

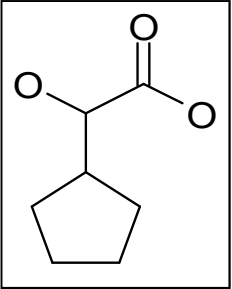
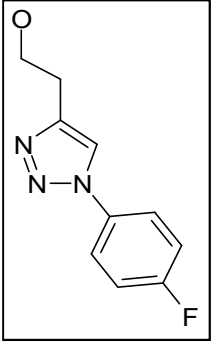
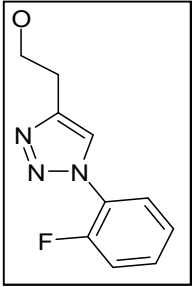
Supplemental Material for

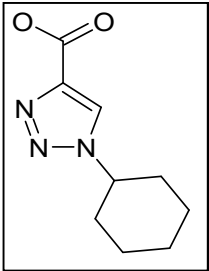
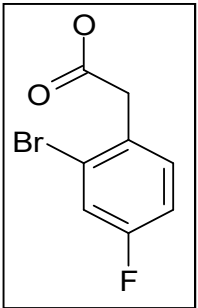
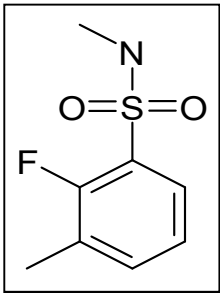
Screening of benzenesulfonamide in combination with chemically diverse fragments against carbonic anhydrase by differential scanning fluorimetry

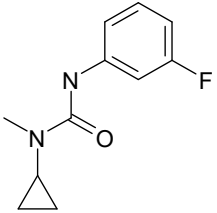
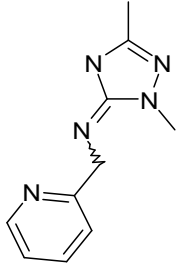
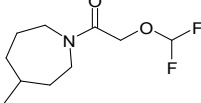
Mikhail Krasavin,^{*} Stanislav Kalinin, Sergey Zozulya, Anastasia Grinuikova. Petro Borysko, Andrea Angeli, Claudiu T. Supuran^{*}

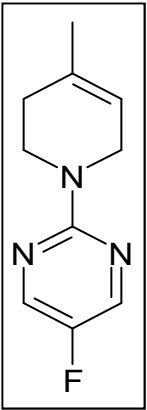
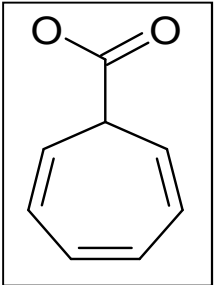
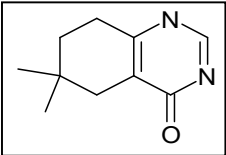
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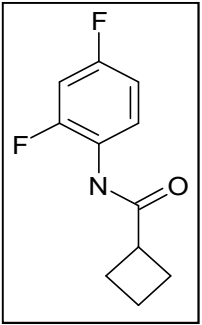
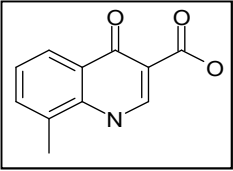
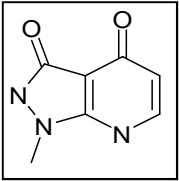
List of 108 validated fragment hits	2-37
Total list of 5,692 fragments screened	38-122

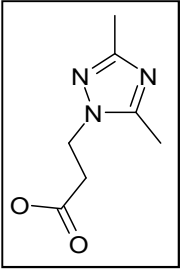
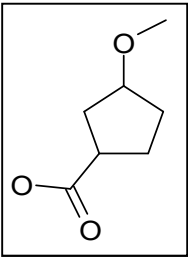
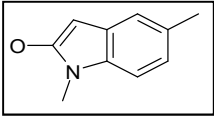
Enamine ID	MW	Formula	Structure
Z1259339771	144,17	C ₇ H ₁₂ O ₃	 Chemical structure of 2-(cyclopentylmethyl)acetic acid, showing a cyclopentane ring attached to a methylene group, which is further attached to a carboxylic acid group.
Z1891749324	207,21	C ₁₀ H ₁₀ FN ₃ O	 Chemical structure of 1-(4-fluorophenyl)-1H-1,2,4-triazole-3-carboxamide, showing a triazole ring system attached to a 4-fluorophenyl group and a carboxamide group.
Z1907767213	207,21	C ₁₀ H ₁₀ FN ₃ O	 Chemical structure of 1-(2-fluorophenyl)-1H-1,2,4-triazole-3-carboxamide, showing a triazole ring system attached to a 2-fluorophenyl group and a carboxamide group.

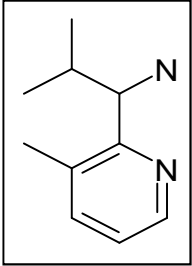
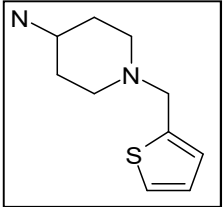
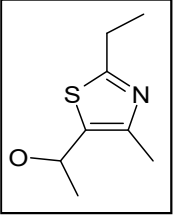
Z1250100765	195,22	C ₉ H ₁₃ N ₃ O ₂	
Z1741967601	233,04	C ₈ H ₆ BrFO ₂	
Z1639162606	203,23	C ₈ H ₁₀ FNO ₂ S	

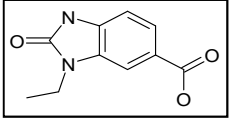
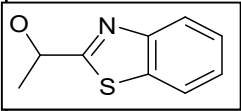
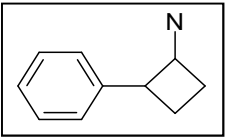
Z973151768	208,24	C ₁₁ H ₁₃ FN ₂ O	<chem>CN1CC1C(=O)Nc2ccc(F)cc2</chem>
Z1699557311	203,25	C ₁₀ H ₁₃ N ₅	<chem>CN1N=CN=C1N=CNc2ccncc2</chem>
Z2068674771	221,25	C ₁₀ H ₁₇ F ₂ NO ₂	<chem>CC1CCN(C1)C(=O)COC(F)(F)F</chem>

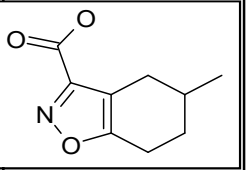
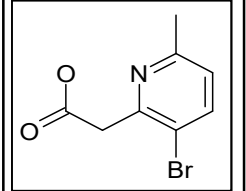
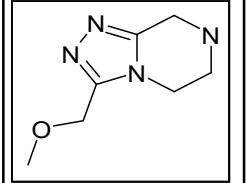
Z1517673547	193,23	C ₁₀ H ₁₂ FN ₃	
Z2327040050	136,15	C ₈ H ₈ O ₂	
Z2235810219	178,24	C ₁₀ H ₁₄ N ₂ O	

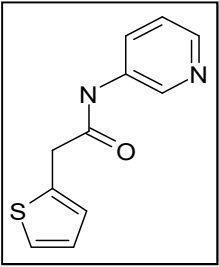
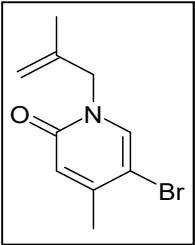
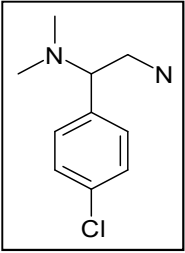
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Z1262246089	203,20	C ₁₁ H ₉ NO ₃	
Z1436105147	165,15	C ₇ H ₇ N ₃ O ₂	

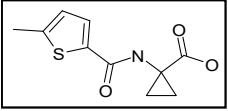
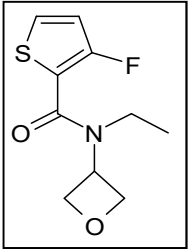
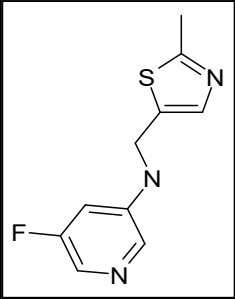
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Z2583036115	144,17	C7H12O3	 <chem>COC1CCCC1CC(=O)O</chem>
Z2168541836	161,20	C10H11NO	 <chem>CC1=CNC(=O)C=C1c2ccc(C)cc2</chem>

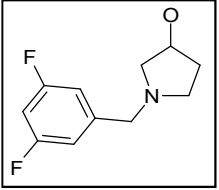
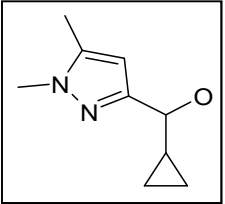
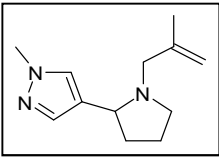
Z1267885765	164,25	C10H16N2	
Z1262237384	196,31	C10H16N2S	
Z1258578217	171,26	C8H13NOS	

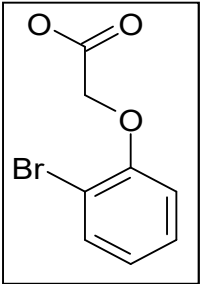
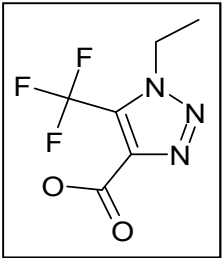
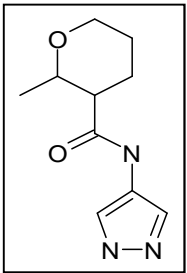
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Z56347071	179,24	C9H9NOS	
Z1269702208	147,22	C10H13N	

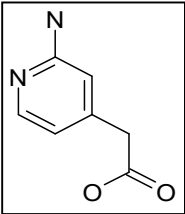
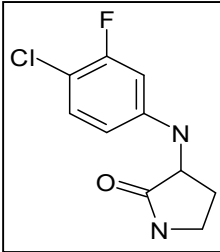
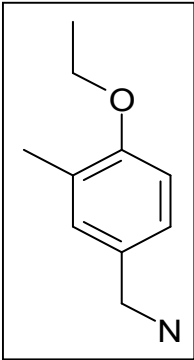
Z1741965991	181,19	C ₉ H ₁₁ NO ₃	 <chem>CC1CCC2=C(C1)C3=NON=C3C(=O)O</chem>
Z1889997414	230,06	C ₈ H ₈ BrNO ₂	 <chem>CC1=CC=C(C(=C1N)C(=O)O)Br</chem>
Z2465620163	168,20	C ₇ H ₁₂ N ₄ O	 <chem>COC1=CN2C(=N1)NCCN2</chem>

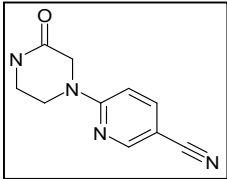
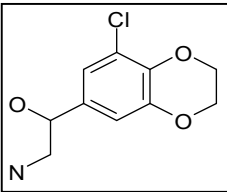
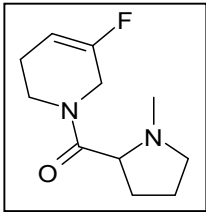
Z31791472	218,27	C11H10N2OS	 <chem>C1=CC=C(S1)CC(=O)Nc2ccncc2</chem>
Z1878408220	242,12	C10H12BrNO	 <chem>CC(=C)CN1C(=O)C=C(Br)C(C)=CN1C</chem>
Z228574062	198,69	C10H15ClN2	 <chem>CN(C)C(C1=CC=C(Cl)C=C1)CN</chem>

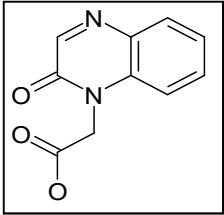
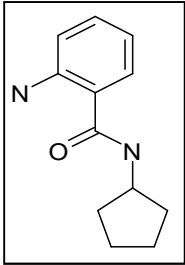
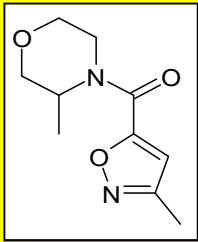
Z1603606287	225,26	C10H11NO3S	 <chem>CC1=CC=C(S1)C(=O)N2CCOC2=O</chem>
Z2285175561	229,27	C10H12FNO2S	 <chem>CCN(C(=O)c1cc(F)sc1)C2OCC2=O</chem>
Z1983897532	223,27	C10H10FN3S	 <chem>CC1=CN=C(S1)CN2C=CC(=CC2=N)N3C=CC(F)=CC3</chem>

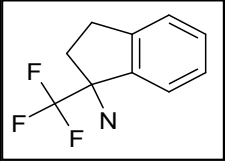
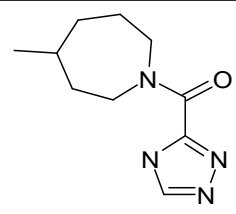
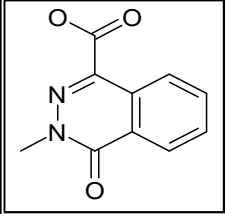
Z1779277596	213,23	C11H13F2NO	 <chem>C1CCN(C1)c2cc(F)c(F)cc2</chem>
Z2301499695	166,22	C9H14N2O	 <chem>Cn1nnc(C1CC2CC2)c1</chem>
Z1103241017	205,31	C12H19N3	 <chem>CC(C)CN1CCCC1</chem>

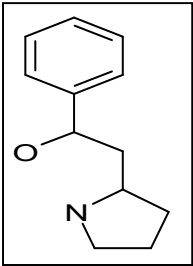
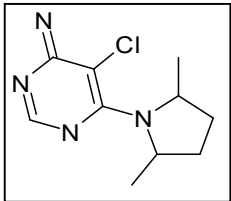
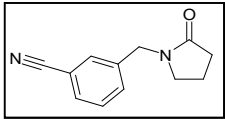
Z111834298	231,05	C ₈ H ₇ BrO ₃	 Chemical structure of 4-bromobenzoic acid benzyl ester. It consists of a benzene ring with a bromine atom at the para position and a benzyl ester group (-CH₂-O-C(=O)-C₆H₅) at the other para position.
Z1365534328	209,13	C ₆ H ₆ F ₃ N ₃ O ₂	 Chemical structure of 1-ethyl-4-(trifluoromethyl)-1H-1,2,4-triazol-5-carboxylic acid. It features a 1,2,4-triazole ring with an ethyl group at position 1, a trifluoromethyl group (-CF₃) at position 4, and a carboxylic acid group (-COOH) at position 5.
Z1838500084	209,25	C ₁₀ H ₁₅ N ₃ O ₂	 Chemical structure of 1-(4-methyl-4,5,6,7-tetrahydro-2H-pyran-2-yl)-1H-pyrazole. It consists of a pyran ring with a methyl group at the 4-position and a 1H-pyrazol-1-yl group at the 2-position.

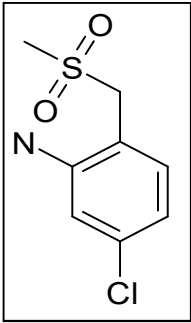
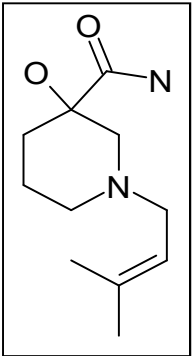
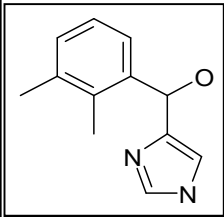
Z2510258100	152,15	C7H8N2O2	 <chem>CC(=O)Cc1ccncc1N</chem>
Z1460224226	228,65	C10H10ClFN2O	 <chem>O=C1CCCN1c2cc(F)c(Cl)cc2</chem>
Z1267773594	165,24	C10H15NO	 <chem>CCN=Cc1cc(OC)c(C)cc1</chem>

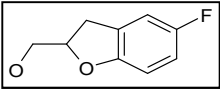
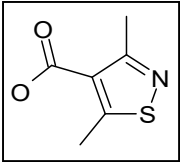
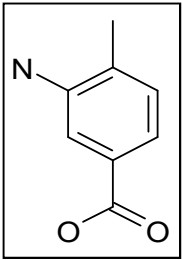
Z219186376	202,22	C ₁₀ H ₁₀ N ₄ O	 <chem>N#Cc1ccc(cc1)N2CCOC(=O)N2</chem>
Z1238835893	229,66	C ₁₀ H ₁₂ ClNO ₃	 <chem>COC1CCOC1c2cc(Cl)ccc2C(C)O</chem>
Z1796224493	212,27	C ₁₁ H ₁₇ FN ₂ O	 <chem>CN1CCCC1C(=O)N2CC(F)CC2</chem>

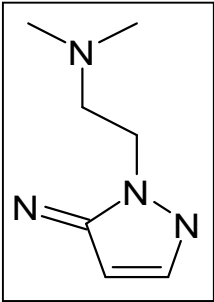
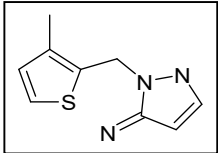
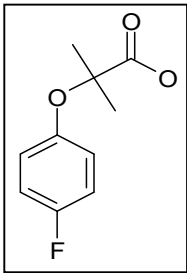
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Z56347236	204,27	C ₁₂ H ₁₆ N ₂ O	
Z364575442	210,23	C ₁₀ H ₁₄ N ₂ O ₃	

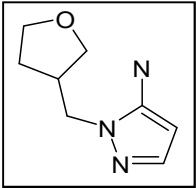
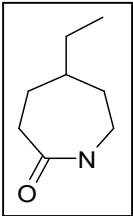
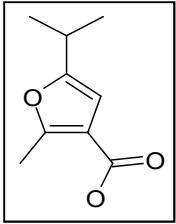
Z1649677579	237,65	C10H11ClF3N	 <chem>ClC1(C(F)(F)F)C2=CC=CC=C2N1</chem>
Z1474242573	208,27	C10H16N4O	 <chem>CC1CCN(C1=CC2=CN=CN2)C3=NC=NC=N3</chem>
Z19629920	204,19	C10H8N2O3	 <chem>CN1C(=O)C(=O)c2ccccc2C1=O</chem>

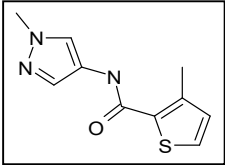
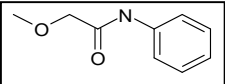
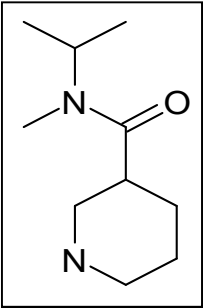
Z1272739430	191,27	C ₁₂ H ₁₇ NO	 <chem>O=C(CCN1CCCC1)c2ccccc2</chem>
Z1874203205	226,71	C ₁₀ H ₁₅ ClN ₄	 <chem>CN1CCCC1C2=CN=C(N=C2)N3CCCC3Cl</chem>
Z1267881725	200,24	C ₁₂ H ₁₂ N ₂ O	 <chem>N#Cc1ccc(cc1)CN2CCCC2=O</chem>

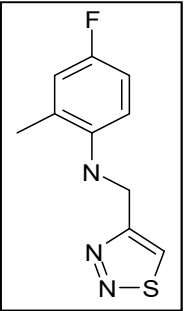
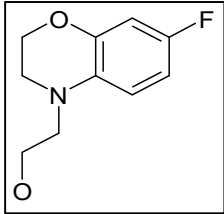
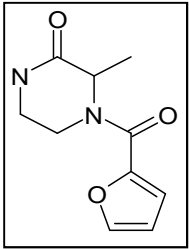
Z1262245653	219,68	C ₈ H ₁₀ ClNO ₂ S	 <chem>Cs1cc(ccc1S(=O)(=O)N)Cl</chem>
Z2054890075	212,29	C ₁₁ H ₂₀ N ₂ O ₂	 <chem>CC(C)CNC(=O)C1CCCN1C</chem>
Z2327531717	202,26	C ₁₂ H ₁₄ N ₂ O	 <chem>CC1=CC=C(C=C1C2=CN=CN2C(=O)N)C</chem>

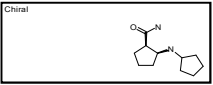
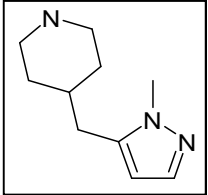
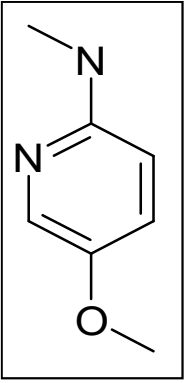
Z1250132763	168,17	C ₉ H ₉ FO ₂	
Z2182115458	157,19	C ₆ H ₇ NO ₂ S	
Z57127001	151,17	C ₈ H ₉ NO ₂	

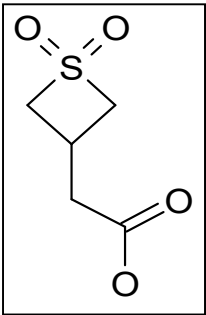
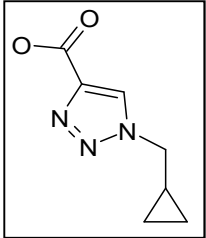
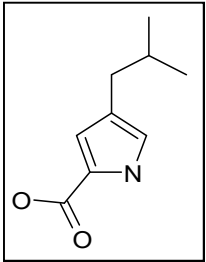
Z2218585849	154,22	C7H14N4	 <chem>CN(C)CC1=NC=CN1</chem>
Z57980675	193,27	C9H11N3S	 <chem>Cc1ccsc1C2=NC=CN2</chem>
Z57047005	198,19	C10H11FO3	 <chem>CC(C)(C)OC1=CC=C(F)C=C1</chem>

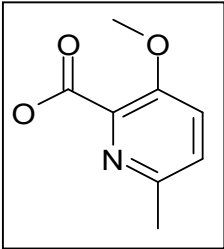
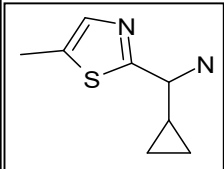
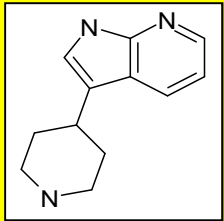
Z1262252948	167,21	C ₈ H ₁₃ N ₃ O	
Z1271843038	141,21	C ₈ H ₁₅ NO	
Z2037273251	168,19	C ₉ H ₁₂ O ₃	

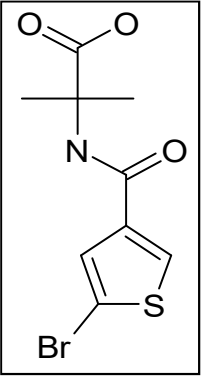
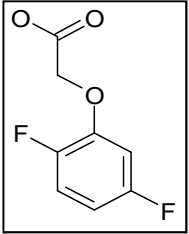
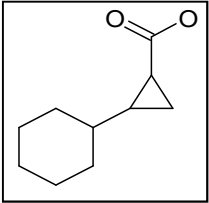
Z373775848	221,28	C10H11N3OS	 <chem>CN1C=NC(=C1)C(=O)N2C=CC=C(C)S2</chem>
Z31504642	165,19	C9H11NO2	 <chem>COC(=O)N=Cc1ccccc1</chem>
Z1262237439	184,28	C10H20N2O	 <chem>CN(C)C(=O)C1CCNCC1</chem>

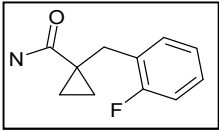
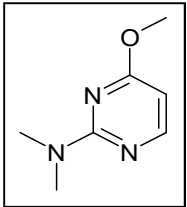
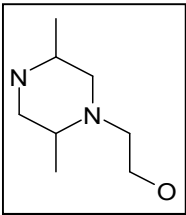
Z1573313752	223,27	C ₁₀ H ₁₀ FN ₃ S	
Z1337784682	197,21	C ₁₀ H ₁₂ FN ₂ O ₂	
Z1082510666	208,22	C ₁₀ H ₁₂ N ₂ O ₃	

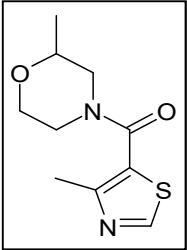
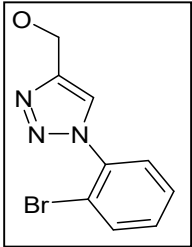
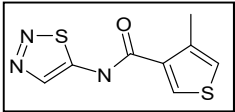
Z2235387992	196,29	C ₁₁ H ₂₀ N ₂ O	Chiral 
Z2574918328	179,27	C ₁₀ H ₁₇ N ₃	
Z2034364269	138,17	C ₇ H ₁₀ N ₂ O	

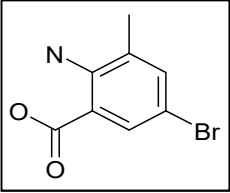
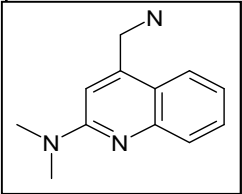
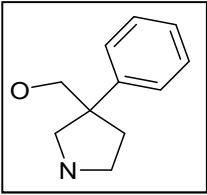
Z2510259511	164,18	C5H8O4S	 <chem>OS(=O)(=O)C1CC(C1)CC(=O)O</chem>
Z2510259303	167,17	C7H9N3O2	 <chem>OC(=O)c1cn[nH]c1CN2CC2</chem>
Z2327531729	167,21	C9H13NO2	 <chem>CC(C)CC1=CC=C(C=C1N)CC(=O)O</chem>

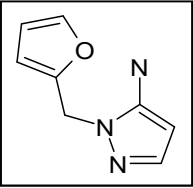
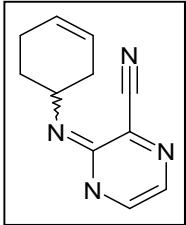
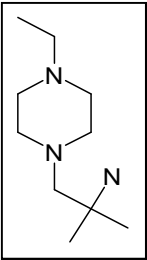
Z2168390419	167,16	C ₈ H ₉ NO ₃	
Z1262237455	168,26	C ₈ H ₁₂ N ₂ S	
Z234897683	201,27	C ₁₂ H ₁₅ N ₃	

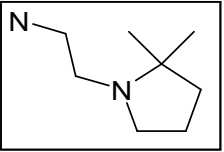
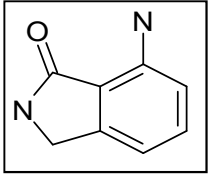
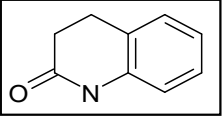
Z929052328	292,15	C ₉ H ₁₀ BrNO ₃ S	 Chemical structure of 2-bromo-4-((2-oxo-2-propylthio)acetyl)thiophene. It features a thiophene ring with a bromine atom at position 2 and a 2-oxo-2-propylthio group at position 4.
Z1259273099	188,13	C ₈ H ₆ F ₂ O ₃	 Chemical structure of 2-(2,4-difluorophenoxy)acetic acid. It consists of a benzene ring with fluorine atoms at positions 2 and 4, and a 2-oxo-2-propoxy group at position 1.
Z1259162080	168,24	C ₁₀ H ₁₆ O ₂	 Chemical structure of cyclohexyl cyclopropanecarboxylate. It shows a cyclohexane ring connected to a cyclopropane ring, which is also attached to a carboxylate group.

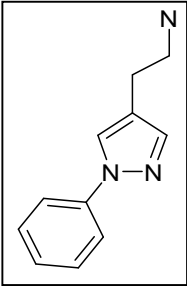
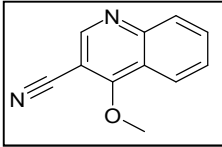
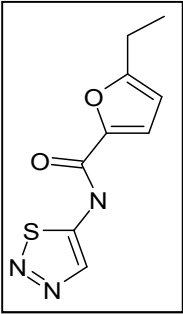
Z1796028750	193,22	C ₁₁ H ₁₂ FNO	
Z281802048	153,19	C ₇ H ₁₁ N ₃ O	
Z2327884032	158,25	C ₈ H ₁₈ N ₂ O	

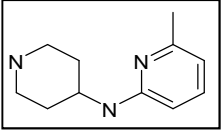
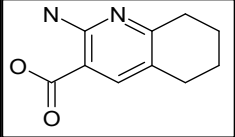
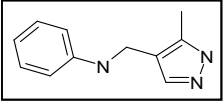
Z422368058	226,29	C ₁₀ H ₁₄ N ₂ O ₂ S	
Z2027049516	254,09	C ₉ H ₈ BrN ₃ O	
Z1820273488	225,28	C ₈ H ₇ N ₃ O ₂ S	

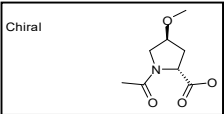
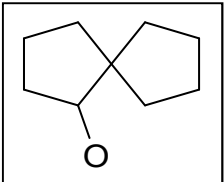
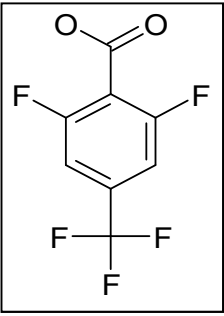
Z1272739859	230,06	C ₈ H ₈ BrNO ₂	 <chem>Cc1cc(Br)cc([N+](=O)[O-])c1C(=O)O</chem>
Z1276496838	201,27	C ₁₂ H ₁₅ N ₃	 <chem>CN(C)c1nc2ccccc2c(c1)CNc3ccccc3[N+](=O)[O-]</chem>
Z2177031006	177,25	C ₁₁ H ₁₅ NO	 <chem>CN1CCCC1Cc2ccccc2</chem>

Z57040473	163,18	C ₈ H ₉ N ₃ O	
Z1232688349	200,25	C ₁₁ H ₁₂ N ₄	
Z2240988377	185,32	C ₁₀ H ₂₃ N ₃	

Z1741815708	142,25	C ₈ H ₁₈ N ₂	
Z234893819	148,17	C ₈ H ₈ N ₂ O	
Z85917566	147,18	C ₉ H ₉ NO	

Z228474642	187,25	C11H13N3	 <chem>CC1=CN=CN=C1C2=CC=CC=C2</chem>
Z1271843050	184,20	C11H8N2O	 <chem>COc1c(C#N)cnc2ccccc12</chem>
Z1791179790	223,25	C9H9N3O2S	 <chem>CC1=CC=C2C(=C1)OC=C2C(=O)N3=NC=SS3</chem>

Z1268152406	191,28	C ₁₁ H ₁₇ N ₃	 <chem>CN1CCN(CC1)Nc2ccc(C)cc2</chem>
Z1267886876	192,22	C ₁₀ H ₁₂ N ₂ O ₂	 <chem>N#Cc1ccc2c(c1)cccnc2C(=O)O</chem>
Z1267882601	187,25	C ₁₁ H ₁₃ N ₃	 <chem>CN(C)Cc1ccccc1Nc2c(C)nn[nH]2</chem>

Z1891772658	187,20	C ₈ H ₁₃ NO ₄	Chiral 
Z2467541171	140,23	C ₉ H ₁₆ O	
Z2168499582	226,10	C ₈ H ₃ F ₅ O ₂	

Enamine ID	SMILES	MW	Molecular Formula
Z1259339771	<chem>OC(C1CCCC1)C(O)=O</chem>	144,17	C7H12O3
Z1891749324	<chem>OCCC1=CN(N=N1)C1=CC=C(F)C=C1</chem>	207,21	C10H10FN3O
Z1907767213	<chem>OCCC1=CN(N=N1)C1=C(F)C=CC=C1</chem>	207,21	C10H10FN3O
Z1250100765	<chem>OC(=O)C1=CN(N=N1)C1CCCC1</chem>	195,22	C9H13N3O2
Z1868316789	<chem>CCOC1=C(C(O)=O)C(C)=CC=N1</chem>	181,19	C9H11NO3
Z2188171616	<chem>CC1=C(C=CC(N)=C1)C1=CC=NC=C1</chem>	184,24	C12H12N2
Z2009840048	<chem>NC1CC(=O)N2CCCCC12</chem>	154,21	C8H14N2O
Z1262237414	<chem>CC(CN)CN1CCCC1=O</chem>	156,23	C8H16N2O
Z1823335958	<chem>CC1=C(C=CO1)S(=O)CC1=NC(C)=CS1</chem>	241,32	C10H11NO2S2
Z1350579526	<chem>CC(N)C1=CC=C(C=C1)N1C=CN=C1C</chem>	201,27	C12H15N3
Z2194169420	<chem>CNCC1CCCOC1C1=CC=CC=C1</chem>	205,30	C13H19NO
Z1267773501	<chem>NCCC1=NN(C=C1)C1=CC=C(F)C=C1</chem>	205,24	C11H12FN3
Z951367728	<chem>CC(CN)C1=NC2=C(S1)C=CC=C2</chem>	192,28	C10H12N2S
Z267168630	<chem>CC1=NOC(CNC2=C(C)C=CC=C2)=C1</chem>	202,26	C12H14N2O
Z1272670424	<chem>CC1(CCC2=C(C1)C=CC=C2)C(O)=O</chem>	190,24	C12H14O2
Z1270207977	<chem>CC1CNC2=C(C=CC=C2)N(C1)C(C)=O</chem>	204,27	C12H16N2O
Z212851096	<chem>CC1CN(CCO1)C(=O)C1=NC=CN=C1</chem>	207,23	C10H13N3O2
Z1238477809	<chem>CCC(O)CN1CCNCC1</chem>	158,25	C8H18N2O
Z101186134	<chem>NC(=O)CC1=NOC2=C1C=CC=C2</chem>	176,18	C9H8N2O2
Z56871715	<chem>COC1=C(C=C(Cl)C=C1)C#N</chem>	167,59	C8H6ClNO
Z2216303152	<chem>NC1=CC2=C(C(OC(CO)=C2)C=C1</chem>	163,18	C9H9NO2
Z2211231539	<chem>COC1=CC2=C(C(NC(=O)C(C)N2)C=C1</chem>	192,22	C10H12N2O2
Z2255626880	<chem>CC1CNCC(O1)C1CC1</chem>	141,21	C8H15NO
Z108566670	<chem>CNC1=C(C(O)=O)C(C)=NS1</chem>	172,20	C6H8N2O2S
Z224184044	<chem>CCC(=O)NC1=C(C=CC=C1C)C(O)=O</chem>	207,23	C11H13NO3
Z14775230	<chem>NC(=O)COC1=C(C(Cl)C=CC(Cl)=C1</chem>	220,05	C8H7Cl2NO2
Z16115067	<chem>CC1=CC(OCC(N)=O)=C(Cl)C=C1</chem>	199,63	C9H10ClNO2
Z212063058	<chem>CC(=O)NC1=CC=C(S1)C(O)=O</chem>	185,20	C7H7NO3S
Z55410632	<chem>CN1N=CC(C(N)=O)=C1N</chem>	140,15	C5H8N4O
Z212062948	<chem>CC1=C(SC(NC(=O)C2CC2)=C1)C(O)=O</chem>	225,26	C10H11NO3S
Z219997506	<chem>OC(=O)CC1=C(Cl)C=C(C(Cl)C=C1</chem>	205,03	C8H6Cl2O2
Z45202427	<chem>CC(NC1=C(C)C(C)=CC=C1)C(N)=O</chem>	192,26	C11H16N2O
Z207209754	<chem>CN1C(=O)C(C)=NC2=C1C=CC=C2</chem>	174,20	C10H10N2O
Z1863617838	<chem>NC1=C2CNCCC2=CC=N1</chem>	149,20	C8H11N3
Z1863617794	<chem>CC(C)NC1=NC=CN1C</chem>	139,20	C7H13N3
Z1667555483	<chem>CN1N=C(C)N=C1NC(=O)C1=CC=CO1</chem>	206,21	C9H10N4O2
Z1729204367	<chem>COC1=C(Cl)C=C(C(N2C=CN=N2)C=C1</chem>	223,66	C10H10ClN3O
Z1743510401	<chem>CC1=CC(NCC2(C)CCOCC2)=NO1</chem>	210,28	C11H18N2O2
Z1860991558	<chem>CC1=CC(=O)C2=C(N1)C=CC(N)=C2</chem>	174,20	C10H10N2O
Z169675004	<chem>CN1C=CC(NC(=O)CN2C=CC=N2)=N1</chem>	205,22	C9H11N5O
Z1833679631	<chem>CCN(C)C(=O)NC1=CN=NS1</chem>	186,23	C6H10N4OS
Z1889902494	<chem>CC1=C(C=CO1)C1=CC(N)=NO1</chem>	164,16	C8H8N2O2
Z1881599143	<chem>OCCC1CCC(CO)CC1</chem>	144,21	C8H16O2
Z1657810189	<chem>CN1C(C)=NN=C1NC(=O)CC1CCC1</chem>	208,27	C10H16N4O
Z1020680176	<chem>NCC(O)C1=CC=C(Cl)C=C1</chem>	171,62	C8H10ClNO
Z228042642	<chem>OC(=O)CN1CC(=O)NC2=C1C=CC=C2</chem>	206,20	C10H10N2O3
Z1575143888	<chem>NCC1CCCN(C1)C1=NC=CC=N1</chem>	192,27	C10H16N4
Z1575143894	<chem>COC1=CC(N)=C(F)C=C1</chem>	141,15	C7H8FNO
Z1575143702	<chem>NCC1=NOC2=C1C=CC=C2</chem>	148,17	C8H8N2O
Z2216711752	<chem>CC(C)C1(CO)CCCN1</chem>	157,26	C9H19NO
Z234893683	<chem>NCCC1=NC=C(C=C1)C(F)(F)F</chem>	190,17	C8H9F3N2
Z1251207602	<chem>CC1=NN=C(S1)N1CCCC1</chem>	183,27	C8H13N3S
Z1255637874	<chem>CCC1=CSC(=N1)C1=C(N)C=CC=C1</chem>	204,29	C11H12N2S
Z324556956	<chem>CNC(=O)C1CCCCN1S(C)(=O)=O</chem>	220,29	C8H16N2O3S
Z1171979277	<chem>OC(=O)C1=CCN=C1C1CCCC1</chem>	194,23	C10H14N2O2
Z993967108	<chem>CCC(C(O)=O)C1=C(C)ON=C1C</chem>	183,21	C9H13NO3
Z1267773535	<chem>NCCC1=C(F)C=C(F)C=C1</chem>	157,16	C8H9F2N
Z1258578241	<chem>CC(C)C(O)C1=NC=CC=C1</chem>	151,21	C9H13NO
Z1020680358	<chem>CC(O)(CN)C1CCCC1</chem>	143,23	C8H17NO
Z1230795906	<chem>CN1C=CN=C1C(=O)NCC=C</chem>	165,20	C8H11N3O
Z53038390	<chem>CNS(=O)(=O)C1=CC(C(O)=O)=C(C)C=C1</chem>	229,25	C9H11NO4S
Z2492774597	<chem>NC1=CC2=C(CS(=O)(=O)C2)C=C1</chem>	183,23	C8H9NO2S
Z2216710432	<chem>CCNS(=O)(=O)C1=CC(C)=C(Cl)C=C1</chem>	233,71	C9H12ClNO2S
Z1416200983	<chem>OC(=O)C1=CN2C(C=C1)=NN=C2C(F)F</chem>	213,14	C8H5F2N3O2
Z1741980409	<chem>C1CNC2=C(C1)C=CC=N2</chem>	134,18	C8H10N2
Z1891772663	<chem>CC(=O)NC(C1CCOCC1)C(O)=O</chem>	201,22	C9H15NO4

Z2509351220	BrC1=CC2=C(OCCNC2=O)C=C1	242,07	C9H8BrNO2
Z1982493933	CN1C(=O)COC2=C1C=CC(N)=C2	178,19	C9H10N2O2
Z344843836	CCN(C)C(=O)CC1=C(CI)C=CC=C1CI	246,13	C11H13Cl2NO
Z1973465555	CC1=C(C=C(O1)C#N)C(O)=O	151,12	C7H5NO3
Z1966484358	CC1=C(C(C)=NO1)C(C)(C)C(O)=O	183,21	C9H13NO3
Z1891775602	CC(=O)NC1=C(N)C=CC=N1	151,17	C7H9N3O
Z57261333	CC1=C(CI)C=C(C=C1)C(=O)NCCO	213,66	C10H12ClNO2
Z1945984210	CN(C)C(=O)NC1=C(C)C(N)=CC=C1	193,25	C10H15N3O
Z272156568	CCOC1=C(C=CC=N1)C(N)=O	166,18	C8H10N2O2
Z1741978641	OC(=O)C1=CN2CCCCC2=N1	166,18	C8H10N2O2
Z229615464	CN1N=C(C)C2=C1SC(=C2)C(N)=O	195,24	C8H9N3OS
Z241898600	CN1N=C(C)C2=C1N=C(C)C=C2C(N)=O	204,23	C10H12N4O
Z239136710	CC(=O)NC1=CC(C)=NN1	139,16	C6H9N3O
Z2692095185	CN1N=CC=C1C(N)C1=CC=NN1C	191,24	C9H13N5
Z2692095209	NC1=NC(=NS1)C1CCOCC1	185,25	C7H11N3OS
Z1255634340	CC(C)C1=NC(=CN1)S(=O)(=O)N(C)C	217,29	C8H15N3O2S
Z2692093625	NC(CCO)C1=CC(F)=C(CI)C=C1	203,64	C9H11ClFNO
Z1821397907	CC(C)CC1(CO)CCCN1	157,26	C9H19NO
Z1259155925	CC1(O)CCC2=C(C1)C=CC=C2	162,23	C11H14O
Z1259155865	COC1=C(C=CC=C1)C1(CC1)C(O)=O	192,21	C11H12O3
Z1741967601	OC(=O)CC1=C(Br)C=C(F)C=C1	233,04	C8H6BrFO2
Z1849008050	CC1=CSC(C(O)=O)=C1Br	221,07	C6H5BrO2S
Z1849010842	CN(C)S(=O)(=O)C1=CN=C(N)C=C1	201,24	C7H11N3O2S
Z1348386878	O=S1CCN(CC1)C1=CN=C(C=C1)C#N	221,28	C10H11N3OS
Z1839475324	OC(=O)C1=CC=CN1CC=C	151,17	C8H9NO2
Z1127744289	NC(=O)C1=CC=C(CN2C=CC=C2)C=C1	200,24	C12H12N2O
Z1837073463	NC1C(CO)CCC2=C1C=CC=C2	177,25	C11H15NO
Z57899965	COC1=CC(=CC(OC)=C1)C#N	163,18	C9H9NO2
Z1183649742	CCC1=CC2=C(C=C1)C(CI)=C(S2)C(N)=O	239,72	C11H10ClNOS
Z1834278447	CN1OC(=CC1=O)C(O)=O	143,10	C5H5NO4
Z1696930122	CC1=CSC=C1C(=O)NC1=NC=CN=C1	219,26	C10H9N3OS
Z1827897963	O=C1CN(CCCN1)C1CC1	154,21	C8H14N2O
Z1682035348	CC1CN(CC2=C5N=N2)C(C)(C)CO1	227,33	C10H17N3OS
Z29692196	CN1C=CC=C1C(=O)NCC1=CC=CS1	220,29	C11H12N2OS
Z1824511099	CC1=CC(=O)C2=C(N1)C=CS2	165,21	C8H7NOS
Z1258992459	OCC1=CC(=CC=C1)C#N	133,15	C8H7NO
Z1258992442	CC(O)C1=NC2=C(N1)C=CC(CI)=C2	196,63	C9H9ClN2O
Z1173707511	OC1(CNC2=NC=C(Br)C=N2)CCC1	258,12	C9H12BrN3O
Z1258854546	CCNC(=O)N1CCC2=C1C=C(N)C=C2	205,26	C11H15N3O
Z1258578989	COC1=C(C=CC=C1)C1(C)CC1C(O)=O	206,24	C12H14O3
Z1258578330	CC(C)C1=NC=NC(O)=C1	138,17	C7H10N2O
Z1258578306	CC(O)C1=CC2=C(NC(=O)C2)C=C1	177,20	C10H11NO2
Z1251222566	NCC1=CC2=C(O1)C=CC=C2	147,18	C9H9NO
Z751811134	CN(C)S(=O)(=O)C1=CN=CC=C1	186,23	C7H10N2O2S
Z1251171287	CC1=CC(CCN)=CC(C)=C1	149,24	C10H15N
Z1259335848	CCN1N=CC2=C1C=C(N)C=C2	161,21	C9H11N3
Z1259341108	CC1=CC(C)=C(C=C1)C1=NN=C(N)S1	205,28	C10H11N3S
Z1259341095	CCOC1=NC=CC(=C1)C(O)=O	167,16	C8H9NO3
Z1259341091	CCC1=C(C=NC(C)=N1)C(O)=O	166,18	C8H10N2O2
Z1259339962	CN1C=C(CCC(O)=O)C(C)=N1	168,20	C8H12N2O2
Z1259162172	NC(C(O)=O)C1=C(C=CC=C1)C(F)(F)F	219,16	C9H8F3NO2
Z1259162070	CC(CC1=C(C)NN=C1C)C(O)=O	182,22	C9H14N2O2
Z1623889816	FC1=CCCN(C1)C1=NC=C(C=C1)C#N	203,22	C11H10FN3
Z1583292118	CC1=NN=C(CNC2=C(F)C=CC=C2)S1	223,27	C10H10FN3S
Z1354370680	CN(CCO)C1=C(F)C=C(CI)C=N1	204,63	C8H10ClFN2O
Z1980875175	CC(NC1=NC(C)=NS1)C1=NNC=C1	209,27	C8H11N5S
Z262247854	COCC(=O)NC1(C)CCS(=O)(=O)C1	221,27	C8H15NO4S
Z1262327459	CC(C)C(=O)NCC1CCCNC1	184,28	C10H20N2O
Z2012523861	CC(=O)NC1=C(F)C=C(OC(F)F)C=C1	219,16	C9H8F3NO2
Z2687203946	NC1(COC2=C(C1)C=CC=C2)C(O)=O	193,20	C10H11NO3
Z1497330165	CNC(=O)C1=C(F)C=C(C=C1)N(C)C	196,23	C10H13FN2O
Z1639162606	CNS(=O)(=O)C1=C(F)C(C)=CC=C1	203,23	C8H10FN2O2S
Z2684295076	OCCC1CCCN1=O	143,19	C7H13NO2
Z2680629390	NC1=C(C=CC=C1)N1CCNC(=O)C1	191,23	C10H13N3O
Z1171979278	CC(C)CC1=NC(C)=C(S1)C(O)=O	199,27	C9H13NO2S
Z1171978788	CN(CC(O)=O)C(=O)C1=NC=CC=C1	194,19	C9H10N2O3
Z1171978806	CC(C(O)=O)C1=C(C)NN=C1C	168,20	C8H12N2O2

Z333523646	CCC(=O)NC1CCCC2=C1C=CO2	193,25	C11H15NO2
Z434911440	CN(CC(N)=O)C(=O)C1=C(Br)C=CS1	277,14	C8H9BrN2O2S
Z31111899	C(NC1=NC=CC=C1)C1=CC=CS1	190,26	C10H10N2S
Z287484230	CN1N=C(C)C(CC(N)=O)=C1C	167,21	C8H13N3O
Z1770193310	CC1=COC(=C1C(O)=O)C1=CC=CC=C1	202,21	C12H10O3
Z1768428973	COC(C)C1=NC=C(S1)C(O)=O	187,21	C7H9NO3S
Z1666810169	FC1=C(NC(=O)C2CC=CC2)N=CC=C1	206,22	C11H11FN2O
Z1762658235	CC1=C(N)C(C(O)=O)=C(Br)C=C1	230,06	C8H8BrNO2
Z1616719042	CN(C)C(=O)N(C)C1(CCCC1)C(N)=O	213,28	C10H19N3O2
Z1593013689	CN(C)C1CN(C1)C1=NC=C(Cl)C=N1	212,68	C9H13ClN4
Z1603606863	OC(=O)C1(CC1)NC(=O)C1=C(Br)C=CS1	290,13	C9H8BrNO3S
Z1742055008	CC1=COC2=C1C=C(N)C=C2	147,18	C9H9NO
Z1741880725	CC1CCCCC1(N)C(O)=O	157,21	C8H15NO2
Z1718361780	NC1=C(C=NC(=N1)C1CC1)C#N	160,18	C8H8N4
Z1272500940	C1C2CC=CCC2CN1C1=NC=CN=C1	201,27	C12H15N3
Z1407004019	CCOC1=NC=C(N)C=C1	138,17	C7H10N2O
Z1681200613	OC1(CC2=NC(=NO2)C2CC2)CCCC1	208,26	C11H16N2O2
Z1289535961	CC1CS(=O)(=O)CCN1CC1CCC1	217,33	C10H19NO2S
Z90517838	C(NC1CC1)C1=CC=CO1	137,18	C8H11NO
Z1271660837	CCNCC1=CN(C)N=N1	140,19	C6H12N4
Z2335495746	CCOC1=CC(F)=C(NC(C)=O)C=C1	197,21	C10H12FNO2
Z2106611472	CC1=CN(CC(O)=O)N=C1C(F)(F)F	208,14	C7H7F3N2O2
Z2689172057	COC1=CC(=CC=C1)C1=C(N)NN=C1C	203,25	C11H13N3O
Z2146515783	CN1C(C)=NC2=C1N=CC(Br)=C2	226,08	C8H8BrN3
Z2146513621	CNS(O)(=O)C(C)C1=CC=CC=C1	199,27	C9H13NO2S
Z2146514261	CC(O)C1=NC=C(C=C1)N(C)C	166,22	C9H14N2O
Z2092369803	COC1=C(OC)C(C)=C(C=C1)C(O)=O	196,20	C10H12O4
Z2092368585	CC1(C)CNC(=O)C(C)(C)N1	156,23	C8H16N2O
Z1265814003	CNC(=O)C1=C(C)C=CC(Br)=C1	228,09	C9H10BrNO
Z1787644587	CC(O)C(=O)NCC1=C(C)C=CC(Br)=C1	272,14	C11H14BrNO2
Z2160914711	COC1=CC2=C(C=C1)C(=O)NN2	164,16	C8H8N2O2
Z1262237375	CNC1=CN=C(OC)C=C1	138,17	C7H10N2O
Z45534888	O=S(=O)(NC1CC1)C1=CC=CS1	203,27	C7H9NO2S2
Z1688198928	OC(=O)C1CC11CCOC1	142,15	C7H10O3
Z1302595798	CN(C)C(=O)C1=CC(=NO1)C1CCCC1	208,26	C11H16N2O2
Z1139507648	CCN1CCCC1C1=C(C)N(C)N=C1C	207,32	C12H21N3
Z1741794221	OC(=O)CC1CCCC=C1	140,18	C8H12O2
Z1741794235	CC1=NC2=C(C=CC=C2)N=C1	144,18	C9H8N2
Z234895091	NCC1CC2=C1C=CC=C2	133,19	C9H11N
Z1696871223	CC(C)C1=NC(=NC=C1)N1CCNCC1	206,29	C11H18N4
Z56040660	CCC(C)NC(=O)C1=C(N)C=CC=C1	192,26	C11H16N2O
Z105197244	NCC1=NC(=NO1)C1=CC=CS1	181,21	C7H7N3OS
Z910841232	CC(=O)NC1=C(C=C(C)C=C1C)C(O)=O	207,23	C11H13NO3
Z85956709	CC(N)C1=CC=C(C=C1)N1C=NC=N1	188,23	C10H12N4
Z57841909	CC(N1C=NC2=C1C=CC=C2)C(O)=O	190,20	C10H10N2O2
Z55692910	C1CC1C1=NC2=C(N1)C=CC=C2	158,20	C10H10N2
Z71501992	CNC(=O)C1=C(C=CS1)C1=CC=CC=C1	217,29	C12H11NOS
Z111781340	CC1=NC2=C(C=NN2C(C)=C1)C(O)=O	191,19	C9H9N3O2
Z228590120	COC1=CC=C(C=C1)C1=NNC(N)=C1C	203,25	C11H13N3O
Z992422568	NCC1=C(C=C(Br)C=C1)C(F)(F)F	254,05	C8H7BrF3N
Z969560582	CNC(=O)C1=CN=C(C)S1	156,20	C6H8N2OS
Z1416282800	NC[C@@H](O)CN1CCOCC1	160,22	C7H16N2O2
Z973151768	CN(C1CC1)C(=O)NC1=CC(F)=CC=C1	208,24	C11H13FN2O
Z280818240	CC(C1CC1)N(C)C(=O)C1=C(C)C=CO1	207,27	C12H17NO2
Z265564928	CC1CCCCN1CC1=NC(C)=NO1	195,27	C10H17N3O
Z382767716	CCC1CCCN(CC2=NC(C)=NO2)C1	209,29	C11H19N3O
Z103891156	OC1CCN(CC2=CC=C(Cl)S2)CC1	231,74	C10H14ClNOS
Z416341642	CC(C)N(C)S(=O)(=O)N1CCOC(C)C1	236,33	C9H20N2O3S
Z1241573367	CC(CC1=NC(C)=CS1)N1C=C(Cl)C=N1	241,74	C10H12ClN3S
Z217102784	CC(N)C1=NC2=C(C=CC=C2)N1C(F)F	211,22	C10H11F2N3
Z2327402244	COC1=CC=C(C=C1)N1C(=O)NC=C1C	204,23	C11H12N2O2
Z2327226168	CN1C=C(C(O)=O)C(=N1)C1CCC1	180,21	C9H12N2O2
Z2327226126	CC1=C(Br)C(F)=CC(N)=C1	204,04	C7H7BrFN
Z274767396	CCN1N=C(C)C(N)=C1C	139,20	C7H13N3
Z1218147280	CC(N1CC(C)C2=C1C=CC=C2)C(O)=O	205,26	C12H15NO2
Z2309759405	CNC1=CC=C(C=C1)C1=NC=CS1	190,26	C10H10N2S
Z2306626038	CN1CC2=C(N)C=CC=C2C1=O	162,19	C9H10N2O

Z2305986981	CCN1C(C)=CC2=C(C(N)=NN2)C1=O	192,22	C9H12N4O
Z274799154	OCC1CN2CCC1CC2	141,21	C8H15NO
Z2293608485	OC(=O)C1CN(C1)C1CCCCC1	183,25	C10H17NO2
Z2293606411	CC1=CC(Br)=C(S1)C(O)=O	221,07	C6H5BrO2S
Z2284390049	BrC1=CC(=CC=C1)N1CCCN1=O	255,12	C10H11BrN2O
Z2284399991		172,22	C9H16O3
Z1891776116	NCC1=CC(NC2CC2)=NC=C1	163,22	C9H13N3
Z1267773690	CC1=C(Br)C=CC(C(O)=O)=C1N	230,06	C8H8BrNO2
Z1266854952	CN(C)C(=O)CN1CCC(N)CC1	185,27	C9H19N3O
Z1266854930	CNS(=O)(=O)C1CCNCC1	178,25	C6H14N2O2S
Z1266823218	CCC(C1=NN=C(N)S1)C1=CC=CC=C1	219,31	C11H13N3S
Z1263824428	CCOC1=C(N)C=C(OC)C=C1	167,21	C9H13NO2
Z1263820490	NC(=O)C1=C(CO)C=CC=C1	151,17	C8H9NO2
Z1263820443	COC1=CC(=NC=C1)N1CCNCC1	193,25	C10H15N3O
Z1263820309	CNS(=O)(=O)C1=C(CN)C=CC=C1	200,26	C8H12N2O2S
Z1263714062	NC(CO)CC1=CNC2=C1C=CC=C2	190,25	C11H14N2O
Z1263602405	CCOC1=C(N)C=C(Br)C=C1	216,08	C8H10BrNO
Z1245735276	OC1(CCCC1)C1=CC=CC=C1	162,23	C11H14O
Z254586068	CCC1=C(SN=N1)C(=O)N(C)C	185,25	C7H11N3OS
Z1891701433	NCC1=NC(=CS1)C1=C(F)C=CC=C1	208,25	C10H9FN2S
Z2273353833	CCC1(CC1)NC1=NC(C)=NS1	183,27	C8H13N3S
Z1575304397	NCCNC1=NN=CC=C1	138,17	C6H10N4
Z1983132756		155,24	C9H17NO
Z1695921554	CN1C=C(C=N1)C(O)C(O)=O	156,14	C6H8N2O3
Z1381271509	CC1=CC(N2CCCC2)=C(CN)C=C1	190,29	C12H18N2
Z1699557311	CN1N=C(C)N=C1NCC1=NC=CC=C1	203,25	C10H13N5
Z1575311949	CN1C=C(N)C(C)=CC1=O	138,17	C7H10N2O
Z2091496785	CN(CC1=NC=CS1)C1=NC=C(F)C=C1	223,27	C10H10FN3S
Z1615132073	CN(CC(C)=C)C1=NC=C(F)C=N1	181,21	C9H12FN3
Z2256514859	CN(CC1=C(F)C=NC=C1)C1CCOC1	210,25	C11H15FN2O
Z1537215768	COC1=C(F)C(C=CC=C1)C(=O)N(C)C	197,21	C10H12FNO2
Z2272040615	CC1(O)CC(C1)C(=O)N1CCC=C(F)C1	213,25	C11H16FNO2
Z1587272989	CC1=NOC(CN2CCC=C(F)C2)=N1	197,21	C9H12FN3O
Z1749360781	CC1=C(C)N(CC2=CC(F)=CN=C2)C=N1	205,24	C11H12FN3
Z2272040604		213,25	C11H16FNO2
Z2068674771	CC1CCCN(CC1)C(=O)COC(F)F	221,25	C10H17F2NO2
Z1517673547	CC1=CCN(CC1)C1=NC=C(F)C=N1	193,23	C10H12FN3
Z1973748497	CC1=CCCN(C1)C1=NC=C(F)C=N1	193,23	C10H12FN3
Z56347489	CN(C)C(CN)C1=CC(F)=CC=C1	182,24	C10H15FN2
Z435369470	CN(CC1=CC(Br)=CS1)C(=O)C1CCC1	288,20	C11H14BrNOS
Z1486705591	CS(=O)(=O)N1CCOCC1CCC1	205,27	C8H15NO3S
Z1188325591	CCN(C)C(=O)NCC1=CC(C)=CC=C1	206,29	C12H18N2O
Z940634048	CCS(=O)(=O)NC1COC2=C1C=CC=C2	227,28	C10H13NO3S
Z1506050651	CN(C(=O)[C@H]1CC1(C)C)C1=CN=CC=C1	204,27	C12H16N2O
Z2327040050	OC(=O)C1C=CC=CC=C1	136,15	C8H8O2
Z2293642517	CC1(CCCC1)C(O)=O	144,17	C7H12O3
Z1263529842	FC(F)OC1=C(C=CC=C1)C#N	169,13	C8H5F2NO
Z89264959	CC1=NC2=C(C=C(N)C=C2)C(N)=C1	173,22	C10H11N3
Z85923113	CC1=C2CCCCC2=NC(N)=N1	163,22	C9H13N3
Z57899732	COC1=CC(=CC(OC)=C1OC)C#N	193,20	C10H11NO3
Z85923173	COC1=C(OC(F)F)C=CC(=C1)C#N	199,16	C9H7F2NO2
Z85932361	OC(=O)C1=CC2=C(OCO2)C(Cl)=C1	214,60	C9H7ClO4
Z57984664	NC1=CC=NN1CC1=CC(Br)=CS1	258,14	C8H8BrN3S
Z26148273	NC(=O)CN1N=NC2=C(C=CC=C2)C1=O	204,19	C9H8N4O2
Z14772440	CNC(=O)COC1=C(Cl)C=CC(Cl)=C1	234,08	C9H9Cl2NO2
Z56347458	OC(=O)CN1C(=O)COC2=C1C=CC=C2	207,19	C10H9NO4
Z57029692	C[C@H](NC(=O)C1=CC(C)=CC=C1)C(O)=O	207,23	C11H13NO3
Z401537598	CCC1=NC(CC(O)=O)=CS1	171,21	C7H9NO2S
Z33547100	NC(=O)C1=CC2=C(OCO2)C=C1	179,18	C9H9NO3
Z31407956	CC1=CC=C(S1)C(=O)NCC1=CC=CO1	221,27	C11H11NO2S
Z263785508	COCC(=O)NC1=NN=C(C)S1	187,22	C6H9N3O2S
Z752370760	CC(C)OC1=C(Cl)C=C(C=N1)C(O)=O	215,63	C9H10ClNO3
Z228589452	OC(=O)CC1=CSC(=N1)C1=CC=CO1	209,22	C9H7NO3S
Z321209398	CC(C)NC(=O)C1=NNC(=C1)C1CC1	193,25	C10H15N3O
Z235449228	COC1=CC(=CC=C1)C1=NC(CO)=CS1	221,27	C11H11NO2S
Z33546492	COC1=CC=C(C=C1)C(N)=O	151,17	C8H9NO2
Z30173060	O=C(NCC1=CN=CC=C1)C1=CC=CS1	218,27	C11H10N2OS

Z345089918	CC1=C(CNC(=O)C2=CC=CO2)SC=C1	221,27	C11H11NO2S
Z50147461	CC1=NN(C(=O)C1)C1=C(C)C=CC(C)=C1	202,26	C12H14N2O
Z235342005	NCC1(CCCCC1)NC1=CC=CC=C1	204,32	C13H20N2
Z235338709	O=C1N(N=NC2=C1C=CC=C2)C1CC1	187,20	C10H9N3O
Z30166515	O=C(NCC1=NC=CC=C1)C1=CC=CS1	218,27	C11H10N2OS
Z332659786	CNC(=O)C1=NNC(=C1)C1=CC=CO1	191,19	C9H9N3O2
Z2469606504	CN1C=NC2=C1N=CNC2=O	150,14	C6H6N4O
Z1551700540	CC(C)C1=CC(NC(=O)CO)=CC=C1	193,25	C11H15NO2
Z2442033754	NC1=C(F)C=CC(=C1)N1CCNC1=O	195,20	C9H10FN3O
Z2429425678	CC1CCN2N=CC(C(O)=O)=C2C1	180,21	C9H12N2O2
Z2429425504	CC1=CC=C(C=C1)N1C=CNC1=O	174,20	C10H10N2O
Z2429425500	CC1=NC(CCO)=CN=C1	138,17	C7H10N2O
Z2429425528	OCC1CNC2=C(C1)C=CC=C2F	181,21	C10H12FNO
Z2418194206	OC1CCCN2C=CN=C12	138,17	C7H10N2O
Z2412196557	CC1=C(C)N=C(C)C(=O)N1	138,17	C7H10N2O
Z137992830	CCN1CCCCC1CO	143,23	C8H17NO
Z1263529734	C(C1CCCCN1)N1CCOCC1	184,28	C10H20N2O
Z1443588951	CC(C(O)=O)C1=CCCC1	140,18	C8H12O2
Z1374788709	CN(C)C1=C(C)NC=CC(C)=C1	164,25	C10H16N2
Z1250132777	CC(N)CC1=C(C)ON=C1C	154,21	C8H14N2O
Z1272672332	CC(CN)C1=C(F)C=C(F)C=C1	171,19	C9H11F2N
Z1272728880	CC(C)C(N)CC1=CC=C(F)C=C1	181,25	C11H16FN
Z1263811754	COC1=C(C)C(C)C(N)C=CC=C1	179,26	C11H17NO
Z1362754425	CC(O)CN1C=CN=C1C	140,19	C7H12N2O
Z1362754408	NC1CCCN2N=CN=C12	138,17	C6H10N4
Z1381287341	NC1CCN(C1)C1=C(F)C=CC=C1F	198,22	C10H12F2N2
Z1350579567	COC1CCC(CN)CC1	143,23	C8H17NO
Z1346370676	CCC1=CN=C(S1)C(C)N	156,25	C7H12N2S
Z1407659697	CCC1CCC(O1)C(O)=O	144,17	C7H12O3
Z1176666054	CCN1CCC(CC1)C(C)O	157,26	C9H19NO
Z89271885	CCS(=O)C(=O)C1=CC2=C(C(OC(N)=N2)C=C1	226,25	C9H10N2O3S
Z106805790	CCC1N(CCN)=O)CCC2=C1C=CS2	224,32	C11H16N2OS
Z168883434	CNS(=O)C(=O)C1=CN(C)C(C=C1)C(O)=O	218,23	C7H10N2O4S
Z223688278	CNC(C(=O)NC)C1=CC=C(CI)C=C1	212,68	C10H13ClN2O
Z228474590	CN1C(=O)N(CC(O)=O)C2=C1C=CC=C2	206,20	C10H10N2O3
Z119993908	CC1=C(C(C(O)=O)C(C)=NC(=O)N1	182,18	C8H10N2O3
Z104341874	CC1=CC2=C(C=CC=C2)N1CC(O)=O	189,21	C11H11NO2
Z56824601	OC(=O)COC1=C(C=CC=C1)C#N	177,16	C9H7NO3
Z1250083006	OC(=O)C1=C2OCCOC2=CC=C1	180,16	C9H8O4
Z1250080927	CS(=O)C(=O)C1(CN)CCOCC1	193,26	C7H15NO3S
Z1238477790	CC(NC(=O)C1CCCC1)C(O)=O	185,22	C9H15NO3
Z2469657345	CS(=O)C(=O)C1=CC2=C(NC=C2)C=C1	195,24	C9H9NO2S
Z1222423406	CC1=CC=C(O1)C1=NC(N)=NN=C1	176,18	C8H8N4O
Z1429750050	COC1=C2C=CC=NC2=CC=C1	159,19	C10H9NO
Z1262395976	CC1=C(C=C(CI)C=C1)N1CCC(CN)C1	224,73	C12H17ClN2
Z1267885772	CC1CN(CCN1)C1=NC(C)=CC=C1	191,28	C11H17N3
Z2235791789	CC1CNCCC1CCC(O)=O	171,24	C9H17NO2
Z2240999272	COC1=CC2=C(N=CC=C2)C(OC)=C1	189,21	C11H11NO2
Z1741964335	C1CNC(CN1)C1=CC=CC=C1	162,24	C10H14N2
Z2238934986	COC1=NC=C(N=C1)C#N	135,13	C6H5N3O
Z1720655573	CC(C)C1=C(C=CC(C)=N1)C(O)=O	179,22	C10H13NO2
Z1198183883	NC1=NC2=C(CCC2)C=C1	134,18	C8H10N2
Z2179938347	CN1N=CC(CCC(O)=O)=N1	155,16	C6H9N3O2
Z2235810122	CC1=CN=C2C=C(C=CN12)C(O)=O	176,18	C9H8N2O2
Z2235810219	CC1(C)CCC2=C(C1)C(O)=NC=N2	178,24	C10H14N2O
Z1263529593		177,25	C11H15NO
Z1983132695	BrC1=C2OCCNC2=CC=C1	214,06	C8H8BrNO
Z1103034534	CC1=CC=CN(CC2=CC=C(CI)S2)C1=O	239,72	C11H10ClNOS
Z1250132460	CC(C)N1C=CC(CN)=N1	139,20	C7H13N3
Z606312288	CN(C)C(=O)CN1C=C(Br)C=N1	232,08	C7H10BrN3O
Z1245646665	OC(C1=CC=C(CI)C=C1)C1=CN=CC=C1	219,67	C12H10ClNO
Z1245633392	CC(O)C1=CC2=C(OCC2)C=C1	164,20	C10H12O2
Z56822177	OC(=O)C1CC2=C(CN1)C=CC=C2	177,20	C10H11NO2
Z1230795916	CC(C)CNC(=O)C1=NC=CN1C	181,24	C9H15N3O
Z1983132706	C1CC2(CO1)COCCN2	143,19	C7H13NO2
Z32803522	CCC(=O)NC1=CC(CO)=CC=C1	179,22	C10H13NO2
Z1729207294	ClC1=C(CCN2C=CN=N2)C=CC=C1	207,66	C10H10ClN3

Z1269702508	CC(N)C1=C(C)C(C)=CC=C1	149,24	C10H15N
Z105197348	CC(N)C1=NC2=C(S1)C=CC=C2	178,25	C9H10N2S
Z803153754	NCC1=CC(=NC=C1)N1CCOCC1	193,25	C10H15N3O
Z1895554285	CC(CCO)C1=CNC2=C1C=CC=C2	189,26	C12H15NO
Z1655103965	CN(C)C1=C(N)N=CC=C1	137,19	C7H11N3
Z1696822333	OC(=O)C1CCCN1C1CCNC1	184,24	C9H16N2O2
Z1998612646	C1CNC(CN1)C1=CN=CC=C1	163,22	C9H13N3
Z1230248368	CN(CCO)C(=O)NC1=C(Br)C=CC=C1	273,13	C10H13BrN2O2
Z1993522703	CN1C(=O)CC2=C1C=CC(Cl)=C2	181,62	C9H8ClNO
Z383202616	CC(=O)NC1=CC2=NNC=C2C=C1	175,19	C9H9N3O
Z2028214360	OC(=O)C[C@H]1C[C@H]1C1=CC=CC=C1	176,22	C11H12O2
Z2027915114	CC(C)C1=NNC(=N1)C(F)F	161,16	C6H9F2N3
Z2027915113	CC1=NN(C(F)F)C(C)=C1CO	176,17	C7H10F2N2O
Z1896598013	CCC1=CC(=O)N2N=C(NC)SC2=N1	210,26	C8H10N4OS
Z1899648075	O=C1N(CC2CC2)C=CC2=C1C=NC=N2	201,23	C11H11N3O
Z1623872052	CC(C)C(O)C1(CN)CC1	143,23	C8H17NO
Z103698666	CC(N1CCCCC1)C(N)=O	156,23	C8H16N2O
Z1582262983	CCC1=CSC(=N1)N1C=C(C=N1)C(O)=O	223,25	C9H9N3O2S
Z1575311614	NC1CCS(=O)(=O)C2=C1C=C(Cl)C=C2	231,69	C9H10ClNO2S
Z1575304427	CC1=NN(CC(O)=O)C2=C1C=CC=N2	191,19	C9H9N3O2
Z1569709055	CCC1=C(C=C(C=C1)C(O)=O)S(C)(=O)=O	228,26	C10H12O4S
Z1569709199	CC1=NNC2=C1C=CC(N)=C2	147,18	C8H9N3
Z1551777829	CCS(=O)(=O)N1CCN(CC1)C(=O)CO	236,29	C8H16N2O4S
Z1642389710	CC1=C(F)C=CC(C(O)=O)=C1N	169,16	C8H8FNO2
Z1642389640	NC1=CC2=C(CCCC2)N=C1	148,21	C9H12N2
Z1642389487	CN(C)C1=C(C=CN=C1)C#N	147,18	C8H9N3
Z755044716	CCNC(=O)C1=CN=N1	140,15	C5H8N4O
Z1119758873	OCC1CCN(CC2=NC=CC=C2)CC1	206,29	C12H18N2O
Z1262396026	CC(N)C1=CC(Br)=CC=C1	200,08	C8H10BrN
Z1981623627	CN(C(=O)C1CCC1)C1=NC=CN=C1	191,23	C10H13N3O
Z1702887672	CC1CN(C1)C(=O)NC1=NC=CC=C1	191,23	C10H13N3O
Z1463254676	NCC1=C2OCCOCC2=CC=C1	179,22	C10H13NO2
Z1575308472	CC1=C(CCN)C=NC=C1	136,20	C8H12N2
Z1695867452	CC1=NC(C)=NC(=C1)N1CCC(N)CC1	206,29	C11H18N4
Z1689341639	CC1=C(Br)C=C(C(O)=O)C(=O)N1	232,03	C7H6BrNO3
Z2054764431	C[C@H]1OCCN(CC=C(C)C)[C@H]1C(N)=O	212,29	C11H20N2O2
Z2235790650	COC1=C(C=C(Cl)C=C1)C(O)CN	201,65	C9H12ClNO2
Z2235681415		176,22	C11H12O2
Z2235681413	CC1(C)CNC2=C(O1)C=CC=N2	164,21	C9H12N2O
Z1939263633	NC(=O)COC1=C2CCCNC2=CC=C1	206,25	C11H14N2O2
Z2235409161	NC1=NC=CC(CCO)=C1	138,17	C7H10N2O
Z2235409319	COC1=NC=NC(=C1)C#N	135,13	C6H5N3O
Z2235330321	NCC1CS(=O)(=O)C2=C1C=CC=C2	197,25	C9H11NO2S
Z85879488	OC(=O)C1=C(C(NC(=O)C2CC2)C=CC=C1	205,21	C11H11NO3
Z2217033053	CN1N=CC=C1[C@H]1[C@H](N)CCC(=O)N1C	208,27	C10H16N4O
Z2106594228	OC(=O)C1=C(Br)C=NN1C1CCCC1	259,10	C9H11BrN2O2
Z1562205518	NC(=O)C1=CN(CCO)N=C1	155,16	C6H9N3O2
Z1516516959	CC(C)(O)CN1C=C(Br)C=N1	219,08	C7H11BrN2O
Z57952782	CC1CC2=C(O1)C=CC(=C2)C(O)=O	178,19	C10H10O3
Z2568758085	CN1C=C(C=N1)N1CCC(CO)C1	181,24	C9H15N3O
Z2568758079	CC1=CC2=C(C=C1)C(N)=NC=C2	158,20	C10H10N2
Z2522940202	CC1=CCC(C)(CC1)C(O)=O	154,21	C9H14O2
Z2517219346	CN1CCC2=C(C=CC(N)=C2)C1=O	176,22	C10H12N2O
Z1508967947		208,21	C11H12O4
Z1993611196	Cl.CNCC(=O)NC1=NC=CC(C)=C1	215,68	C9H14ClN3O
Z2515207540	COC1=CC=C(C=C1)C1=NC(N)=NO1	191,19	C9H9N3O2
Z345556840	CC(=O)NCC1=C(Cl)C=CC=C1Cl	218,08	C9H9Cl2NO
Z228585484	OCC(=O)NC1=CC=C(Cl)C=C1	185,61	C8H8ClNO2
Z1741967387	NC(CO)C(=O)C1=CC=C(Br)C=C1	244,09	C9H10BrNO2
Z54745174	CNC1=NSC2=C1C=CC=C2	164,23	C8H8N2S
Z2513337538	OCCC1=C2C=CC=CC2=NC=C1	173,22	C11H11NO
Z1889909750	CC(C)C1OCCCC1C(O)=O	172,22	C9H16O3
Z166605304	CC1=NC2=NN=C(CN)N2C(C)=C1	177,21	C8H11N5
Z57983005	OC(=O)CC1OC2=C(NC1=O)C=CC=C2	207,19	C10H9NO4
Z85917495	OC(=O)CC1=CSC(=N1)C1=NC=CC=C1	220,25	C10H8N2O2S
Z56945486	OC(=O)CNC(=O)C1=C(Br)C=CC=C1	258,07	C9H8BrNO3
Z56939169	CC1=C(C(O)=O)C(C)=NO1	141,13	C6H7NO3

Z56886259	OC(=O)CNC(=O)C1=CC=CS1	185,20	C7H7NO3S
Z56921163	NC(CC(O)=O)C1=CC=C(F)C=C1	183,18	C9H10FNO2
Z56914816	CCOC1=CC=C(C=C1)C1=NN=C(N)O1	205,22	C10H11N3O2
Z56862696	CC(=O)NC1=CC(OC(F)F)=C(Br)C=C1	280,07	C9H8BrF2NO2
Z30802725	FC1=CC(F)=C(NC(=O)C2CCC2)C=C1	211,21	C11H11F2NO
Z56827184	CCOC1=C(Br)C=C(NC(C)=O)C=C1	258,12	C10H12BrNO2
Z56827160	OC(=O)CNC(=O)C1=C(Cl)C=CC=C1	213,62	C9H8ClNO3
Z56795887	CC1=CC(=O)C2=NN=CN2N1	150,14	C6H6N4O
Z234969411	CC1=NN(CCO)C(C)=C1C(O)=O	184,20	C8H12N2O3
Z56757135	NC(=O)C12CCC(CC1)C2	139,20	C8H13NO
Z1431905456	CCC(O)(C(N)=O)C1=CC=C(Br)C=C1	258,12	C10H12BrNO2
Z1428159818	OC(=O)C1CCNC(=O)C1	143,14	C6H9NO3
Z1416282423	CC1=C(CS(C)(=O)=O)C=C(S1)C(O)=O	234,28	C8H10O4S2
Z1316699693	CC1=CC(C)=NC(NCC2(O)CCC2)=N1	207,28	C11H17N3O
Z1416200910	COC1=C(OC)C=C(C(O)=O)C(F)=C1	200,17	C9H9FO4
Z1416200891	COC1=CC(N)=C(C)C=C1	137,18	C8H11NO
Z1316700062	CC1=NC(C)=NC(NCC2(O)CCC2)=C1	207,28	C11H17N3O
Z1270081818	CC1(CO)CCCC1NC1=NC=CC=N1	207,28	C11H17N3O
Z166605426	CN1C(C)=CC=C1C(O)=O	139,15	C7H9NO2
Z1374884282	COC1=NC2=C(O1)C=CC(N)=C2	164,16	C8H8N2O2
Z1210869358	NC1CCC(CC1)C1=CC=CC=C1	175,28	C12H17N
Z140561750	CNC(C)C1=C(OC)C=CC=C1	165,24	C10H15NO
Z1259161793	CC1=CC=C(O1)C(C)(O)CN	155,20	C8H13NO2
Z927412230	CC1CCCCN1C(=O)CCN	170,26	C9H18N2O
Z1162910733	NCC1CCCN1CC1CCCCC1	196,34	C12H24N2
Z1318357717	CCOC1=NC(N)=CC=C1	138,17	C7H10N2O
Z234897649	NCC1=CC(=NC=C1)N1CCCCC1	205,31	C12H19N3
Z369045030	CCC1=NC(CN2CCOCC2C)=CS1	226,34	C11H18N2OS
Z55002275	N#CC1=C(CN2CCCC2)C=CC=C1	186,26	C12H14N2
Z1343332730	CN(CC1CCOC1)C1=NC=C(Br)C=N1	272,15	C10H14BrN3O
Z2234631223	CC1=C(C=C(C=C1)C(O)=O)C(O)=O	180,16	C9H8O4
Z1222285084	COC1CCN(CC1)C1CCCCC1N	212,34	C12H24N2O
Z2130657289	CC(C)OC1=C(CO)C=NC=C1	167,21	C9H13NO2
Z1899842917	CC1=NN(CC2=C(C)ON=C2C)C(=O)S1	225,27	C9H11N3O2S
Z229424542	C1CC2=C(CN1C1=NC=CC=N1)C=CS2	217,29	C11H11N3S
Z2037257299	OCC1CCCC(=O)(=O)C1	164,22	C6H12O3S
Z1841067347	OC1CCCC1NCC1=CC=C(Br)O1	260,13	C10H14BrNO2
Z1787761777	COC1CN(CC2=CN=CS2)CCC1C	226,34	C11H18N2OS
Z1899855407	CCC1=NC(CN2N=C(C)SC2=O)=CS1	241,33	C9H11N3OS2
Z2028236283	CN(C)CC(N)C1=CC=C(Cl)C=C1	198,69	C10H15ClN2
Z2010052046	COCC1(CCC1)C(O)=O	144,17	C7H12O3
Z33546677	NC(=O)CC1=CC=C(Cl)C=C1	169,61	C8H8ClNO
Z370745502	CNC(=O)C1=CC=C(O1)S(=O)(=O)N(C)C	232,25	C8H12N2O4S
Z242435796	FC1=CC=CC(F)=C1C(=O)NCC=C	197,19	C10H9F2NO
Z1101435050	CN1C=C(CC(O)=O)C=N1	140,14	C6H8N2O2
Z54128519	CCC(C)(C)NC(=O)C1CC1	155,24	C9H17NO
Z441756998	CCC(C)(C)NC(=O)C1=NNC=C1	181,24	C9H15N3O
Z409510704	CC1CN(CCO1)C(=O)NC1=NN=CS1	228,27	C8H12N4O2S
Z285675388	CNC(=O)C1=CN=C(C=C1)N1CCCC1	205,26	C11H15N3O
Z332751146	CN(C)C(=O)C1=NNC(=C1)C1CC1	179,22	C9H13N3O
Z45462907	O=C1CN(CCN1)S(=O)(=O)C1=CC=CS1	246,30	C8H10N2O3S2
Z740611958	CC(C)C(=O)NC(C)C1=C(C)N=C(C)S1	226,34	C11H18N2OS
Z853055300	CC1(C)COCCN1C(=O)C1=NSN=C1	227,28	C9H13N3O2S
Z1272949026	CCOC1=C(C=CC=C1F)C(O)=O	184,17	C9H9FO3
Z1271843096	CC(C)C1CCNC(=O)CC1	155,24	C9H17NO
Z734736324	CCC(C)(C)NC(=O)C1=CC(C)=NN1C	209,29	C11H19N3O
Z1318356930	CC1=CC(CC(O)=O)=C(C)S1	170,23	C8H10O2S
Z1318356922	CC(C1=CC=CC=C1)C(C)(O)C(O)=O	194,23	C11H14O3
Z1310750949	NC1(CCOCC1)C(O)=O	145,16	C6H11NO3
Z274554320	CC(CN1N=C(C)C=C1C)C(O)=O	182,22	C9H14N2O2
Z274554370	CC(CC(O)=O)N1N=C(C)C(Br)=C1C	261,12	C9H13BrN2O2
Z274554330	CC(CN1C=NC=N1)C(O)=O	155,16	C6H9N3O2
Z1281658025	OC(=O)CCC1=NC2=C(S1)C=CC(Br)=C2	286,14	C10H8BrNO2S
Z56324724	CN(C)C(=O)NC1=CC(Cl)=C(C)C=C1	212,68	C10H13ClN2O
Z1921389504	CC(=C)CN1CC(O)CC2=C1C=CC=C2	203,29	C13H17NO
Z1481101458	FC1=CN=C(NC2CC2)N=C1	153,16	C7H8FN3
Z2219513504	CC1CN(CC2=C(C)N(C)N=C2C)C1C	207,32	C12H21N3

Z1250132461	CCC(N)C1=C(F)C=C(F)C=C1	171,19	C9H11F2N
Z1222285079	COC1=CC(=CC=C1)N1CCC(CN)C1	206,29	C12H18N2O
Z234897221	NCC1=CN=C(OC2CCCCC2)C=C1	206,29	C12H18N2O
Z1272480091	COCC1CN(CC01)C1=NC=CC=C1	208,26	C11H16N2O2
Z1262395911	COC1=NC(CN)=CC=C1	138,17	C7H10N2O
Z1333043394	CNCC1=NC2=C(C(CCC2)S1	182,29	C9H14N2S
Z1224460119	OCCNC1CCCC2=C1C=CC=C2	191,27	C12H17NO
Z1614721070	OC(=O)C1(CC1)C(=O)NC1CCCC=C1	209,25	C11H15NO3
Z1918366445	FC1=C(CI)C=CC(NCC2=NNC=C2)=C1	225,65	C10H9ClFN3
Z2065464240	CC1=NOC(CN2N=NC(N)=C2C)=C1	193,21	C8H11N5O
Z32367965	FC1=C(CC(=O)NC2CC2)C(Cl)=CC=C1	227,66	C11H11ClFNO
Z1848951744	FC1=C(NCC2=CN=CS2)C=CN=C1	209,24	C9H8FN3S
Z1983199026	COC(CI)C(=O)NC1=NC(C)=CC=N1	209,25	C10H15N3O2
Z1796281450	CN(C)CC(=O)NC1=C(F)C=CC=C1C	210,25	C11H15FN2O
Z1791179060	CC1=C(OC=C1)C(=O)NC1=CN=NS1	209,22	C8H7N3O2S
Z1270403514	OC(=O)C1CCS(=O)(=O)CC1	178,20	C6H10O4S
Z414834498	OC(=O)[C@H]1C[C@H](C1)C(O)=O	144,13	C6H8O4
Z57157168	CC1=CCC(C(C1)C(O)=O)C(O)=O	184,19	C9H12O4
Z85887020	OC(=O)CNC(=O)C1=CC2=C(CCC2)S1	225,26	C10H11NO3S
Z959151608	O[C@@H]1CCOC2=C1C=CC=C2F	168,17	C9H9FO2
Z1020680168	NCC1(O)CCCCC1	143,23	C8H17NO
Z1268152304	O=S1CCNC2=C1C=CC=C2	181,25	C9H11NOS
Z29672824	CC1=NN=C(NC(=O)C2=CC=CO2)S1	209,22	C8H7N3O2S
Z927306976	NCCNC(=O)C1=NC=CN=C1	166,18	C7H10N4O
Z1262246158	CC(C)N1N=CC2=C1C=C(N)C=C2	175,24	C10H13N3
Z1262246089	CC1=C2NC=C(C(O)=O)C(=O)C2=CC=C1	203,20	C11H9NO3
Z220383506	NC(=O)CC1=C(CI)C=C(C(N1)C(F)F	238,59	C8H6ClF3N2O
Z2658865866	COC1=CC2=C(C(=O)C=CN2)C(OC)=C1	205,21	C11H11NO3
Z846981274	CC1=CC(CS(C)(=O)=O)=C(C)S1	204,30	C8H12O2S2
Z2106591704	OC(=O)C1=CC=C(CN2C=CC=N2)S1	208,24	C9H8N2O2S
Z2106593035	OC(=O)CN1C=CC(=N1)C1CC1	166,18	C8H10N2O2
Z2060348232	CN(CC(O)=O)C1=C(C(F)C=C(C=C1)C#N	208,19	C10H9FN2O2
Z2106601348	CC(C)N1C=C(C(O)=O)C(C)=N1	168,20	C8H12N2O2
Z2510258132	COC1=CC2=C(C(CCC2C(O)=O)C=C1	192,21	C11H12O3
Z2412196567	CCOC1=NC(N)=CN=C1	139,16	C6H9N3O
Z1624945782	CC(=CC1=CC=C(CI)S1)C1=NC=CN=C1	236,72	C11H9ClN2S
Z1217960891	CN1CCC(OC2=CC(F)=CC=C2)C1=O	209,22	C11H12FNO2
Z2379802745		191,23	C11H13NO2
Z2379802683	CN1N=C(N)C2=C1C=C(C)N(C)C2=O	192,22	C9H12N4O
Z1413929716	OCCNC1=CC(F)=C(F)C=C1	173,16	C8H9F2NO
Z2379087651	OC(=O)CC1=CC=C(C=C1)N1C=NN=C1	203,20	C10H9N3O2
Z275169862	CN1N=C(C(O)=O)C(Cl)=C1C	174,58	C6H7ClN2O2
Z2346081588	CC(C)(O)C1=C(N)C=C2C=CC=CC2=N1	202,26	C12H14N2O
Z2327883945	O=S1(=O)CCCN1C1CCNCC1	204,29	C8H16N2O2S
Z2327883755	CCN1C(=O)C(O)=NC2=C1C=CC=C2	190,20	C10H10N2O2
Z2327883839	CC1=CSC2=C1N=CN=C2	150,20	C7H6N2S
Z111808714	CC1=NC2=C(C=CC=C2N)C=C1	158,20	C10H10N2
Z227823010	CCNC1=NC=CC(=C1)C(O)=O	166,18	C8H10N2O2
Z1262398568	CC(=O)N1CCNC2=C1C=CC=C2	190,25	C11H14N2O
Z28134680	CC(=O)NC1=CC=C(C)C=C1	149,19	C9H11NO
Z1697079442	CC1=NC=NC(=C1)N1CCC=C(F)C1	193,23	C10H12FN3
Z1262327470	CNS(=O)(=O)C1=C(C)C=C(N)C=C1	200,26	C8H12N2O2S
Z1262327418	CC1CNC(=O)N1C1=CC(N)=CC=C1	191,23	C10H13N3O
Z1262254339	OC(C1CCCCN1)C1=CC=CC=C1	191,27	C12H17NO
Z1259339084	CN1N=CC=C1C1CCNCC1	165,24	C9H15N3
Z1262252941	NCC1=C(F)C=C(F)C=C1	143,14	C7H7F2N
Z1272267454	CC1=NSC(=N1)N1CCC[C@H]1CO	199,27	C8H13N3OS
Z1836338670	CC1NCCN2C=NN=C12	138,17	C6H10N4
Z1827898544	CCC1=C(N)C=NN1C1CCCC1	179,27	C10H17N3
Z1250132437	OC(=O)CCC1CCOC1	144,17	C7H12O3
Z1823262976	CCNC1=CC2=C(NC=C2)C=C1	160,22	C10H12N2
Z1815149220	CCC(C)N1N=CC(N)=C1C1CC1	179,27	C10H17N3
Z1516316257	CCC1=NOC(C)=C1CN1C=CC(C)=N1	205,26	C11H15N3O
Z1741963038	CC1=C(CN)C=C(CI)C=C1	155,63	C8H10ClN
Z1801361876	C1COC(C1)C1CCNCC1	155,24	C9H17NO
Z1820007381	CC(C)N1N=CC(C(O)=O)=C1N	169,18	C7H11N3O2
Z1891775929	OC1CCNC2=C1C=C(F)C=C2	181,21	C10H12FNO

Z2242946524	NC1=C(Br)C=C2CNCC2=C1	213,08	C8H9BrN2
Z1893446212	CC1=C(N)ON=C1C1=C(F)C=CC(C)=C1	206,22	C11H11FN2O
Z1889917194	OC(=O)C1CCCN1C1=CC=CC=C1	191,23	C11H13NO2
Z1837073492	CC1=C(CO)C=CC(=C1)N1C=CN=C1	188,23	C11H12N2O
Z1723633687	CC1=C(C=C(F)C=C1)C1=NN=C(N)O1	193,18	C9H8FN3O
Z2226312235	CC1=NOC=C1CN1CCC=C(F)C1	196,23	C10H13FN2O
Z2329283105	OC1(CCN2CCC=C(F)C2)CCC1	199,27	C11H18FNO
Z1619984629	CN1CCC(N2CCC=C(F)C2)C1=O	198,24	C10H15FN2O
Z2034487295	CN(CC1CCOC1)C1=NC=C(F)C=C1	210,25	C11H15FN2O
Z1929757385	CC1(C)CN(CC1O)C1=C(F)C=CC=N1	210,25	C11H15FN2O
Z1748646799	C[C@H](NC(=O)CO)C1=C(Cl)C=CC(Cl)=C1	248,10	C10H11Cl2NO2
Z1675358685	CN(CC1(O)CCC1)C1=C(Cl)C=NC=C1	226,70	C11H15ClN2O
Z1985112155	CCN(C(=O)C1CC1)C1=C(C)C=CC=N1	204,27	C12H16N2O
Z1463350841	CC(C)CN1C=CN=C1N	139,20	C7H13N3
Z2087745225		205,30	C13H19NO
Z2092579816	CC(N)CN(C)C1CCN(C)CC1	185,32	C10H23N3
Z2442044577	OCC(F)=C1CCCNC1	145,18	C7H12FNO
Z1348559502	CNC1(CCCC1)C(N)=O	142,20	C7H14N2O
Z1526503471	CC1=C(C)N=C(C(O)=O)C(O)=N1	168,15	C7H8N2O3
Z1501469698	CC(C)C1=C(N)N=CC=C1	136,20	C8H12N2
Z1333043520	CN1C(=O)CNC2=C1C=CC=C2	162,19	C9H10N2O
Z1492781233	CC(C)(C1=NOC(N)=C1)S(C)(=O)=O	204,24	C7H12N2O3S
Z1480642142	COC1(CN)CCOCC1	145,20	C7H15NO2
Z1459946056	COCC1=NC=NC(O)=C1	140,14	C6H8N2O2
Z57990849	OC(=O)CCC1=NC2=C(O1)C=CC=C2	191,19	C10H9NO3
Z1442018040	CC1=C(C(O)=O)C(N)=C(Cl)C=C1	185,61	C8H8ClNO2
Z1436472922	COCC1=NC=NC(N)=C1	139,16	C6H9N3O
Z1436105147	CN1NC(=O)C2=C1NC=CC2=O	165,15	C7H7N3O2
Z274779140	CC(CN)OC1=CC=C(F)C=C1	169,20	C9H12FNO
Z1428019338	CCC1CN(CCC1N)S(C)(=O)=O	206,30	C8H18N2O2S
Z1266823391	COCCN1CCNCC1C	158,25	C8H18N2O
Z1342884092	CC(C1CCCC1)C(O)=O	142,20	C8H14O2
Z1222285092	COC1=C(C=CC=C1)N1CCC(N)CC1	206,29	C12H18N2O
Z1238477839	CC(N)CN1CCCCC1	142,25	C8H18N2
Z1263529706	COC1=C2OC(CN)=CC2=CC=C1	177,20	C10H11NO2
Z1262237458	NC(C1CC1)C1=NC=CS1	154,23	C7H10N2S
Z454097862	CC(C)NC(=O)C1=NNC(=C1)C(C)C	195,27	C10H17N3O
Z1455009926	CC1=C(Cl)C=CC(=C1)C(=O)NCC(O)=O	227,64	C10H10ClNO3
Z647156496	CC(O)CNC(=O)C1=C(C)C=C(Br)C=C1	272,14	C11H14BrNO2
Z1741975280	CC1=NC(N)=C(CO)C=N1	139,16	C6H9N3O
Z1945695955	OC(=O)CCC1=CC2=C(C=CC=C2)N=C1	201,23	C12H11NO2
Z1273312303	CCNC(=O)C1=CC(Br)=CN1C(C)C	259,15	C10H15BrN2O
Z1934400485	NCC1=NN=C(S1)C1=C(F)C=NC=C1	210,23	C8H7FN4S
Z1699521115	CN1N=CN=C1NCC1=C(C)N=C(C)S1	223,30	C9H13N5S
Z1896597109	CNC1=NC=C(N=C1)C#N	134,14	C6H6N4
Z1901071385	CN(C)C1=NC=C(N=C1)C#N	148,17	C7H8N4
Z1783879420	N#CC1=CSC(CNC2=NC=CC=N2)=C1	216,26	C10H8N4S
Z1895582742		202,65	C8H7ClO2S
Z744593250	OC(=O)C1=C2NCCCN2N=C1	167,17	C7H9N3O2
Z56763896	OC(CN1C=NC=N1)C1=CC=C(Cl)C=C1	223,66	C10H10ClN3O
Z373775846	CN1C=C(NC(=O)C2=CC=C(C)S2)C=N1	221,28	C10H11N3OS
Z372503386	CCC1=CC=C(O1)C(=O)NC1=CCN=C1	205,22	C10H11N3O2
Z145545076	BrC1=CNC(=C1)C(=O)N1CCNC(=O)C1	272,10	C9H10BrN3O2
Z57074586	CC(NC(=O)C1=CC=C(Br)O1)C(O)=O	262,06	C8H8BrNO4
Z744754540	CN1CC(=O)NC2=C1C=CC(=C2)C(O)=O	206,20	C10H10N2O3
Z228586716	O=C(NCC1=CC=CS1)C1CCNCC1	224,32	C11H16N2OS
Z1259339138	CNC1CCN(CC2=CC=NC=C2)CC1	205,31	C12H19N3
Z1258620051	CC1=C2NC=C(CCN)C2=CC=C1	174,25	C11H14N2
Z228581550	CC1=NN(C=C1C(O)=O)C1=CC=CC=C1	202,21	C11H10N2O2
Z1170039578	CC1CCC2=C(C1)C=C(C#N)C(=O)N2	188,23	C11H12N2O
Z955526726	CNC(=O)C1CC1C1=CC(Cl)=CC=C1	209,67	C11H12ClNO
Z228584312	OCC1=NC2=C(S1)C=CC(=C2)C(F)F	233,21	C9H6F3NO5
Z1171978821	OC(=O)CN1N=CC2=C1C=CC=C2	176,18	C9H8N2O2
Z432066794	NC1=NN=C(O1)C1CCNCC1	168,20	C7H12N4O
Z224841742	NC1=C(N=CC=N1)C(=O)NC1CCCC1	206,25	C10H14N4O
Z274553586	CC1=NN(CCC(O)=O)C(C)=N1	169,18	C7H11N3O2
Z2588063830	CCOC1=CC(CO)=CN=C1	153,18	C8H11NO2

Z751928604	CC1=NNC=C1CNC1=CC(F)=CC=C1	205,24	C11H12FN3
Z1925944096	CC(C)CC1=C(N)ON=C1C(F)(F)F	208,18	C8H11F3N2O
Z1324812698	CC(=O)NCC1=NOC=C1	140,14	C6H8N2O2
Z2583036115	COC1CCC(C1)C(O)=O	144,17	C7H12O3
Z2568771122	C=CCOC1=CN=CC=C1	135,17	C8H9NO
Z2188253056	C[C@@H](O)CN(C)C(=O)C1=NC(C)=CC=C1	208,26	C11H16N2O2
Z228586320	CCC(O)C1=CC=C(OC)C=C1	166,22	C10H14O2
Z2216303091	OC(=O)COC1=CC(F)=C(Cl)C=C1	204,58	C8H6ClFO3
Z2211231664	COC1=C2C(CCC2=CC=C1)C(O)=O	192,21	C11H12O3
Z2001336017	CC1(C)CNC(=O)CN1S(=O)(=O)C1CC1	232,30	C9H16N2O3S
Z2205958778	CC1=C(SC2=C1C=C(C=C2)C#N)C(O)=O	217,24	C11H7N2O2S
Z2189283988	OC(=O)CCC1=CN=CN=C1	152,15	C7H8N2O2
Z2188172118	OC(=O)CC1=CCOCC1	142,15	C7H10O3
Z1952438221	CC(NC(=O)C1=C(Br)C=CC=N1)C=C	255,12	C10H11BrN2O
Z2168541814	CC(N1CC(C)C1)C(O)=O	143,19	C7H13NO2
Z2168541836	CN1C(=O)CC2=C1C=CC(C)=C2	161,20	C10H11NO
Z2168499534	CS(=O)(=O)[C@@H]1CCCC[C@H]1O	178,25	C7H14O3S
Z2168282749	OC(=O)C1CCN(C1)C1=C(F)C=CC=C1	209,22	C11H12FN2O2
Z183465912	CC(C)CNC(=O)C1=C(O)N=CC=C1	194,23	C10H14N2O2
Z108544480	CN1C=CC(NC(=O)C2=CC=C(C)S2)=N1	221,28	C10H11N3O5
Z28139094	COC1=CC=C(NC(=O)C2CC2C)C=C1	205,26	C12H15NO2
Z30612266	CCC(=O)NC1=CC=C(C=C1)C#N	174,20	C10H10N2O
Z324552980	Cl.CC1=CC(CN2CCNCC2)=NO1	217,70	C9H16ClN3O
Z104586966	CC(NC1=CC=C(Br)C=C1)C(N)=O	243,10	C9H11BrN2O
Z317046464	NC1=C(C=CC=C1)S(=O)(=O)N1CCCC1	226,29	C10H14N2O2S
Z228589506	CC1=CN2C(C=C1)=NC=C(C(O)=O)C2=O	204,19	C10H8N2O3
Z295451518	CS(=O)(=O)C1=C(C(NC(=O)CO)C=CC=C1	229,25	C9H11NO4S
Z89324450	COC1=C(C=C(C)C=C1)S(=O)(=O)N(C)C	229,29	C10H15NO3S
Z101185962	COC1=C2OCCOC2=CC(=C1)C(N)=O	209,20	C10H11NO4
Z235345619	COC1=C(OC)C=C(C=C1)C(O)=O	182,18	C9H10O4
Z30612298	CC(C)CC(=O)NC1=CC=C(C=C1)C#N	202,26	C12H14N2O
Z234897551	NC1=C(C=C(C=C1)N1CCCC1)C(O)=O	206,25	C11H14N2O2
Z1169949823	C1CC(C1)C1=NC(=NO1)C1=CN=CC=C1	201,23	C11H11N3O
Z133743156	CC(NS(C)(=O)=O)C1=CC(F)=CC=C1	217,26	C9H12FNO2S
Z1335657450	CCN1N=CC2=C1CCCC2N	165,24	C9H15N3
Z228585382	OCC(=O)N1CCCCC1	157,21	C8H15NO2
Z1276751957	CC1CCNC(C1)C1=CC=CO1	165,24	C10H15NO
Z1255523342	CC1=CC=C(O1)C(O)CN	141,17	C7H11NO2
Z1333043516	COC1=CC2=C(C=C1)C(O)CO2	166,18	C9H10O3
Z1333717727	OC(=O)CCC1CCCOC1	158,20	C8H14O3
Z1250132472	CC1NCCS(=O)(=O)C1C	163,24	C6H13NO2S
Z1267885765	CC(C)(N)C1=C(C)C=CC=N1	164,25	C10H16N2
Z1267882052	C=CCOC1CCNCC1	141,21	C8H15NO
Z1262237384	NC1CCN(CC2=CC=CS2)CC1	196,31	C10H16N2S
Z149387406	C=CCN1N=NN(C1=O)C1=CC=CC=C1	202,22	C10H10N4O
Z1258578217	CCC1=NC(C)=C(S1)C(C)O	171,26	C8H13NOS
Z1354416067	COC1=NC(=O)C(F)=CN1	144,11	C5H5FN2O2
Z1347206020	CNS(=O)(=O)C1=C(C)C=C(Cl)C(C)=C1	233,71	C9H12ClNO2S
Z1342879029	COC1=CC=C(CN2C=NC(N)=N2)C=C1	204,23	C10H12N4O
Z1342879027	CNS(=O)(=O)CC1CCCN1	178,25	C6H14N2O2S
Z1342208417	FC1=C2CN=C3CCCN3C2=CC=C1	190,22	C11H11FN2
Z1335657678	CCC1=NC(=CN1)C(O)=O	140,14	C6H8N2O2
Z1333761880	CC(C(O)=O)C1=CC2=C(O1)C=CC=C2	190,20	C11H10O3
Z27805821	CC(=O)NC1=CC=C(F)C=C1	153,16	C8H8FNO
Z1281718596	C(NC1=NC=CN2C=NN=C12)C1CCCC1	203,25	C10H13N5
Z1357774299	NC(C(O)=O)C1=CC=CS1	157,19	C6H7NO2S
Z1357774297	CC1(O)CCC2=C1C=CC=C2	148,21	C10H12O
Z1357774199	OC(CC1CCCN1)C1=CC=CS1	197,30	C10H15NOS
Z1816233640	NC1=CN(CC(O)=O)N=C1	141,13	C5H7N3O2
Z1378430661	CN(C)S(=O)(=O)C1=CC2=C(O1)C=CC=C2	225,26	C10H11NO3S
Z276754694	CC(C)N(C(C)C)C(=O)C1=CC=CC=C1	205,30	C13H19NO
Z1801307734	CC(C)(O)C1=NN=C(N)O1	143,15	C5H9N3O2
Z1801307814	O=C1NCC2=C1C=CC=N2	134,14	C7H6N2O
Z1800620533	CC(O)(CCN)C1=CC=CC=C1	165,24	C10H15NO
Z228585444	OCC(=O)NC1=CC=CC=C1	151,17	C8H9NO2
Z1778350582	OC(=O)C1(CC2=C(Cl)C=CC=C2)CC1	210,66	C11H11ClO2
Z1601556832	CN(C)C(=O)CNC1=C(F)C=CC=C1C	210,25	C11H15FN2O

Z94597856	CN(C)S(=O)(=O)C1=C(C)NN=C1C	203,26	C7H13N3O2S
Z449369024	CC1=NC(N)=C(C=N1)C#N	134,14	C6H6N4
Z449369112	CCC1=C(C=NC=N1)C(O)=O	152,15	C7H8N2O2
Z444349766	OC(=O)C1CCC(=O)NC1	143,14	C6H9NO3
Z367858598	CCC1=CC=C(O1)C(=O)NC1=NN=CS1	223,25	C9H9N3O2S
Z363121080	CC1=C(C=CC(=N1)C(=O)NC1CC1)C#N	201,23	C11H11N3O
Z432102204	CC1=C(CCC(O)=O)C(C)=NC(=O)N1	196,21	C9H12N2O3
Z244345748	CNC(=O)C1=C(C=CS1)N1C=CC=C1	206,26	C10H10N2O5
Z425389620	OC(=O)C1=CC=C(C=C1)N1CCNC1=O	206,20	C10H10N2O3
Z415636688	CC1=CC2=NC=C(C(O)=O)C(=O)N2C=C1	204,19	C10H8N2O3
Z406680082	OC(=O)C1=CC(=CC=C1)N1CCNC1=O	206,20	C10H10N2O3
Z398557072	CS(=O)(=O)NCC1CCCNC1	192,28	C7H16N2O2S
Z234894111	NC1=NN=C(C(O1)C1=CC2=C(CCCC2)S1	221,28	C10H11N3O5
Z398513148	CC(C)C1=C(C=NN1)C(O)=O	154,17	C7H10N2O2
Z398513314	CC(C)C1=NC(C)=C(S1)C(O)=O	185,24	C8H11NO2S
Z242124466	CNC(=O)C1=NOC(=C1)C1=CC=CS1	208,24	C9H8N2O2S
Z108544622	CN1C=CC(NC(=O)C2=CC=CS2)=N1	207,25	C9H9N3O5
Z57068946	NC(C(O)=O)C12CC3CC(C(C3)C1)C2	209,29	C12H19NO2
Z383822280	NC1=C(N=CC=N1)C(=O)NCC1CCC1	206,25	C10H14N4O
Z27167166	O=C(NC1=NN=C(S1)C1CC1)C1CC1	209,27	C9H11N3O5
Z935140740	Cl.CC1=CC(C)=C(CN)C(C)=C1	185,70	C10H16ClN
Z916919184	CC(=O)NC1=C(C=CC=C1Cl)C(O)=O	213,62	C9H8ClNO3
Z1741963648	OC(=O)C1CC2=C(C1)C=CC=C2	162,19	C10H10O2
Z1250080932	OC(=O)C1(O)CC2=C(C1)C=CC=C2	178,19	C10H10O3
Z1742054869	OC(=O)CN1N=CN2C=CC=C2C1=O	193,16	C8H7N3O3
Z1171978864	CC(C)C(N1CCCC1=O)C(O)=O	185,22	C9H15NO3
Z812517016	OC(=O)CN1C(=O)NC2=C1C=CC=C2	192,17	C9H8N2O3
Z2327039956	CC(C)N1C(=O)NC2=C1C=C(F)C=C2	194,21	C10H11FN2O
Z1258578180	NCC1=CC2=C(C=CO2)C=C1	147,18	C9H9NO
Z1273048546	CC1=CC2=C(C=C1)N=C(CCN)O2	176,22	C10H12N2O
Z2234631222	OC(=O)C1CCCC1C1=CC=CC=C1	190,24	C12H14O2
Z2087745156	NCC1CCC2=NC(=CN2C1)C(F)(F)F	219,21	C9H12F3N3
Z255150112	CC1=NC2=C(C(C(N)CC2)C=N1	163,22	C9H13N3
Z1827889368	NCC1CCOC2(CCO2)C1	171,24	C9H17NO2
Z1262395967	NCCC1=NN(C=C1)C1=CC(F)=CC=C1	205,24	C11H12FN3
Z1335657813	CC(O)CC1=NC2=C(S1)C=CC=C2	193,26	C10H11NO5
Z1335657668	OC(=O)C1CC11CCC2=C1C=CC=C2	188,23	C12H12O2
Z1276751393	CC(N)C1=CC=C(C=C1)N1C=CC=N1	187,25	C11H13N3
Z1272684691	O=C1CC2(CN1)CCOCC2	155,20	C8H13NO2
Z1207823996	CN(CC(C)(C)O)C1=NC=C(Br)C=N1	260,14	C9H14BrN3O
Z1263602401	CN1C2=C(C=CC=C2)C(=O)NCC1=O	190,20	C10H10N2O2
Z449369118	CC(C)C1=C(C=NC=N1)C(O)=O	166,18	C8H10N2O2
Z1868430499	CN1N=C(C(C(O)=O)CC1=O	156,14	C6H8N2O3
Z1945708568	CC(C)C1=NC(CC(F)(F)F)=NN1	193,17	C7H10F3N3
Z1820077409	CNC(CN)C1=CC=C(F)C=C1	168,22	C9H13FN2
Z1820078920	CC(C)CN1N=CC(N)=C1C(C)C	181,28	C10H19N3
Z2255334838	OC(=O)C12CCCC1CNC2	155,20	C8H13NO2
Z1820078487	NCC1=NC2=C(C=CC=C2)N1C1CC1	187,25	C11H13N3
Z33448386	COCC(=O)NC1=CC2=C(CCC2)C=C1	205,26	C12H15NO2
Z29693768	O=C(NCC1=CC=CS1)C1=CC=CC=C1	217,29	C12H11NO5
Z30624434	CCC(=O)N1CCC2=C1C=CC=C2	175,23	C11H13NO
Z139720892	COC1=NC=C(C=C1)C(O)=O	153,14	C7H7NO3
Z131022006	CC1=C(C)C(C#N)=C(N)O1	136,15	C7H8N2O
Z45528360	CCNS(=O)(=O)C1=C(C)C=CC(C)=C1	213,30	C10H15NO2S
Z57228584	CC(NC(=O)C1=CC=CS1)C(O)=O	199,22	C8H9NO3S
Z217102738	CN1N=C(C)C(C(O)=O)=C1C	154,17	C7H10N2O2
Z30280214	CCNC(=O)C1=C(Br)C=CC(OC)=C1	258,12	C10H12BrNO2
Z1849012892	CC1=CC(=O)C2=C(N1)C=CC=C2	159,19	C10H9NO
Z1889861359	CCC1=CC=C(C=C1)N1CCNC1=O	190,25	C11H14N2O
Z1889706353	OC(=O)C1=C2OCCOC2=C(Cl)C=C1	214,60	C9H7ClO4
Z1881599258	OCC1(CCOCC1)C1=CC=CC=C1	192,26	C12H16O2
Z1881599850	OC1CCN(C1=O)C1=CC(Br)=CC=C1	256,10	C10H10BrNO2
Z1874937335	CN(C)C(=O)C1(CC1)C(O)=O	157,17	C7H11NO3
Z1260735513	CNC(=O)C1=CN=C(S1)C1=CC=NC=C1	219,26	C10H9N3O5
Z1259273134	OC(=O)C1(O)CCOCC1	146,14	C6H10O4
Z1176890038	CC1CC2=C(C=CC=C2)C1NS(C)(=O)=O	225,31	C11H15NO2S
Z1188322569	CCN(C)C(=O)NC1=CC(Cl)=C(F)C=C1	230,67	C10H12ClFN2O

Z1222283885	NCCNC1=C(Cl)C=C(Cl)C=N1	206,07	C7H9Cl2N3
Z1222283884	NC(=O)C1=CC2=C(NCCC(=O)N2)C=C1	205,22	C10H11N3O2
Z1222278648	CN1C=C(C(O)=O)C(=N1)C1CCCCC1	208,26	C11H16N2O2
Z1217170566	CN1NC(=O)C2=C1N=CC=C2	149,15	C7H7N3O
Z1127124543	O[C@@H]1CCN(C1)C1=NC2=C(S1)C=CC=C2	220,29	C11H12N2O5
Z755015062	O=C(NC1CCCCC1)C1=CN=N1	208,27	C10H16N4O
Z335675800	OCCOC1=CC(Cl)=CC(Cl)=C1	207,05	C8H8Cl2O2
Z1245633199	CC(C)C(N)C1=NC=CN1C	153,23	C8H15N3
Z1575143878	CC(N)CCN1C=NC=N1	140,19	C6H12N4
Z1575082122	C1CNC(C1)C1=NNC=C1	137,19	C7H11N3
Z737615774	CN(CC1CC1)C(=O)C1=C(C)SC(C)=C1	223,33	C12H17NOS
Z422952578	CN(CC(N)=O)C(=O)C1=CC(Br)=CN=C1	272,10	C9H10BrN3O2
Z422344882	CC1=C(SC=N1)C(=O)N1CCNC(=O)C1	225,27	C9H11N3O2S
Z1172115917	CN1CCC(CC1=O)C(O)=O	157,17	C7H11NO3
Z1172068250	CC(C(O)=O)C1=CC2=C(OCCO2)C=C1	208,21	C11H12O4
Z1172068150	OC(=O)CN1CCCN1=O	158,16	C6H10N2O3
Z1171979242	CCN1C=C(CC(O)=O)C2=C1C=CC=C2	203,24	C12H13NO2
Z1232874903	CCNS(=O)(=O)N1CCN2CCCC2C1	233,33	C9H19N3O2S
Z1526453862	CC(C)(CO)C1CCCC1	142,24	C9H18O
Z1268153220	CC(CN)OC1=CC(Br)=CC=C1	230,11	C9H12BrNO
Z1407654393	CC1CC(N)CN1CC1=CC=CC=C1	190,29	C12H18N2
Z2509351132	CCC1=C(N)N=C(C)C=C1	136,20	C8H12N2
Z2492774465		211,26	C11H17NO3
Z2489418727	CC1=C(OC(=O)C2=C1C=CC=C2)C(O)=O	204,18	C11H8O4
Z2472860046	CCN1C(=O)NC2=C1C=C(C=C2)C(O)=O	206,20	C10H10N2O3
Z2471547774	OC(=O)C1=C2NC(=O)COC2=CC=C1	193,16	C9H7NO4
Z1982493929	CN1N=CC2=C1CC(CC2)C(O)=O	180,21	C9H12N2O2
Z2509351166	CCN(C(C)=O)C1=NC=C(N)C=C1	179,22	C9H13N3O
Z1973466038	OC(=O)C1=C(C(OC=C1)C1CC1	152,15	C8H8O3
Z1455010668	OC(=O)CNC(=O)C1=C(Br)C=CC=C1F	276,06	C9H7BrFNO3
Z353237440	CC(CO)NC(=O)C1=C(C)C=CC(F)=C1	211,24	C11H14FNO2
Z1946684511	OC1CCCOC2=C1C=CC=C2F	182,19	C10H11FO2
Z29692416	CC1=CC=C(O1)C(=O)NCC1=CC=CS1	221,27	C11H11NO2S
Z1891775701	CN1CCC(O)(CN)CC1	144,22	C7H16N2O
Z1992316417	NC1=CC(CN2CCOCC2)=C(Cl)C=C1	226,70	C11H15ClN2O
Z1992316403	CN1C=C(C(O)=O)C(=O)C=C1C	167,16	C8H9NO3
Z1983100835	OC(=O)CC1CCCC(=O)N1	171,20	C8H13NO3
Z1983080176	OC(=O)CC1CCCCNC1=O	171,20	C8H13NO3
Z1983079259	OC(=O)C1=CC(=NO1)C1CC1	153,14	C7H7NO3
Z993967154	CNC(C(O)=O)C1=CC(Cl)=C(Cl)C=C1	234,08	C9H9Cl2NO2
Z993967218	CC1=CC=C(S1)C1=NC(N)=NN=C1	192,24	C8H8N4S
Z19739650	CC(OC1=CC=C(C=C1)C#N)C(N)=O	190,20	C10H10N2O2
Z2453029853	CC1=CC(C2=NNC(N)=C2)=C(F)C=C1	191,21	C10H10FN3
Z2692095159	CCC1(CCNCC1)N1CCOCC1	198,31	C11H22N2O
Z2692095103	CC1(COC2=C(O1)C=CC=C2)C(O)=O	194,19	C10H10O4
Z2692095025	OC(=O)C1=C(NC(=C1)C1CC1)C1CC1	191,23	C11H13NO2
Z2692093988	COC1=NC(N)=C2C=CC=CC2=C1	174,20	C10H10N2O
Z2273464199	FC1=C(N[C@H]2CCCN2=O)N=CC=C1	209,22	C10H12FN3O
Z1259155996	CC1CN(CC(CO1)C1=NC=C(N)C=C1	207,28	C11H17N3O
Z1259155942	CC1=C(CO)OC2=C1C=CC=C2	162,19	C10H10O2
Z254580486	CN(C)C(=O)CN1C=CC=N1	153,19	C7H11N3O
Z1846840792	C(NC1CCCCC1)C1=CN=N1	180,26	C9H16N4
Z1667560467	CN1N=C(C)N=C1NC(=O)C1CC=CC1	206,25	C10H14N4O
Z1837073496	O=C1CCC(CC2=CC=CC=C2)N1	175,23	C11H13NO
Z1837073270	C(NC1=CC=CC=C1)C1=CN=N1	174,21	C9H10N4
Z1836338761	CN1CCCCC1CC(O)=O	157,21	C8H15NO2
Z1741962792	CC1=CSC(C(O)=O)=C1Cl	176,61	C6H5ClO2S
Z1836338742	COC1(CC(O)=O)CCC1	144,17	C7H12O3
Z1836181359	CC(C)N1C=C(NC(=O)C2(N)CC2)C=N1	208,27	C10H16N4O
Z1834278543	CC1=C2C=CC=C(Br)C2=NN=C1	223,07	C9H7BrN2
Z1827897920	CC1C(CCN1C1=CC=CC=C1)C(O)=O	205,26	C12H15NO2
Z1258992713	CC1CCCC(C)C(=O)N1	141,21	C8H15NO
Z135897268	NC(=O)C1C2CC3CC(C2)CC1C3	179,26	C11H17NO
Z1255523379	CC1=NC2=C(C=CC=C2C(O)=O)C=C1	187,20	C11H9NO2
Z1250132718	OC(=O)C1=CC(=CC=C1)N1CC=CC1	189,21	C11H11NO2
Z1250132694	CC(CC1=C(C)ON=C1C)C(O)=O	183,21	C9H13NO3
Z410097646	CN(C)C(=O)NC1=CC(=CC=C1)C#N	189,22	C10H11N3O

Z1250132381	OCC1CN(C(=O)C1)C1=CC=CC=C1	191,23	C11H13NO2
Z1610998441	CC1=NSC(NCC2=CN=CS2)=N1	212,29	C7H8N4S2
Z1629024437	C[C@H](NC(=O)C1=NC=C(Br)C=C1)C(N)=O	272,10	C9H10BrN3O2
Z1259341037	CC(C)NC1=CN=CC=C1	136,20	C8H12N2
Z1259340994	CC1=C(C)C(=O)N=C(N1)C1=CC=NC=C1	201,23	C11H11N3O
Z1259335789	COC1=C(C(O)=O)C(C)=NN1C	170,17	C7H10N2O3
Z1259335778	CC1=CC(=CC=C1)C(N)C(O)=O	165,19	C9H11NO2
Z1259335770	CN1C=C(C=N1)C1=NC=C(S1)C(O)=O	209,22	C8H7N3O2S
Z1259273402	OC(=O)COC1CCOCC1	160,17	C7H12O4
Z1259161763	CC(N)C1=CN(C)N=C1C	139,20	C7H13N3
Z1460222813	FC1=C(NC2CCNC2=O)C=CC(Cl)=C1	228,65	C10H10ClFN2O
Z1267773633	CCC1=NC=C(CNC)S1	156,25	C7H12N2S
Z1268168726	CC(=O)NCC1=CNC=N1	139,16	C6H9N3O
Z2169086459	CN1C=C(Br)C=C(F)C1=O	206,01	C6H5BrFNO
Z2037267084	CC1=NC2=C(N1)C=CC=C2C(O)=O	176,18	C9H8N2O2
Z2218249029	CNS(=O)(=O)C1=C(F)C=CS1	195,23	C5H6FNO2S2
Z2684295940	CN1CCC(CC(N)C(O)=O)CC1	186,26	C9H18N2O2
Z734660320	CNC(=O)C1=CC2=C(C=CC=C2)N1C	188,23	C11H12N2O
Z2681277212	CN1C=C(N)C(=N1)C1=CC=CO1	163,18	C8H9N3O
Z1741980128	COC1=C2CNC(=O)C2=CC=C1	163,18	C9H9NO2
Z135504726	CN(C)C(=O)C1=CC=CN1	138,17	C7H10N2O
Z1171979256	CC1=NC=CN1C1=CC(=NC=C1)C(O)=O	203,20	C10H9N3O2
Z1171979243	CCN1C=C(Br)C=C1C(O)=O	218,05	C7H8BrNO2
Z1171978890	CC1=NC2=C(C=NN2C=C1)C(O)=O	177,16	C8H7N3O2
Z85895893	CC(=O)N1CCCCC1C(O)=O	171,20	C8H13NO3
Z1094758722	OC(=O)C1=C2OCC(=O)NC2=CC=C1	193,16	C9H7NO4
Z1171978880	CC1=NC(=CS1)C1=CC(=CO1)C(O)=O	209,22	C9H7NO3S
Z1171978866	COC1=CC=C(C=C1)C1(CCC1)C(O)=O	206,24	C12H14O3
Z54082288	CN1C=CC=C1C(=O)NCC1=CC=CO1	204,23	C11H12N2O2
Z85525679	CC(NC(C)=O)C(=O)NC1=NC=CC=C1	207,23	C10H13N3O2
Z354838940	CCNC(=O)C1CCN(CC1)C(C)C	198,31	C11H22N2O
Z954532756	CCNC(=O)C1=CNC2=C1C=CC(Cl)=C2	222,67	C11H11ClN2O
Z55928890	NC1=CC=NN1C1CCCC1	165,24	C9H15N3
Z1162910732	OC(C1=CC=CS1)C1=NC=CC=C1	191,25	C10H9NO5
Z1160899501	COC1=C(N)C=C(CN2CCCC2)C=C1	206,29	C12H18N2O
Z1770192727	CC1(C)CC(O)C(C)(C)O1	144,21	C8H16O2
Z1768160555	CN1C(=O)CCC2=C1C=CC(=C2)C(O)=O	205,21	C11H11NO3
Z1768160552	OC(=O)C1CCCN2C(=O)NN=C12	183,17	C7H9N3O3
Z1767916692	CC(=O)NC1C(=O)NC2=C(C)C=CC=C12	204,23	C11H12N2O2
Z1766245361	CCC1=CC2=C(C=C1)N=C(O)N2	162,19	C9H10N2O
Z1762997280	C[C@](N)(C1CCCCC1)C(O)=O	171,24	C9H17NO2
Z1753033011	CC(C)OC1=NN=C(N)C=C1	153,19	C7H11N3O
Z1610969627	N#CC1=CSC(CNC2=NN=CS2)=C1	222,28	C8H6N4S2
Z275170072	CCN1N=CC=C1C(O)=O	140,14	C6H8N2O2
Z85888094	CC(=O)NC1(CCCCC1)C(O)=O	185,22	C9H15NO3
Z1295559816	CCC(N)C1=NC(=CS1)C(F)(F)F	210,22	C7H9F3N2S
Z2211246487	COC1=C2CCNC2=CC=C1	163,22	C10H13NO
Z1558209772	CCN1C=CC(=O)C(N)=C1	138,17	C7H10N2O
Z1335657438	C1CNC(C1)C1=CC=CO1	137,18	C8H11NO
Z1262237470	C1CNCC2(C1)CCOCC2	155,24	C9H17NO
Z1367012439	COC1=NC(CO)=CC=C1	139,15	C7H9NO2
Z1900627279	FC1=CCCN(C1)C1=CN=C(C=C1)C#N	203,22	C11H10FN3
Z2689172043	CN1C(=O)COC2=C1C=C(C=C2)C(O)=O	207,19	C10H9NO4
Z2130642054	COC1=C(CO)C=NC=C1	139,15	C7H9NO2
Z2130642358	CC1=C(C=CC(N)=N1)C1=CC=CC=C1	184,24	C12H12N2
Z2130643237	CCNC1=C(N)C=NC=C1	137,19	C7H11N3
Z2130641782	CC1=C2OC(N)=NC2=CC=C1	148,17	C8H8N2O
Z2120061007	OCC1=C(N=CC=C1)N1CCCC1	178,24	C10H14N2O
Z2092370541	ClC1=CC=C(C=C1)N1CCNC1=O	196,63	C9H9ClN2O
Z2658867442	OC(=O)C1(CCN1=O)C1CCCC1	197,23	C10H15NO3
Z1603606725	OC(=O)C1(CCN1)NC(=O)C1=CC=CC=C1	205,21	C11H11NO3
Z2034719242	C[C@H](NS(C)=O)C1=NC=C(Cl)C=C1	234,70	C8H11ClN2O2S
Z1492804399	CC1CCN(CC2=NC(N)=CC=N2)C1	192,27	C10H16N4
Z2160914592	C(C1=CNC=N1)C1=CC=CC=C1	158,20	C10H10N2
Z1741957818	CC1=C(Cl)C(=NN1)C(F)(F)F	184,55	C5H4ClF3N2
Z159528828	CN(CCO)C1CCCC1	157,26	C9H19NO
Z1547844612	CC(C)(O)C1CCCN1CC1CCOC1	213,32	C12H23NO2

Z1473963139	C1COC2CCNCC2C1	141,21	C8H15NO
Z1428018528	ClC1=C2OCCNC2=CC=C1	169,61	C8H8ClNO
Z1436472689	CN1C=C(C)C=C(N)C1=O	138,17	C7H10N2O
Z56347292	NC1=CC=NN1C1CCCC1	151,21	C8H13N3
Z1742056046	CN(C)C1=NN(C=N1)C1=CC(N)=CC=C1	203,25	C10H13N5
Z1741794237	CC1CNCCN1CCO	144,22	C7H16N2O
Z1266823341	CC(C)(N)CNC1=CC=CC=C1	164,25	C10H16N2
Z1527148054	CN(CCO)C(=O)C1=C(C)C=C(F)C=C1	211,24	C11H14FNO2
Z1704693923	CC(C)C1=NC=C(C=C1)C#N	146,19	C9H10N2
Z1546887028	CC(CO)N(C)C1=NC=C(Cl)C=N1	201,65	C8H12ClN3O
Z165137254	CC(=O)NC1=NN=C(S1)C1=CC=CO1	209,22	C8H7N3O2S
Z234896383	CNC1CCCCNC1=O	142,20	C7H14N2O
Z237578634	CC(C)(O)C1=NC2=C(N1)C=CC=C2	176,22	C10H12N2O
Z19725438	CNC(=O)COC1=CC=C(Br)C=C1	244,09	C9H10BrNO2
Z234853694	CC(C)CC1=NNC(=C1)C(O)=O	168,20	C8H12N2O2
Z57834657	CN1C(=O)N(C)C2=C1C=CC(N)=C2	177,21	C9H11N3O
Z119081056	CC1=C(OC=C1)C(=O)NCC1=CC=CS1	221,27	C11H11NO2S
Z363071686	CN(CCl(=O)N1CCCCC1)S(C)(=O)=O	234,31	C9H18N2O3S
Z314448400	CCN(C1CC1)C(=O)C1CCCO1	183,25	C10H17NO2
Z1456185598	CC(N)C1CN(C)CCO1	144,22	C7H16N2O
Z1267773576	NC1CCN(C1)C1=C(Br)C=CC=C1	241,13	C10H13BrN2
Z513575288	CCNC(=O)N1CCC(O)CC1	172,23	C8H16N2O2
Z1172231059	CC1CCC(C)N1CC(O)=O	157,21	C8H15NO2
Z280813686	CC(C1CC1)N(C)C(=O)C1CCC=CC1	207,32	C13H21NO
Z314446644	CCN(C1CC1)C(=O)C1CCCC1	167,25	C10H17NO
Z314790120	CN1C=CC=C1C(=O)NCCN	167,21	C8H13N3O
Z752989208	CC1=C(N=C(CN)S1)C1=CC=CC=C1	204,29	C11H12N2S
Z270730164	NC1=C(C=CC=C1)N1CCCCC1	190,29	C12H18N2
Z2327226178	CC1=C(F)C(F)=CC=C1N	143,14	C7H7F2N
Z2327226118	CN1N=NC=C1CC(O)=O	141,13	C5H7N3O2
Z407486572	COC1=CC2=C(NC=C2CC(N)=O)C=C1	204,23	C11H12N2O2
Z2327039924	CC1=NC=C2C=CC=C(N)C2=C1	158,20	C10H10N2
Z2326990062	CC1=CC=C(CN2CCNC2=O)C=C1	204,27	C12H16N2O
Z2309759496	COC1=C(C=NN1C)C(O)=O	156,14	C6H8N2O3
Z2301499788	CCN1CCC(=O)NC(C)C1=O	170,21	C8H14N2O2
Z2293608802	OC(=O)C1=C(C=CN1)C1CC1	151,17	C8H9NO2
Z2293606507	COC1=CC(N)=CC(OC)=C1Cl	187,62	C8H10ClNO2
Z1945709775	CC1=C(C=NO1)C1=CSC(C)=N1	180,23	C8H8N2OS
Z2285376686	CN1C(=O)OC2=C1C=C(F)C(N)=C2	182,15	C8H7FN2O2
Z126933712	CCNC1=CC=C(C=C1)C#N	146,19	C9H10N2
Z927632696	CCNC(=O)C1=C(N)C=CC(Cl)=C1	198,65	C9H11ClN2O
Z1266854868	CC(C)C1=NC(N)=NC(C)=N1	152,20	C7H12N4
Z1266854826	COC1=CC2=C(OC(C)C(=O)N2)C=C1	193,20	C10H11NO3
Z1266823232	CNC(C)C1=C(C)N=C(C)S1	170,27	C8H14N2S
Z1262253450	O=C(N1CCNCC1)C1=CNC(=O)N1	196,21	C8H12N4O2
Z1266823151	CCC(C1=NN=C(N)O1)C1=CC=CC=C1	203,25	C11H13N3O
Z87615031	CC(=O)NC1=CC=C(C(N)=O)C=C1	192,22	C10H12N2O2
Z1263714154	COC1=C(C=C(Cl)C=C1)C1=NN=C(N)O1	225,63	C9H8ClN3O2
Z1208171827	CC1=CC=C(S1)C1CCCN1S(C)(=O)=O	245,36	C10H15NO2S2
Z1741815643	NCCN1CCC2=C(C1)C=CC=C2Cl	210,71	C11H15ClN2
Z57102476	COC1=C(CN)C=CC=C1	137,18	C8H11NO
Z414477974	CS(=O)(=O)NC1CCCCNC1=O	206,26	C7H14N2O3S
Z1436472855	COC1=NN=C2CCNCC2=C1	165,20	C8H11N3O
Z1782591374	C=CCNC1CCCOC2=C1C=CC=C2	203,29	C13H17NO
Z2001754599	COCCC(=O)N1CC(=O)NCC1(C)C	214,27	C10H18N2O3
Z1263529750	NC(CN1CCCC1)C1=CC=CC=C1	204,32	C13H20N2
Z2157438002	BrC1=CN=C(N=C1)N1CCCCN1	243,11	C8H11BrN4
Z1446874472	CC(N)CC1=CC(C)=NN1	139,20	C7H13N3
Z1717424532	FC1=CCCN(CC2=CSN=N2)C1	199,25	C8H10FN3S
Z1900628669	CC1=NC(=CN=C1)N1CCC=C(F)C1	193,23	C10H12FN3
Z1613884074	CC1=C(OC=C1)C(=O)N1CCC=C(F)C1	209,22	C11H12FNO2
Z1899838847	CC1=NN(CC2=NC=C(F)C=C2)C(=O)S1	225,24	C9H8FN3OS
Z1587273510	CN1C=CN=C1CN1CCC=C(F)C1	195,24	C10H14FN3
Z1551815330	OCC(=O)NC1(CC1)C1=C(F)C=CC=C1	209,22	C11H12FNO2
Z1974574407	CC(=O)N[C@H]1C[C@H]1C1=C(Cl)C=CC=C1F	227,66	C11H11ClFNO
Z1357827227	CNC1=C(N=CC=C1)N(C)C	151,21	C8H13N3
Z1333761736	C1CN(CCN1)C1CCOCC1	170,26	C9H18N2O

Z1168422657	C1CC1C1=CSC(=N1)C1=CC=NC=C1	202,28	C11H10N2S
Z1231609616	ClC1=CN=C(C=C1)C(=O)NC1CC1	196,63	C9H9CIN2O
Z1891774432	CC(CN)N1CCC2=C1C=CC=C2	176,26	C11H16N2
Z2106606815	NC1=CC2=C(CCCC2)C=C1	147,22	C10H13N
Z2234185604	OC(=O)CC1=CC2=C(S1)C=CC=C2	192,23	C10H8O2S
Z2213893012	NC1CCCC2=C1C=C(Cl)S2	187,69	C8H10CINS
Z2234631175	CCC1CCCC1C(O)=O	142,20	C8H14O2
Z1717761806	CC(C)(C1CCC1)C(O)=O	142,20	C8H14O2
Z1860991693	CCC1OCCCC1C(O)=O	158,20	C8H14O3
Z2235330356	CCOC1=CC(N)=C(Cl)C=C1	171,62	C8H10CINO
Z2327531741	CN(C)C1=C(C)N=C(C)C(C)=N1	165,24	C9H15N3
Z1575245647	CN1C=C(CCO)C(C)=N1	140,19	C7H12N2O
Z104377982	Cl.COC1=C2CNCC(O)C2=C(OC)C=C1	245,70	C11H16CINO3
Z57728665	OC(=O)CCN1C(=O)OC2=C1C=CC=C2	207,19	C10H9NO4
Z57066685	CC1=CC2=C(OC(=CC2=O)C(O)=O)C=C1	204,18	C11H8O4
Z57985380	CCN1CCN(CC1)C1=C(N)C=CC=C1	205,31	C12H19N3
Z90122368	CC(=O)N1CCN(CC1)C(N)=O	171,20	C7H13N3O2
Z85932257	CC(O)C1=NC2=C(C=CC=C2)N1C(F)F	212,20	C10H10F2N2O
Z57683752	CC1=C(C(C(O)=O)C(C)=NN1	154,17	C7H10N2O2
Z57625083	CN1CCN(CC1)C1=C(N)C=CC=C1	191,28	C11H17N3
Z26743827	CCC(=O)NC1=CC(Cl)=C(OC)C=C1	213,66	C10H12CINO2
Z56347071	CC(O)C1=NC2=C(S1)C=CC=C2	179,24	C9H9NOS
Z45527657	CNS(=O)(=O)C1=CC=C(OC)C=C1	201,24	C8H11NO3S
Z240299438	CN1C=CC(NC(=O)C2=CC(Br)=CN2)=N1	269,10	C9H9BrN4O
Z818727398	CC(N)COC1=C(C)C=CC=C1C	179,26	C11H17NO
Z812516948	CCC1=C(SC=C1)C(O)=O	156,20	C7H8O2S
Z422426600	CC(C)C(C)NC(=O)C1=C(C)N=CS1	212,31	C10H16N2OS
Z295814046	CNC(=O)C1=C(C)SC(=N1)C1=CC=CO1	222,26	C10H10N2O2S
Z102345362	CC(NC(=O)C1=NNC(=O)C=C1)C1CC1	207,23	C10H13N3O2
Z803145246	CC(C)C(N1CCN(C)CC1)C(O)=O	200,28	C10H20N2O2
Z422952260	CN(CC(N)=O)C(=O)C1=CC=C(Br)S1	277,14	C8H9BrN2O2S
Z383001878	CNS(=O)(=O)C1=CC=C(O1)C(=O)N(C)C	232,25	C8H12N2O4S
Z226408766	CN1N=C(OC1=O)C1=CC=C(F)C=C1	194,17	C9H7FN2O2
Z397955404	NC(=O)CN1C(=O)OC2=C1C=CC(Br)=C2	271,07	C9H7BrN2O3
Z71179597	COC1=C(C=CC=N1)C(O)=O	153,14	C7H7NO3
Z26968795	COC1=CC(Cl)=C(OC)C=C1NC(C)=O	229,66	C10H12CINO3
Z212277696	CC(=O)NC1=CC=C(S1)C(=O)NC1CC1	224,28	C10H12N2O2S
Z394693554	NCC(O)C1=CC(Cl)=CC=C1	171,62	C8H10CINO
Z33546734	CC(CC(N)=O)C1=CC=CC=C1	163,22	C10H13NO
Z108547236	CCC(=O)NC1=CC(=CC=C1)S(C)(=O)=O	227,28	C10H13NO3S
Z381785690	OC(=O)C1=CC=C(CN2C=CC=N2)O1	192,17	C9H8N2O3
Z2025666292	NC(=O)N1CCOC2=C(C1)C=C(Br)C=C2	271,11	C10H11BrN2O2
Z235352209	NC1=CC(=CC=C1)C1=NN=C2CCCN12	200,25	C11H12N4
Z235352197	CC1=NC=C(O1)C1=CC=C(N)C=C1	174,20	C10H10N2O
Z235346973	NC1=NC=C(C=C1)N1CCOCC1	179,22	C9H13N3O
Z235345305	CC1=C(CC(O)=O)N=C(O1)C1=CC=CS1	223,25	C10H9NO3S
Z235341203	CNC1=NC2=C(O1)C=CC=C2	148,17	C8H8N2O
Z56886301	CC1=C(Cl)C(N)=NC=C1Cl	177,03	C6H6Cl2N2
Z32367959	O=C(NC1CC1)C1=CC=C(C=C1)C#N	186,21	C11H10N2O
Z57966275	CC1=NN2CCC(=O)NC2=C1	151,17	C7H9N3O
Z332770958	CC1=CC(NC(=O)C2=COC(Br)=C2)=NO1	271,07	C9H7BrN2O3
Z367451004	O=C1NCC2=C1C=CC=C2	133,15	C8H7NO
Z2470210350	COC1=CNCC2=C1C=C(F)C=C2	165,17	C9H8FNO
Z2469680276	COC1=CC2=C(NC(C)=C2)C=C1	161,20	C10H11NO
Z2469606526	O=C1NCC(=C1)C1=CC=CC=C1	159,19	C10H9NO
Z2469606458	OC(=O)C1=C(F)C=C(C=C1)C(F)F	190,12	C8H5F3O2
Z2469606506	CCC(C1CNC(=O)C1)C1=CC=CC=C1	203,29	C13H17NO
Z2467454623	FC1=C(F)C=C2OCCNC2=C1	171,15	C8H7F2NO
Z2467454621	COCC1=CC(N)=NC=C1	138,17	C7H10N2O
Z1954800557	N#CC1=NC2=C(NCCC2)C=C1	159,19	C9H9N3
Z2418194168	CC1=CC=C(C=C1)C1(CCC1)C(O)=O	190,24	C12H14O2
Z2418193694	OC1CCCN1CCC1=CC=CC=C1	205,30	C13H19NO
Z2412196538	CC1(C)C2CC1NC(=O)CC2	153,23	C9H15NO
Z2412196506	CC1=C(C(O)=O)C(N)=CC=C1F	169,16	C8H8FNO2
Z212230762	CC1CN(CCO1)C(=O)CN1CCCC1	212,29	C11H20N2O2
Z1252468609	COCCN1N=C(C)C=C1C	154,21	C8H14N2O
Z1262252989	NCCC1=C(Br)C=CC=C1	200,08	C8H10BrN

Z426201150	OCCOC1=CC(Br)=CC=C1	217,06	C8H9BrO2
Z1374788746	NC1(CC1)C1=CC(F)=C(F)C=C1	169,18	C9H9F2N
Z1269702393	CCC(N)C1=C(C)N(C)N=C1C	167,26	C9H17N3
Z235336557	OC(C1CCNCC1)C1=CC=CC=C1	191,27	C12H17NO
Z235333131	CC1=NN2C(=C1)N=CC(C(O)=O)=C2C	191,19	C9H9N3O2
Z235333081	OC(=O)C1=CN(CC2=CC=CC=C2)N=N1	203,20	C10H9N3O2
Z168883346	CC1=C(C(O)=O)C(C)=CC(=O)O1	168,15	C8H8O4
Z89268045	CC1=CC=C(CN2N=CC=C2N)S1	193,27	C9H11N3S
Z1159152696	NC(=O)C1CCCCN1C1CCCC=C1	208,31	C12H20N2O
Z1238477760	CN(C)C(=O)C1=C(N)C=C(Cl)C=C1	198,65	C9H11ClN2O
Z195562120	CNCC1=NC2=C(C(=CC=C2)C(N)=N1	188,23	C10H12N4
Z1725496598	CC(=O)NC1=C2NC=CC2=CC=C1	174,20	C10H10N2O
Z1145207891	CS(=O)(=O)NC1CCC2=C1C=C(F)C=C2	229,27	C10H12FNO2S
Z1222331444	CC(C)OC1=NC(C(O)=O)=C(Cl)C=C1	215,63	C9H10ClNO3
Z1222331409	OC(=O)C1CCC2=NN=C(C3CC3)N2C1	207,23	C10H13N3O2
Z2255112112	CC1(CCC(=O)N1)C(O)=O	143,14	C6H9NO3
Z1437171658	CNC(C)C1=CN(C)N=C1	139,20	C7H13N3
Z1245633213	CC(N)C1=CC(OC(F)F)=CC=C1	187,19	C9H11F2NO
Z1251171288	CC1=CC(NC2CCNCC2)=CC=C1	190,29	C12H18N2
Z31192919	N#CC1=C(N=CC=C1)N1CCCCC1	187,25	C11H13N3
Z1250132548	OC1CCCC1C1=CC=C(F)C=C1	180,22	C11H13FO
Z1267882056	NCCC1=CC(=N1)N1CCCCC1	197,30	C9H15N3S
Z1267773558	CN1CCC(CC1)N1CCC(N)C1	183,30	C10H21N3
Z1259161657	CNC1CCCCC1S(C)(=O)=O	191,29	C8H17NO2S
Z1350579651	CC(O)C(C)C1=NC2=C(S1)C=CC=C2	207,29	C11H13NOS
Z1262252970	CCC1=CC(=CC=C1)N1CCC(N)CC1	204,32	C13H20N2
Z422471910	CC(C1CC1)N(C)C(=O)C1=C(C)N=CS1	224,32	C11H16N2OS
Z1268153229	CC(C)CN1C=C(N)C=N1	139,20	C7H13N3
Z2242946408	CC(O)C1NCC2=C1C=CC=C2	163,22	C10H13NO
Z1741969705	CC1=NC2=C(O1)C=CC=C2N	148,17	C8H8N2O
Z2235831713	CN1C=C(N)C(=N1)C(=O)NCC1CC1	194,24	C9H14N4O
Z1262564339	C(C1=NN=CN1)C1=CC=CC=C1	159,19	C9H9N3
Z2238934532	BrC1=CC(=CC=C1)C1CCNC1=O	240,10	C10H10BrNO
Z1980894300	CC1=NC(CO)=NC(=C1)N1CCCCC1	207,28	C11H17N3O
Z1266823371	CN(C)CC1CNCCO1	144,22	C7H16N2O
Z1437173851	CNC1CCCC2=C1C=NN2C	165,24	C9H15N3
Z2255110160	CC1=C2SC(=O)NC2=CC=C1	165,21	C8H7NOS
Z90517827	C(NC1CC1)C1=CN=CC=C1	148,21	C9H12N2
Z1983132442	CC(O)C1=NC=C(C=C1)C(F)(F)F	191,15	C8H8F3NO
Z372962240	CN(C)C1=C(C=CC=C1)C#N	146,19	C9H10N2
Z745184320	CN(C)C(=O)CCN1C=C(Br)C=N1	246,11	C8H12BrN3O
Z137588472	NC(=O)CNC1=C(Br)C=CC=C1	229,08	C8H9BrN2O
Z1992316316	CC(C)CC1(CC1)C(O)=O	142,20	C8H14O2
Z1347251965	CC(C)(O)CCN1CCCCC1	157,26	C9H19NO
Z1953500072	CC(N)C1CN(C)CCN1C	157,26	C8H19N3
Z803153238	CC(C)C1=NC(CCN)=CS1	170,27	C8H14N2S
Z1945984181	COC1(CN)CCC(C)CC1	157,26	C9H19NO
Z1945984192	CC1=NC(CCN)=CC=C1	136,20	C8H12N2
Z1949075885	CC1=C(Br)C(N)=C(F)C=C1	204,04	C7H7BrFN
Z183344018	CC(C)NC(=O)N(C)CC1=CN(C)N=C1	210,28	C10H18N4O
Z1480642078	CC(N)C(C)N1C=CC=N1	139,20	C7H13N3
Z1913645786	OCC12CCCN1CCC2	141,21	C8H15NO
Z1723418925	CC1(C)CCCC1C(O)=O	142,20	C8H14O2
Z1545196403	FC1=C(NCC2=NNC=C2)C=CC=C1	191,21	C10H10FN3
Z1664348558	CC1=NC(C)=C(N)C(N)=C1	137,19	C7H11N3
Z1148165337	CN(C)C(=O)CN1N=CC2=C1C=CC=C2	203,25	C11H13N3O
Z1696860270	CC1=NC(=CS1)C1=C(C)OC(=C1)C(O)=O	223,25	C10H9NO3S
Z1696844798	CC1=NC2=CC(=NN2C(C)=C1)C(O)=O	191,19	C9H9N3O2
Z360056164	C[C@@H](O)C1=CC=C(C=C1)N1C=NC=N1	189,22	C10H11N3O
Z1696091879	OC(=O)[C@@H]1C[C@@]1(C(O)=O)C1=CC=CC=C1	206,20	C11H10O4
Z1695921492	CC(C)(OC1=CC=C(C=C1)C#N)C(O)=O	205,21	C11H11NO3
Z2004547759	BrC1=C2NCCCN2N=C1	202,06	C6H8BrN3
Z1631503812	CC(=O)NC1=NC=CC(=C1)C(F)(F)F	204,15	C8H7F3N2O
Z932997760	CNC(=O)CNC(=O)C1=CC(N)=CC=C1	207,23	C10H13N3O2
Z354263462	CN(C)C1=NC(N)=NC(C)=C1	152,20	C7H12N4
Z1993522718		192,21	C11H12O3
Z1702887683	CC1CN(C1)C(=O)NC1=CC=CC=C1	190,25	C11H14N2O

Z1439138555	BrC1=C(NC2CC2)N=CN=C1	214,07	C7H8BrN3
Z2028214407	OC(=O)C1CCS(=O)(=O)C2=C1C=CC=C2	226,25	C10H10O4S
Z2028214362	CC1=C(OC(CO)=C1)C(O)=O	156,14	C7H8O4
Z2028214426	FC(F)(F)C1=CC2=C(C=C1)C(=O)NC2	201,15	C9H6F3NO
Z1741967141	COC1=C(Cl)C=C(C=N1)C(O)=O	187,58	C7H6ClNO3
Z2027049490	OC(=O)C1=C(NC=C1)C1CC1	151,17	C8H9NO2
Z2027049525	NCCC1=CC2=NNC=C2C=C1	161,21	C9H11N3
Z1682064802	COC1=C(OC)C(Br)=CC(=C1)C(O)=O	261,07	C9H9BrO4
Z208334426	CN(C1CCS(=O)(=O)C1)C(=O)NC1CC1	232,30	C9H16N2O3S
Z1642061413	CN1C=NC(=N1)C1=CC=C(C=C1)C(O)=O	203,20	C10H9N3O2
Z1623872209	CNCC1CCCCC1O	143,23	C8H17NO
Z1623864185	CCC1=NC2=C(C=C(N)C=C2)C(N)=C1	187,25	C11H13N3
Z57370050	CC(O)C1=NC2=C(C(N1)C=CC(C)=C2	176,22	C10H12N2O
Z198264916	C=CCNC(=O)C1=CC2=C(NN=N2)C=C1	202,22	C10H10N4O
Z1575311809	CN1C=CC(=N1)N1CCC(N)C1=O	180,21	C8H12N4O
Z1569709170	OC(=O)C1=NC(=NC=C1)C1CCCC1	192,22	C10H12N2O2
Z929183718	CC(C)(N(C=O)C1=CC=CC=C1)C(O)=O	207,23	C11H13NO3
Z1230797900	CC(C1CC1)N(C)C(=O)C1=NC=CN1C	207,28	C11H17N3O
Z103698412	N#CC1=C(CN2CCCC2)C=CC=C1	200,29	C13H16N2
Z1834223522	CC1(C)CC2=C(O1)C(N)=CC=C2	163,22	C10H13NO
Z1820225788	CCNC1=C2C=CNC2=CC=C1	160,22	C10H12N2
Z992422556	CC(N)CCC1CCCO1	143,23	C8H17NO
Z1416200831	CC(N)C1=C(C=CC=C1)N1C=CC=N1	187,25	C11H13N3
Z32064550	C=CCNC(=O)C1=CC=NC=C1	162,19	C9H10N2O
Z1269702208	NC1CCC1C1=CC=CC=C1	147,22	C10H13N
Z90122603	CC(N)C1=CC=C(F)C=C1	139,17	C8H10FN
Z1695709587	OC(=O)C1=C(C(NN=C1)C1CC1	152,15	C7H8N2O2
Z1683067954	N#CC1=NC(=CC=C1)N1CCNCC1	188,23	C10H12N4
Z1265813904	CN(C)C(=O)C1=CC2=C(O1)C(F)=CC=C2	207,20	C11H10FNO2
Z1665033540	CC1CC(C)(C)CNC1=O	141,21	C8H15NO
Z2158786427	O=C(NC1=CC=NC=C1)N1CCCCN1	206,25	C10H14N4O
Z2235681471	OC(=O)C1=CN=C(C=C1)N1CCC1	178,19	C9H10N2O2
Z2235330314	BrC1=CC2=C(OC2)N=C1	200,04	C7H6BrNO
Z2061490609	C[C@@H]1CN(C[C@H]1C(N)=O)C(=O)C1(C)CC1	210,28	C11H18N2O2
Z275127490	CC(CC(O)=O)C1=CNC2=C1C=CC=C2	203,24	C12H13NO2
Z2218556484	OCC1CS(=O)(=O)C2=C1C=CC=C2	198,24	C9H10O3S
Z2218555969	CC1=C2OCCCN2N=C1C(O)=O	182,18	C8H10N2O3
Z2217033030	NC1=C(N=NN1)C(=O)N1CCCC1	181,20	C7H11N5O
Z2216711607	NCCC(=O)NC1=CC(Cl)=CC(Cl)=C1	233,09	C9H10Cl2N2O
Z2568751802	COCC1=CSC(=C1)C(O)=O	172,20	C7H8O3S
Z2568751702	BrC1=CC2=C(OC2)N=C1	216,03	C7H6BrNO2
Z2515207600	NC(=O)C1=NC2=C(C(CCN2)C=C1	177,21	C9H11N3O
Z2515207630	CN1N=CC(C2CCC2)=C1C(O)=O	180,21	C9H12N2O2
Z2515207554	OC(=O)C1=C2COCCC2=CC=C1	178,19	C10H10O3
Z2513333903	NC1=CC2=C(C(CCCC2O)C=C1	177,25	C11H15NO
Z2512451323	CC1=CC2=C(N=CN2C=C1)C(O)=O	176,18	C9H8N2O2
Z99600018	CC1=CSC2=C(C#N)C(C)=CC(=O)N12	204,25	C10H8N2OS
Z99598988	CC1=CC(C)=C(C#N)C(=O)N1	148,17	C8H8N2O
Z198194122	CN(CC1=CC=CS1)C(N)=O	170,23	C7H10N2OS
Z46190592	CNCC(=O)NC1=NOC(C)=C1	169,18	C7H11N3O2
Z96091967	CC1=CC=NN1C1=CC=C(C=C1)C(O)=O	202,21	C11H10N2O2
Z55723242	CC1=C(C)N=C2C=C(C=CC2=N1)C(O)=O	202,21	C11H10N2O2
Z90664470	OC(=O)CC1=C(Br)C=C2OCCOC2=C1	273,08	C10H9BrO4
Z55993084	CC(N)C1=CC=C(C=C1)N1C=CN=C1	187,25	C11H13N3
Z208155046	CC1=CC(C)=C(CCC(O)=O)C=C1	178,23	C11H14O2
Z29177127	CC(C)C(=O)NC1=CC(=CC=C1)C(N)=O	206,25	C11H14N2O2
Z28296645	CCC(=O)NC1=CC2=C(C=C1)N=C(C)S2	220,29	C11H12N2OS
Z56754337	OC(=O)C12CCCC(CCC1)(C2)C(O)=O	212,25	C11H16O4
Z56964368	NCCC1=CC2=C(OC2)C=C1	179,22	C10H13NO2
Z44507989	Cl.CNCC1=NC2=C(C=CC=C2)C(=O)N1	225,68	C10H12ClN3O
Z56912006	OC(=O)CNC(=O)C1=CC=C(Br)O1	248,03	C7H6BrNO4
Z56913114	CN1(C)C=CC(C)=C(C#N)C1=O	164,16	C8H8N2O2
Z28292377	CC(=O)NC1=C(C)C(Cl)=CC=C1	183,64	C9H10ClNO
Z31480423	O=C(N1CCCC1)C1=CC=C(C=C1)C#N	200,24	C12H12N2O
Z31480727	FC1=CC(Cl)=C(C=C1)C(=O)N1CCCC1	227,66	C11H11ClFNO
Z56839652	OC(=O)C1COC2=C(O1)C=CC=C2	180,16	C9H8O4
Z56753990	CC1=C(C)CC(C(C1)C(O)=O)C(O)=O	198,22	C10H14O4

Z1428158834	OC(=O)C1=C(C=C(C=C1)C(F)(F)F)C#N	215,13	C9H4F3NO2
Z1428018535	NC1=CC=NN1CC1CC1	137,19	C7H11N3
Z1424669442	CCN1C=C(N)C(=N1)C(O)=O	155,16	C6H9N3O2
Z1421528826	OC(=O)C1=CC2=C(CCS(=O)(=O)C2)S1	232,27	C8H8O4S2
Z1416282601	OC(=O)CN1C=C(N=N1)C1CC1	167,17	C7H9N3O2
Z1143584382	CCC1N(CCN1=O)C(=O)NC(C)C	213,28	C10H19N3O2
Z1328968520	CS(=O)(=O)C1=NC=CN1CC1=CSC=N1	243,30	C8H9N3O2S2
Z1407659631	CC(C)CC1(CN)CCC1	141,26	C9H19N
Z1407007505	O[C@H](C[C@@H]1CCCN1)C1=CC=CC=C1	191,27	C12H17NO
Z1217526242	CN1C=CC=C1C(=O)NC1=NNC=C1C	204,23	C10H12N4O
Z1398461994	CN1N=NC(C(O)=O)=C1C(F)(F)F	195,10	C5H4F3N3O2
Z1381260620	OC(=O)C1=C(C)C(=NN1)C1CC1	186,60	C7H7CIN2O2
Z959151860	O[C@H]1CCC2=C1C=CC(F)=C2	152,17	C9H9FO
Z234897043	CC1=C(C)C=C(C=C1)C1CC1N	161,25	C11H15N
Z818727446	CC(CN)N1CCOCC1	144,22	C7H16N2O
Z401097872	CCC1CCCN(C2=NN=C(C)O2)C1	209,29	C11H19N3O
Z803153704	NCCC1=C(C=C=C1)C(F)(F)F	189,18	C9H10F3N
Z1217910516	CC(C)C(CN)C1=CC=CC=C1	163,26	C11H17N
Z1219738993	NC1CCN(C1)C1=CC=CC=C1	162,24	C10H14N2
Z1262237381	NCCC1=C(F)C=CC(Br)=C1	218,07	C8H9BrFN
Z763367910	CC(N)COC1=C(F)C=C(F)C=C1	187,19	C9H11F2NO
Z375692826	CC(C)C(=O)N(C)CC1=NOC(C)=C1	196,25	C10H16N2O2
Z223327076	CC(C)C(=O)NCC1=NN=C2CCCN12	208,27	C10H16N4O
Z104924088	CC(C)N1CCN(C1)C1=NC=CC=N1	206,29	C11H18N4
Z1348289436	CC(=C)CN1C=CC(=O)C2=C1C=CS2	205,28	C11H11NOS
Z1267773545	CC(C)C1=C(C)SC(CN)=N1	170,27	C8H14N2S
Z2234631245	CNC1=NC(=CO1)C(F)(F)F	166,10	C5H5F3N2O
Z2065788535	NC1C2CC1CC1=C(C2)C=CC=C1	187,29	C13H17N
Z90504169	C(NC1CCCC1)C1CCCO1	169,27	C10H19NO
Z1900548518	CC1=CN=C(CNC2=CC(C)=NC=C2)O1	203,25	C11H13N3O
Z2065464393	CCC1OCCC1C(O)=O	144,17	C7H12O3
Z1373414370	OCC1CCCN(C1)C1=C(F)C=CC=N1	210,25	C11H15FN2O
Z2050724987	CCC(O)C1=NC=C(F)C=C1	155,17	C8H10FNO
Z2044949019	CC(O)C1=NC=C(F)C=C1	141,15	C7H8FNO
Z2033459081	COC1=C(C=CC=C1)C1CCC(C)CN1	205,30	C13H19NO
Z1896858260	ClC1=CC(CCN2C=NC=N2)=CC(Cl)=C1	242,10	C10H9Cl2N3
Z145545120	ClC1=CNC(=C1)C(=O)N1CCNC(=O)C1	227,65	C9H10ClN3O2
Z1101435401	CC(C)C(=O)NC1CCCN1	170,26	C9H18N2O
Z422952944	CN(CCN(=O)C(=O)C1=C(Cl)SC(Cl)=C1	267,12	C8H8Cl2N2O2S
Z54226006	FC1=CC=CC(F)=C1C(=O)N1CCCC1	211,21	C11H11F2NO
Z247484750	CC1=C(OC=C1)C(=O)NC1=NN=CS1	209,22	C8H7N3O2S
Z54953371	CCOC1=C(C=CC=C1)C(N)=O	165,19	C9H11NO2
Z31432009	CC(NC(C)=O)C(=O)N1CCCCC1	212,29	C11H20N2O2
Z324505866	CCS(=O)(=O)N1CCC(CC1)NC(C)=O	234,31	C9H18N2O3S
Z328695024	CC(C)N(C)C1=C2C=NN(C)C2=NC=N1	205,27	C10H15N5
Z285641686	C=CCNC(=O)C1=C2N=CC=CN2N=C1	202,22	C10H10N4O
Z1273089263	CCC(N)C(C(O)=O)C1=CC=CC=C1	179,22	C10H13NO2
Z1310763003	CC1(C)CCN1C(=O)NC1=NN=CS1	212,27	C8H12N4OS
Z1318356921	COC1=CC=C(C=C1)C1=CC=C(CN)S1	219,30	C12H13NOS
Z1318268950	COC1=CC=C(C=C1)C1=CSC(CN)=C1	219,30	C12H13NOS
Z1247413608	CS(=O)(=O)N1CCC(O)CC1	179,23	C6H13NO3S
Z1278581710	CNC(C(O)=O)C1=CC=C(F)C=C1	183,18	C9H10FNO2
Z1037287770	CCN(C)C(=O)NC1=NN=C(S1)C1CC1	226,30	C9H14N4OS
Z803153714	CC(N1CCC(N)C1)C1=CC=CC=C1	190,29	C12H18N2
Z1373438018	CN(C1CCOC1)C1=C(F)C=CC=N1	196,23	C10H13FN2O
Z2313104779	COC1CN(C2=C(F)C=NC=C2)C1	196,23	C10H13FN2O
Z2219019614	CC1=NOC=C1CNC1CCCCC1	194,28	C11H18N2O
Z1921387755	CC#CCN1CC(O)CC2=C1C=CC=C2	201,27	C13H15NO
Z287256168	CC(NC(=O)C1=NC(C)=CC=C1)C1CC1	204,27	C12H16N2O
Z228587528	O=C(C1CCCC1)N1CCCNCC1	196,29	C11H20N2O
Z1318357730	COCC(N)C1=CC=CO1	141,17	C7H11NO2
Z1259087088	CC1=CC=C(O1)C1CCCCN1	165,24	C10H15NO
Z434621834	COC(C(=O)N(C)C)C1=CC=CC=C1	193,25	C11H15NO2
Z280806616	CC(C1CC1)N(C)C(=O)C1CC1	167,25	C10H17NO
Z1575325610	NCC1CCC2=C1C=CC=C2	147,22	C10H13N
Z31190928	CC(C)NC1=NC=CC=N1	137,19	C7H11N3
Z1258578171	CC1=CC(=C(C)O1)C(C)(O)CN	169,22	C9H15NO2

Z1753051259	CCC1(O)CN(C1)C1=C(C=CC=N1)C#N	203,25	C11H13N3O
Z1918453451	CCC1(O)CN(C1)C(=O)C1=NN=C(C)S1	227,28	C9H13N3O2S
Z2065788225	CNC(=O)C1=C(Br)C(N)=CC=C1	229,08	C8H9BrN2O
Z1918542164	CCC1(O)CN(C1)C1=NC=C(Cl)C=N1	213,67	C9H12ClN3O
Z2045006645	CC1=NC2=C(N1)C=CC=C2C#N	157,18	C9H7N3
Z2044769537	CN1C=NC2=C1C=CN=C2	133,15	C7H7N3
Z2044770199	C1CCC(NC1)C1=NNC=C1	151,21	C8H13N3
Z1780230281	BrC1=CC=C(CNC(=O)C2=CC=CO2)O1	270,08	C10H8BrNO3
Z1220054876	NC(=O)CCN1N=C2C=CC=CN2C1=O	206,21	C9H10N4O2
Z274783176	COC1=C(N)C=C(C=C1)C(O)=O	167,16	C8H9NO3
Z420276166	CC1=C(SC=N1)C(=O)NCC1CCCC1	224,32	C11H16N2OS
Z1270387259	CC(C)(OC1=CC=CC=C1)C(O)=O	180,20	C10H12O3
Z1270384392		198,17	C10H8F2O2
Z1270358401	OC(=O)CC1CCC2=C1C=CC=C2	176,22	C11H12O2
Z1270358383	CN1C=C(C=N1)C1=NC(C)=C(S1)C(O)=O	223,25	C9H9N3O2S
Z1270207964	CC1=C(SC(=N1)C1CCCC1)C(O)=O	211,28	C10H13NO2S
Z1269638425	OC1CCCC2=CN=C1C2	138,17	C7H10N2O
Z1268703748	CC1=C(C=CC(=C1)C(O)=O)N1C=NC=N1	203,20	C10H9N3O2
Z1267881762	COC1=C(SC(C)=C1Br)C(O)=O	251,09	C7H7BrO3S
Z2658867260	CC1(C)CCCC(N)(C1)C(O)=O	171,24	C9H17NO2
Z461898648	CN(C)C(=O)C1=CN=C1	139,16	C6H9N3O
Z1127744301	NC(=O)C1CCC2=C1C=CC=C2	161,20	C10H11NO
Z2588063700	OC(=O)C1C2CCCCCCC12	168,24	C10H16O2
Z2588063726	CC1=NC2=C(O1)N=CC(Br)=C2	213,03	C7H5BrN2O
Z2587654857	OC1(CCNCC1)C1CC1	141,21	C8H15NO
Z271138028	OC(=O)CCC1=C(C=CC=C1)C#N	175,19	C10H9NO2
Z2582143599	CCC1=CN(C(=O)C(C=C1)C(O)=O)	167,16	C8H9NO3
Z992753752	C1CC2=C(CN1)SC(=N2)C1=CC=CC=C1	216,30	C12H12N2S
Z1741974486	NC1=NC=NC(=C1)C(F)(F)F	163,10	C5H4F3N3
Z275177252	CC(C)NC(=O)C1=NN(C)C(=C1)C(O)=O	211,22	C9H13N3O3
Z2106601619	CN1N=C(C)C2=C1NC(=O)C=C2C(O)=O	207,19	C9H9N3O3
Z1741965991	CC1CCC2=C(C1)C(=NO2)C(O)=O	181,19	C9H11NO3
Z1813130067	CC1=C(C=CN1C1CC1)C(O)=O	165,19	C9H11NO2
Z2510258226	COC1=CC2=C(C=C1)C(=NS2)C(O)=O	209,22	C9H7NO3S
Z2510258278	COC1=CC2=C(C=C1)C(CCC2)C(O)=O	206,24	C12H14O3
Z2510258276	CC1=CC=C(S1)C1=C(C=NO1)C(O)=O	209,22	C9H7NO3S
Z2510258156	OC(=O)CC1=CC2=C(C=C1)N=CS2	193,22	C9H7NO2S
Z2510258214	CC(C)CC1=NC(C)=C(O1)C(O)=O	183,21	C9H13NO3
Z2380439254	CC1=C(C)CC(CC1)C(O)=O	154,21	C9H14O2
Z2379802699	CN1N=CC=C1C1NCCC2=C1N=CN2	203,25	C10H13N5
Z1269145581	COC1=C(C(O)=O)C(C)=CC=C1Br	245,07	C9H9BrO3
Z2379087683	COC1=NSC(=C1)C(O)=O	159,16	C5H5NO3S
Z1561884809	NC(=O)C1CCN(CC2CCC=CC2)C1	208,31	C12H20N2O
Z2350907435	CCC1C(=O)NC2=C1C=CC=C2	161,20	C10H11NO
Z2335632234	CN1C(C)=C(Br)C=C(C(O)=O)C1=O	246,06	C8H8BrNO3
Z1289592972	CN(CC(O)=O)C1CCC1	143,19	C7H13NO2
Z2327883869	CC1=C(C2CCCC(=O)N2)C(C)=NN1	193,25	C10H15N3O
Z2327883861	CC1(C)CCCC(C)(O)C1	142,24	C9H18O
Z2327883833		206,24	C12H14O3
Z1263529610	CNC1=NC2=C(C=C1)C=C(N)C=C2	173,22	C10H11N3
Z1213669627	CC1=CC2=C(C=C1)C(=O)C=C(O2)C(O)=O	204,18	C11H8O4
Z1188325566	CCN(C)C(=O)NCC1=CC(F)=CC=C1	210,25	C11H15FN2O
Z1173925785	CNC(=O)C1CC1C1=C(Cl)C(Cl)=CC=C1	244,12	C11H11Cl2NO
Z1263529549	CNC(=O)C1=CN=C(C)NC1=O	167,17	C7H9N3O2
Z1262691682	CC1=NC(O)=C(C)C(C)=N1	138,17	C7H10N2O
Z1262398434	CNC(=O)C1=C(N)C=CC=C1C	164,21	C9H12N2O
Z1741965065	CS(=O)(=O)C1=CC2=C(C=CN2)C=C1	195,24	C9H9NO2S
Z1262327477	CC(C)C1=NOC(=N1)C1=CC=C(N)C=C1	203,25	C11H13N3O
Z1889909664	COCC(O)C1=NC=CS1	159,20	C6H9NO2S
Z1889709962	CC(N1CCNCC1)C1=NC=C(C)S1	211,33	C10H17N3S
Z1271660882	CC1CCC(C1)NCCO	143,23	C8H17NO
Z1823334918	CC1=CC(CS(=O)C2=C(C)OC=C2)=NO1	225,26	C10H11NO3S
Z1527154441	CN(CCO)C(=O)C1=CC(C)=C(Cl)C=C1	227,69	C11H14ClNO2
Z1815149173	COC1=C(C=CC=C1)C(N)CN	166,22	C9H14N2O
Z1815149192	NCC(N)C1=CSC2=C1C=CC=C2	192,28	C10H12N2S
Z1778561006	CNCCC1CCOCC1	143,23	C8H17NO
Z1738061139	O=C1SC=NN1CC1=NOC=C1	183,19	C6H5N3O2S

Z1824511473	CC(=O)N1C[C@H](O)C[C@H]1C(O)=O	173,17	C7H11NO4
Z2379203156	NC1=NCC2=C1C=CC=C2	132,17	C8H8N2
Z2070537303	CC1=C(N=C(O1)C1CC1)C(O)=O	167,16	C8H9NO3
Z1993522705	O=C1C=CNC(=N1)C1CCOCC1	180,21	C9H12N2O2
Z1891776137	C1CC(CN1)N1N=CC2=C1C=CC=C2	187,25	C11H13N3
Z198262914	CNC(=O)C1=CC2=C(NN=N2)C=C1	176,18	C8H8N4O
Z1945984127	OC(=O)CC1=CC2=C(NN=C2)C=C1	176,18	C9H8N2O2
Z1918018808	CC1=C(N=NN1CC1CCCC1)C(O)=O	209,25	C10H15N3O2
Z1918018307	CN1N=C(C)C2=C1NC=CC2=O	163,18	C8H9N3O
Z1918018438	CN1N=C(C=C1N)C1=CC=C(C1)S1	213,68	C8H8CIN3S
Z1913660931	CN1N=C(C=C1N)C1=C(F)C=C(F)C=C1	209,20	C10H9F2N3
Z1839480564	ClC1=C(C2CCNCC2=O)C=CC=C1	223,70	C12H14ClNO
Z1839481042	O=C1NCCCC1CC1=CC=CC=C1	189,26	C12H15NO
Z1262327505	C(NC1=NC=CC=C1)C1CCNC1	177,25	C10H15N3
Z1572855477	FC1=CC=C(NCC2=CSN=N2)C=C1	209,24	C9H8FN3S
Z1460223342	FC1=C(F)C=C(NC2CCNCC2=O)C=C1	212,20	C10H10F2N2O
Z729726738	CC1=NOC(NC(=O)C2CCCC2)=N1	209,25	C10H15N3O2
Z1139696203	CC(C)N1CCCC(CN2C=NC=N2)C1	208,31	C11H20N4
Z2429435052	CC(C)(O)CN1CC[C@H](N)C1	158,25	C8H18N2O
Z1755532218	CC(C)C1=NC2=C(C(C2)C(N)=O)N1	207,28	C11H17N3O
Z2582962531	OC(=O)C1CC(C1)OC(F)F	166,12	C6H8F2O3
Z1552027015	CC1=CC=C(OCC2=NC(N)=NO2)C=C1	205,22	C10H11N3O2
Z1378382208	ClC1=C(C=C1N)N1CCS(=O)(=O)CC1	246,71	C9H11ClN2O2S
Z1526503435	CC1=C(C)C(=CC(=C1)S(C)(=O)=O)C(O)=O	228,26	C10H12O4S
Z1516394948	NC1=CN=C(OCCO)C=C1	154,17	C7H10N2O2
Z1511494807	OC(=O)C1CCCC1C(O)=O	158,15	C7H10O4
Z1495385259	Cl.CC1=CC(C)=C(CCN)C(C)=C1	199,72	C11H18ClN
Z85956704	CNCC1=CC(F)=C(OC)C=C1	169,20	C9H12FNO
Z1741966332	CCN1C=C(C(C)N)C(C)=N1	153,23	C8H15N3
Z1492781275	CC1=C(C=CC(=C1)C#N)C(O)=O	161,16	C9H7NO2
Z31112041	C(NC1=NC=CN=C1)C1=CC=CS1	191,25	C9H9N3S
Z1446854759	CC1(C)C(=O)NC2=C1C=C(C=C2)C(O)=O	205,21	C11H11NO3
Z57683743	CC1=NNC(=O)C1CCC(O)=O	170,17	C7H10N2O3
Z85923411	C(NC1=CN=CC=C1)C1=CC=CO1	174,20	C10H10N2O
Z1250132399	CN(C)CCN1C=CC2=C1C=C(N)C=C2	203,29	C12H17N3
Z636406392	FC1=CC(NCC2=CC=CO2)=CC=C1	191,21	C11H10FNO
Z32014822	CN(C)C(=O)C1=CC(C)=C(C)C=C1	177,25	C11H15NO
Z1650040241	CCC(=O)NC1CCNC1	142,20	C7H14N2O
Z1263529632	CN(C)C(=O)CN1C=C(N)C=N1	168,20	C7H12N4O
Z1945700460	NC1=NOC(=N1)C1=CC2=C(CCC2)C=C1	201,23	C11H11N3O
Z1891774786	CC1=C(C)N2CCNCC2=N1	151,21	C8H13N3
Z1945708091	CN1C(=O)CC2=C1N=CC(Br)=C2	227,06	C8H7BrN2O
Z352704742	CC(O)CNC(=O)C1=C(F)C=C(Br)C=C1	276,11	C10H11BrFNO2
Z1916655429	CNC1=NN=C(C=C1)C1=CC(F)=CN=C1	204,21	C10H9FN4
Z1907760164	OC(=O)C1=C(C(F)F)N2N=CC=C2N=C1	213,14	C8H5F2N3O2
Z1907760167	CC1=NN=C(O1)C1=C(N)C=CC(F)=C1	193,18	C9H8FN3O
Z1895741677	CC1=NC2=C(CCCC2C(O)=O)S1	197,25	C9H11NO2S
Z1889997414	CC1=NC(CC(O)=O)=C(Br)C=C1	230,06	C8H8BrNO2
Z1889996343	OCC1=NOC(=C1)C1=CC(F)=CC=C1	193,18	C10H8FNO2
Z1889917206	OC(=O)CCN1CCCS1(=O)=O	193,22	C6H11NO4S
Z1889902457	CC(C)(C1CCC(O)CC1)C(O)=O	186,25	C10H18O3
Z594970960	CC1CCC(C1)NC(=O)C1=NSN=C1	225,31	C10H15N3OS
Z28880966	CC(NC(=O)C1=CC=CS1)C1=CC=CS1	237,34	C11H11NOS2
Z600428394	NC1=NN=C(O1)C1=CC2=C(CCC2)C=C1	201,23	C11H11N3O
Z600428384	CC1=NN2C(N=C(C)C=C2)=C1C(O)=O	205,22	C10H11N3O2
Z600428386	CC1=NN2C=CC=NC2=C1C(O)=O	177,16	C8H7N3O2
Z133804144	CC(NS(C)(=O)=O)C1=CN=CC=C1	200,26	C8H12N2O2S
Z85887069	OC(=O)CNC(=O)C1=CC=C(Br)S1	264,09	C7H6BrNO3S
Z64780602	CC1=NN(CCO)C(C)=C1	140,19	C7H12N2O
Z240137278	O=S(=O)(N1CCCC1)N1CCOCC1	220,29	C8H16N2O3S
Z372499004	CC1=CC=C(O1)C(=O)NC1=CN=C1	191,19	C9H9N3O2
Z228589198	CN(C)C1=NC2=C(S1)C=C(S2)C(O)=O	228,28	C8H8N2O2S2
Z29672803	CC1=NN=C(NC(=O)C2=NC=CC=C2)S1	220,25	C9H8N4OS
Z1234028446	CNS(=O)(=O)C1=CNC=N1	161,18	C4H7N3O2S
Z410633222	CC1=NN=C(NC(=O)N2CCOCC2)S1	228,27	C8H12N4O2S
Z1258578315	CC1=NC(N2CCCC2)=C(C=C1)C#N	187,25	C11H13N3
Z1162470566	CC1CCCC2=C1NC(=O)C(=C2)C#N	188,23	C11H12N2O

Z990231828	CC(=C)CN1CCC(CC1)C1=CN=C1	205,31	C12H19N3
Z295892696	CC(C)NC(=O)C1=C2N=CC=CN2N=C1	204,23	C10H12N4O
Z875024178	CC1=CC(=O)NC(=N1)C1=CC=C(N)C=C1	201,23	C11H11N3O
Z217038356	CC1CN(CCO1)C(=O)CN1C=CC=N1	209,25	C10H15N3O2
Z466628048	CC1=CSC(CNC(=O)C2=NNC=C2)=N1	222,27	C9H10N4OS
Z32015800	CNC(=O)C1=CC(=CC=C1)S(C)(=O)=O	213,25	C9H11NO3S
Z2072621991	FC(F)OCC(=O)N1CC2CCCC2C1	219,23	C10H15F2NO2
Z2587654879	CC(O)C1=C(C)N=CC=C1	137,18	C8H11NO
Z1040397258	CC1(C)COCCN1CC1=CN=CC=C1	206,29	C12H18N2O
Z2379564057	CC1=NSC(=N1)N1CC=CC1	167,23	C7H9N3S
Z2492802465	COCC(N)C1CCOCC1	159,23	C8H17NO2
Z2465620163	COCC1=NN=C2CNCNC12	168,20	C7H12N4O
Z2442103067	COCCN1CCNC(C)(C)C1	172,27	C9H20N2O
Z31791472	O=C(CC1=CC=CS1)NC1=CN=CC=C1	218,27	C11H10N2OS
Z1233341893	CC(C)C(C)C(=O)N(C)C1=NC=CC=C1	206,29	C12H18N2O
Z2574915591	NC1CCCC1CC1=NC=CC=C1	176,26	C11H16N2
Z2574915593	CN1N=C(C)C=C1CC1CCCC1N	193,29	C11H19N3
Z1444214858	CC(C)(NC(=O)C1=CC=NC=C1)C(O)=O	208,22	C10H12N2O3
Z1172068241	OC(=O)CCC1CCCCO1	144,17	C7H12O3
Z2213893336	CC1=CC(=O)NC(=C1)C(O)=O	153,14	C7H7NO3
Z2213893369	CN1C=NC2=C1C(=CC(=O)N2)C(O)=O	193,16	C8H7N3O3
Z2213893376	CC1CNC(=O)CN(C1)C1CC1	168,24	C9H16N2O
Z2205958606		206,25	C11H14N2O2
Z2186882035	CC1=CN2C(S1)=NC(C)=C2C#N	177,23	C8H7N3S
Z2186882188	CC1=C(N)C2=NC=NN2C=C1	148,17	C7H8N4
Z118333670	O=C1CCCCN1C1=CC=CC=C1	175,23	C11H13NO
Z2182115414	CC1COC2=C1C=C(C=C2)C(O)=O	178,19	C10H10O3
Z1878408220	CC(=C)CN1C=C(Br)C(C)=CC1=O	242,12	C10H12BrNO
Z32014367	CN(C)C(=O)C1=CC=CO1	139,15	C7H9NO2
Z274762944	OC(=O)CN1C(=O)OC2=C1C=C(C)C=C2	227,60	C9H6CINO4
Z29659913	COC1=C(OC)C=C(NC(C)=O)C(C)=C1	209,25	C11H15NO3
Z285139200	CC(C)C(=O)NC1=CC(CN)=CC=C1	192,26	C11H16N2O
Z278101766	CC1=C(F)C=C(C=C1)C#N	135,14	C8H6FN
Z256708488	CCOC1=C(C=CC=N1)C(O)=O	167,16	C8H9NO3
Z1828858406	COC(C)(C)C1=NC(=NO1)C1=CC=CS1	224,28	C10H12N2O2S
Z363104186	CNC(=O)C1CCCN(C1)C(=O)C(C)C	212,29	C11H20N2O2
Z1816725432	NCC1(O)CCN(CC2=CC=CC=C2)C1	206,29	C12H18N2O
Z1259339838	CC(N)C1=C(C)N=C(C)S1	156,25	C7H12N2S
Z995389448	CCN1C(=O)ON=C1C1=C(C)C=CC=C1	204,23	C11H12N2O2
Z1259339743	COC1=C(C=CC=C1)C(C)(C)O	166,22	C10H14O2
Z1250132810	CN1CCC(CN)C1C1=CC=CS1	196,31	C10H16N2S
Z228574062	CN(C)(C)CN1C1=CC=C(C)C=C1	198,69	C10H15CN2
Z1354416068	CC(=O)N1CC2=C(C1)C=C(N)C=C2	176,22	C10H12N2O
Z1342208350	C1CNC2=C(N1)C=CC=N2	135,17	C7H9N3
Z1336457497	CNC1=C(N=CC=C1)N1CCCC1	177,25	C10H15N3
Z1816233707	CNC(=O)C1=NC(=CC=C1)C(O)=O	180,16	C8H8N2O3
Z1816233763	CC1=C(SC=N1)C1=CNC=C1C(O)=O	208,24	C9H8N2O2S
Z1815156932	CN1C=CC(CC(O)=O)=N1	140,14	C6H8N2O2
Z2897268424		159,14	C6H9NO4
Z1815155424	NC(=O)C1(CCOCC1)N1CCCC1	198,27	C10H18N2O2
Z1675346324	CN(C1CC(O)C1)C1=NC(C)=NC(C)=C1	207,28	C11H17N3O
Z1247413461	CS(=O)(=O)N1CCCC(CO)C1	193,26	C7H15NO3S
Z364368134	CC(=O)NC1=C(C)C(=CC=C1)C(O)=O	193,20	C10H11NO3
Z1331708376	O=C(NCC1=CN=N1)C1CCC=CC1	206,25	C10H14N4O
Z449369146	OC(=O)CCC1=CC=C(C)S1	190,64	C7H7ClO2S
Z445226250	CC(N)(C(O)=O)C1=CC=C(C)C=C1	199,63	C9H10ClNO2
Z328695000	CC(C)N(C)C1=CC(C)=NC2=NC=NN12	205,27	C10H15N5
Z220564202	C1CC(CCN1)C1=CNC2=C1C=CC=C2	200,29	C13H16N2
Z432066788	CC1=C(F)C=C(C=C1N)C(N)=O	168,17	C8H9FN2O
Z29672805	CC(C)C(=O)NC1=NN=C(C)S1	185,25	C7H11N3OS
Z415636820	CC1=C(N=C(O1)C1=CC=CS1)C(O)=O	209,22	C9H7NO3S
Z71176766	OC(=O)C1=C(N=CC=C1)N1CCCC1	206,25	C11H14N2O2
Z397585784	OC(=O)C1=CSC(CC2=CC=CC=C2)=N1	219,26	C11H9NO2S
Z442033408	O=C(NCC1=CC=CS1)C1=NNC=C1	207,25	C9H9N3OS
Z240297184	CN1C=CC(NC(=O)C2=C(C)OC=C2)=N1	205,22	C10H11N3O2
Z992716870	CN1N=CC(C2=NC(=NO2)C2CC2)=C1N	205,22	C9H11N5O
Z119654718	CN1C=CC(NC(=O)C2=C(C)C=CO2)=N1	205,22	C10H11N3O2

Z951367936	CC1=C(N)C(=CC(F)=C1)C(O)=O	169,16	C8H8FNO2
Z364411884	CCC(=O)NC1=CC(Cl)=C(C=C1)C(N)=O	226,66	C10H11ClN2O2
Z220784950	CC1=C(OC=C1)C(=O)N1CCNC(=O)C1	208,22	C10H12N2O3
Z916919192	CN(C(C)=O)C1=C(C=CC=C1F)C(O)=O	211,19	C10H10FNO3
Z1868430567	OC(C1CCCCC1)C(O)=O	158,20	C8H14O3
Z1868316830	OC(=O)C1CC=CCC1C(=O)NC1CC1	209,25	C11H15NO3
Z1695906701	CC1=NN(C=C1C(O)=O)C1CCOC1	196,21	C9H12N2O3
Z2574910420	OC(=O)CN1CCN(C2CC2)C1=O	184,20	C8H12N2O3
Z1224459567	CN(C(C)=O)CC1(CCCC1)C(O)=O	199,25	C10H17NO3
Z815264062	CN1C=C(C(O)=O)C(=N1)C1=CC=NC=C1	203,20	C10H9N3O2
Z2327226200	O=C1COCC(CC2=CC=CC=C2)N1	191,23	C11H13NO2
Z1446243816	NC1CCOC2(CCC2)C1	141,21	C8H15NO
Z401964204	CC1CCCCC1NCC1=CN=C1C	207,32	C12H21N3
Z2087745281	COC1=C(C=CC=C1)[C@H]1CCC[C@H](C)N1	205,30	C13H19NO
Z2205998814	CN1CCC2OCCNC2C1	156,23	C8H16N2O
Z3244905268	Cl.Cl.Cl.NC1CCN(CCN2CCOCC2)C1	308,67	C10H24Cl3N3O
Z927323342	O=C(C1CC1)N1CCCNCC1	168,24	C9H16N2O
Z57148445	COC1=CC=C(C=C1)C1=NN=C(N)S1	207,25	C9H9N3OS
Z1263602345	COC1=NC2=C(C=CC=C2)C(CN)=C1	188,23	C11H12N2O
Z1415893830	NC1=NN(CC2=CC=NC=C2)C=N1	175,20	C8H9N5
Z1350606444	OC(=O)CCC1=CSC2=C1C=CC=C2	206,26	C11H10O2S
Z285782452	CNC1=C(C=CC=C1)S(C)(=O)=O	185,24	C8H11NO2S
Z1318516260	CC(=O)N1CCC(C)(C1)C(O)=O	171,20	C8H13NO3
Z2216303104	OCC1=CC2=C(ON=C2)C=C1	149,15	C8H7NO2
Z2189170996	OC(=O)C1=C(CC2=CC=CC=C2)SC=N1	219,26	C11H9NO2S
Z2690260832	N#CC1=C2OCCOC2=CS1	167,18	C7H5NO2S
Z26317437	NC(=O)CN1C=C(Br)C=CC1=O	231,05	C7H7BrN2O2
Z53825414	CCS(=O)(=O)N1CCCC1C(O)=O	207,24	C7H13NO4S
Z85890240	CC(NC(=O)C1=CC=CO1)C(O)=O	183,16	C8H9NO4
Z147579704	OC(=O)C1=CC2=C(OC1)C=CC(Cl)=C2	210,61	C10H7ClO3
Z85886788	OC(=O)CNC(=O)C1CCCC1	171,20	C8H13NO3
Z234898187	CC1=C(C=CC=C1N)C(O)=O	151,17	C8H9NO2
Z90122509	NC(=O)N1CCC(CC1)C(O)=O	172,18	C7H12N2O3
Z25080630	CNC(=O)COC1=C(Br)C=C(F)C=C1	262,08	C9H9BrFNO2
Z384361454	CC1=NOC(=C1)C(=O)NCC1CCOC1	210,23	C10H14N2O3
Z44585799	CC1=CC(NC(=O)N2CCCC2)=CC=C1	204,27	C12H16N2O
Z44585777	O=C(NC1=CC=CC=C1)N1CCCC1	190,25	C11H14N2O
Z220616840	NC1=CN=C(C=C1)N1CCOCC1	179,22	C9H13N3O
Z26548083	CC(C)C(=O)NC1=CC(=CC=C1)C#N	188,23	C11H12N2O
Z30841068	BrC1=CC(=CC=C1)C(=O)NC1CC1	240,10	C10H10BrNO
Z359419748	CC1=C(SC2=C1C(C)=CC=N2)C(O)=O	207,25	C10H9NO2S
Z1863617804	COCC1=CC(=O)NC(=N1)N1CCCC1	209,25	C10H15N3O2
Z1530301542	CCC1=CSC(=N1)C1=CNC=N1	179,24	C8H9N3S
Z1180112116	NC1=C(C=CC=C1)C1CCNCC1	176,26	C11H16N2
Z1874937386	OC1=CC(=O)NC(=N1)C(F)(F)F	180,09	C5H3F3N2O2
Z1869801232	CC1(CCCNC1=O)C(O)=O	157,17	C7H11NO3
Z1222331407	CC(C)(CO)NC1=NC=C(Br)C=C1	245,12	C9H13BrN2O
Z1127695826	CC(C)NC(=O)CC1=C(Br)C=CC=C1	256,14	C11H14BrNO
Z165304624	CC1=NC(COC2=C(F)C=CC=C2)=NO1	208,19	C10H9FN2O2
Z320990506	OC(CN1C=CN=C1)C1=CC(Br)=CC=C1	267,13	C11H11BrN2O
Z103739202	CN1CCN(CCO)CC1	144,22	C7H16N2O
Z1098687825	CC1=CC(=NO1)C(=O)N1CCCC1(C)C	208,26	C11H16N2O2
Z241200732	CC(C)C(C)NC(=O)C1=CC=C(C)N1C	208,31	C12H20N2O
Z351222172	OC(=O)C(N1CCCC1)C1=CC=CC=C1	205,26	C12H15NO2
Z1172115933	CC1=C(C=CC(=N1)C1=CC=CO1)C(O)=O	203,20	C11H9NO3
Z649583112	CNCC1=NN=C(C)N1C	140,19	C6H12N4
Z1385328783	CNC(=O)N(C(C)C1=CC=CO1)C1CC1	208,26	C11H16N2O2
Z1526453856	CN1C=CN=C1C1CCNC1	151,21	C8H13N3
Z1262395923	COC1=C(C=CC=C1)C(C)CN	165,24	C10H15NO
Z1270087714	CC1CN(CC(C)O1)C1=NC(C)=NS1	213,30	C9H15N3OS
Z1250132637	CCC(C)(N)C1=NC=CS1	156,25	C7H12N2S
Z1166181228	CC1CN(C)CCN1C(=O)C1=NSN=C1	226,30	C9H14N4OS
Z340498698	CC(C)N(C1CC1)C(=O)C1=C(C)OC=C1	207,27	C12H17NO2
Z324712988	CC(C)N(C1CC1)C(=O)C1=CC=CO1	193,25	C11H15NO2
Z2507919901	C1CC(CO1)C1=NC=CN1	138,17	C7H10N2O
Z1259273141	OC(=O)C1(CCC1)C(=O)NC1CC1	183,21	C9H13NO3
Z2492800383	COCC1=C(N)N=CC=C1	138,17	C7H10N2O

Z2471547875	CN1C(=O)C=CC2=C1CCCC2N	178,24	C10H14N2O
Z295228412	CN(C)(C(=O)C1=CN=C(C=C1)C(O)=O	194,19	C9H10N2O3
Z1982493923	CC1(CCC(=O)NC1)C(O)=O	157,17	C7H11NO3
Z1973465514	O=C1NN=C(C=C1)C1CC1	136,15	C7H8N2O
Z1971703350	CN1N=C(CN2CCCC2)C=C1C(O)=O	209,25	C10H15N3O2
Z90122431	CC1=CC(C)=C(C(O)=O)C(=O)N1	167,16	C8H9NO3
Z1962222453	CN1N=CC(C(O)=O)=C1O	142,11	C5H6N2O3
Z32014557	CN(C)(C(=O)CC1=C(Cl)C=CC=C1F	215,65	C10H11ClFNO
Z32014670	CN(C)(C(=O)CC1=C(Cl)C=CC=C1Cl	232,10	C10H11Cl2NO
Z274740244	CC1=C(N2C=C(Br)C=CC2=N1)C(O)=O	255,07	C9H7BrN2O2
Z1945698150	CN1C(C)=NC2=C1C=C(C=C2)C(O)=O	190,20	C10H10N2O2
Z1983079687	FC(F)(F)C1=CC(=O)NC2=C1C=NN2	203,12	C7H4F3N3O
Z381357590	C1CNC(C1)C1=CC=CN1	136,20	C8H12N2
Z380844598	NCC(O)C1=CC=C(F)C=C1	155,17	C8H10FNO
Z741016936	CC1=CC(NC(=O)C2=CSN=N2)=CC=C1	219,26	C10H9N3OS
Z234855772	CC(C)N1N=CC2=C1NC(=O)C=C2C	191,23	C10H13N3O
Z56767623	C1CN(CCO1)C1=NC2=C(S1)C=CC=C2	220,29	C11H12N2OS
Z227830218	CN(C)C1=NC=C(N)C=C1	137,19	C7H11N3
Z56761814	CC(=O)NC1=C2SC(C)=NC2=CC=C1	206,26	C10H10N2OS
Z56760165	CC1(C)CC2=C(C1)C(=NS2)C(N)=O	196,27	C9H12N2OS
Z55293719	CN(C)(C(=O)NC1=CC=C(Cl)C=C1	198,65	C9H11ClN2O
Z235352019	OC(=O)CN1N=C2CCCCN2C1=O	211,22	C9H13N3O3
Z2692093998	CN1N=C(O)C2=C1CNCC2	153,19	C7H11N3O
Z1741979488	OC(=O)CCC1=CC(F)=C(Cl)C=C1	202,61	C9H8ClFO2
Z2692093605	NC(C1CCCO1)C(O)=O	145,16	C6H11NO3
Z2365130785	C[C@@]1(O)C[C@@H](C1)NC1=C(F)C=CC=N1	196,23	C10H13FN2O
Z2273972081	CC1CN(CC(=O)N1)C1=C(F)C=CC=N1	209,22	C10H12FN3O
Z1373445602	CN1CCN(CC1=O)C1=C(F)C=CC=N1	209,22	C10H12FN3O
Z234897483	OC(=O)C1=C(CN2CCOCC2)C=CO1	211,22	C10H13NO4
Z1821397701	CC1=C(SC(CC2CC2)=N1)C(O)=O	197,25	C9H11NO2S
Z409511958	OC1CCN(CC1)C(=O)NC1=NN=CS1	228,27	C8H12N4O2S
Z1816507673	CN(C)(C(O)=O)C1=C(Cl)C=CC=C1	213,66	C10H12ClNO2
Z1699518303	CN1N=CN=C1NCC1=NC=C(C)C=C1	203,25	C10H13N5
Z1836338757	CN1C=C(C(O)=O)C(=N1)C1=CC=C(Cl)S1	242,68	C9H7ClN2O2S
Z1836338785	OC(CC1CCCCC1)C(O)=O	172,22	C9H16O3
Z1741957000	OC(=O)C1=C(C=CC=C1F)C(F)(F)F	208,11	C8H4F4O2
Z1729240147	CC1=CC(OCC2=NOC=C2)=CC(C)=N1	204,23	C11H12N2O2
Z1259041087	CC1(C)CCNC(=O)CC1	141,21	C8H15NO
Z1258992517	O=C1NN=C2CCCCN12	139,16	C6H9N3O
Z56823545	OC(=O)CNC(=O)C1=C(Cl)C=C(Cl)C=C1	248,06	C9H7Cl2NO3
Z1258578430	CC1=C(C#N)N2C=CSC2=N1	163,20	C7H5N3S
Z56801375	O=C1NCCC2=C1C=CC=C2	147,18	C9H9NO
Z1137726171	CNCC1=C2NC=CC2=CC=C1	160,22	C10H12N2
Z1259341112	N#CC1=CC2=C(OCCO2)C=C1	161,16	C9H7NO2
Z1259340040	CC1=CC(C(O)=O)=C(C=C1)N1CCCC1	205,26	C12H15NO2
Z1259339939	CC1=CC(CC(O)=O)=NO1	141,13	C6H7NO3
Z1259273386	CN1N=C(C=C1C1CC1)C(O)=O	166,18	C8H10N2O2
Z1259273264	CN1C=C(C=N1)C1=CC(=CN=C1)C(O)=O	203,20	C10H9N3O2
Z1259162160	CC(=O)NC(C)(C1CC1)C(O)=O	171,20	C8H13NO3
Z1601639621	FC1=C(NC2CCOCC2)N=CC=C1	210,25	C11H15FN2O
Z1262254278	CC(C)NC(=O)CN1CCCNCC1	199,30	C10H21N3O
Z1262252889	CN1CCC(CCN)CC1	142,25	C8H18N2
Z1262253026	NC1CCCC2=C1C=CO2	137,18	C8H11NO
Z339881488	CC(C)N1CCN(CC1)C(=O)N(C)C	199,30	C10H21N3O
Z2687190967	CC1(C)CC(=O)NCCN1	142,20	C7H14N2O
Z1730522163	CC1CN(C(C)=O)C2=C(O1)C(F)=CC=C2	209,22	C11H12FN2O2
Z2681277106	CC1=C(OC(=C1)C(F)F)C(O)=O	176,12	C7H6F2O3
Z1171979267	CC(=O)NCC1=CC=C(O1)C(O)=O	183,16	C8H9NO4
Z1171978818	COC1=C(SC=C1)C(O)=O	158,17	C6H6O3S
Z844852064	CN(C1CC1)C(=O)C1=CC=C(C)NC1=O	206,25	C11H14N2O2
Z25637733	CC1=C(C)C(OCC(N)=O)=C(C)C=C1	193,25	C11H15NO2
Z1770193507	OC(=O)C1(CC2=CC=C(F)C=C2)CC1	194,21	C11H11FO2
Z1769859569	CC1=CC(=NN1C1=NC=CC=C1)C(O)=O	203,20	C10H9N3O2
Z1768428971	CN1C(C(C1=O)C(O)=O)C1=CC=CS1	225,26	C10H11NO3S
Z1677760062	CC(C)N(C)(C(=O)NC1=C(F)C=NC=C1	211,24	C10H14FN3O
Z1762997287	COC1=CC(Br)=C(C(O)=O)C(N)=C1	246,06	C8H8BrNO3
Z1753013037	CC(N)CS(=O)(=O)C1=CC=C(C)C=C1	213,30	C10H15NO2S

Z1741785925	CC1CCNC(C1)C(N)=O	142,20	C7H14N2O
Z319891284	CC1=CC(=NO1)C1CCCN1S(C)(=O)=O	230,28	C9H14N2O3S
Z1723549274	CCC1=C(CC)N=C(N)N=N1	152,20	C7H12N4
Z1603606287	CC1=CC=C(S1)C(=O)NC1(CC1)C(O)=O	225,26	C10H11NO3S
Z1444213486	CN1N=CC=C1C(=O)NC(C)(C)C(O)=O	211,22	C9H13N3O3
Z295847540	C(N1CCCCC1)C1=NC(=NO1)C1CC1	207,28	C11H17N3O
Z1217910521	CC(CN)CN1N=C(C)C=C1C	167,26	C9H17N3
Z1809263534	COCCN1CCCNCC1=O	172,23	C8H16N2O2
Z1899615150	CC(C)CN1C=NC2=C(C=CN2)C1=O	191,23	C10H13N3O
Z1333717721	CC1=NN2CCNCC2=N1	138,17	C6H10N4
Z2467540742	OCC(O)CN1C=CC=C1	141,17	C7H11NO2
Z1335657421	O=C1CNCCN1C1CC1	140,19	C7H12N2O
Z1245580422	CC1CCCN(CCN)C1	142,25	C8H18N2
Z1998104358	CN(C)C(=O)N1CCOCC11CCOC1	214,27	C10H18N2O3
Z1238540099	C1C1=C(NC2CCNCC2)C=CC=C1	210,71	C11H15CIN2
Z2235330350	CC1=C(CCO)N=CC=C1	137,18	C8H11NO
Z2689946992	OC(=O)C1=CC(=CN=C1)N1CCCC1=O	206,20	C10H10N2O3
Z2158481117	COC1=C(C=CC(=C1)N(C)C)C(O)=O	195,22	C10H13NO3
Z2111525940	N#CC1=CN(CC2=CC=CC=C2)N=N1	184,20	C10H8N4
Z2096087693	OC1CCC2=C1N=CC(Br)=C2	214,06	C8H8BrNO
Z217102788	C1CNC2=C(C1)N=CC=C2	134,18	C8H10N2
Z2168277541	O=C1NCCC1CC1=CC=CC=C1	175,23	C11H13NO
Z2160887406	COC1=C(N)C=C(F)C(F)=C1	159,14	C7H7F2NO
Z1415893980	CCC1(CCCC1)C(O)=O	142,20	C8H14O2
Z1245580461	CC1CCN(CCN)CC1	142,25	C8H18N2
Z1360063124	CN(C)C(=O)C1=C(Br)C=CO1	218,05	C7H8BrNO2
Z57036273	CN(C)C1=C(N)C=C(C=C1)C(F)(F)F	204,20	C9H11F3N2
Z1162778919	CCC1=NC(CN2C=CC=CC2=O)=NO1	205,22	C10H11N3O2
Z818732104	CC(N)CN1CCOCC1	144,22	C7H16N2O
Z1696870012	NC1CCCC1NC1=NC=CN=C1	192,27	C10H16N4
Z1891776227	NC1CCOC2(CCOC2)C1	157,21	C8H15NO2
Z2510258210	COCC1=C(SC=N1)C(O)=O	173,19	C6H7NO3S
Z373773422	CN1C=C(NC(=O)CN2C=CC=N2)C=N1	205,22	C9H11N5O
Z910841006	CCC(=O)NC1=C(C=C(C)C=C1)C(O)=O	207,23	C11H13NO3
Z234897203	NC1=C(CN2CCC(O)CC2)C=CC=C1	206,29	C12H18N2O
Z234896705	NCC1=CC(F)=C(Br)C=C1	204,04	C7H7BrFN
Z234853700	CC1=NC(=O)N(CC(O)=O)C(C)=C1	182,18	C8H10N2O3
Z31190999	CC(C)NC1=C2C=CSC2=NC=N1	193,27	C9H11N3S
Z111781394	OC(=O)C1=CC(=NN1)C1CC1	152,15	C7H8N2O2
Z30271924	CNC(=O)C(C)OC1=CC=C(C=C1)C#N	204,23	C11H12N2O2
Z240297434	CN1C=CC(NC(=O)C2=CC(C)=NO2)=N1	206,21	C9H10N4O2
Z969560526	CC1=NC=C(C(N1)N=CC=C2	133,15	C7H7N3
Z969559596	NC(C(O)=O)C1=CC(Br)=CC=C1	230,06	C8H8BrNO2
Z314449926	CCN(C1CC1)C(=O)C1CCC=CC1	193,29	C12H19NO
Z382738034	CC1=NOC(CN2CCOC(C)(C)C2)=C1	210,28	C11H18N2O2
Z228574258	CN(C)C(CN)C1=C(F)C=CC=C1F	200,23	C10H14F2N2
Z137705484	CC1CCCN(CC2=C(CI)SN=N2)C1	231,74	C9H14CIN3S
Z90507765	C(NC1CCCCC1)C1=CN=CC=C1	204,32	C13H20N2
Z241827180	CN1CCN(CC1)C(=O)C1=NOC(C)=C1	209,25	C10H15N3O2
Z992717376	C1CN(CCN1)C1=NN=CC=C1	164,21	C8H12N4
Z31490283	CC1=C(SC=C1)C(=O)NCC1CCCO1	225,31	C11H15NO2S
Z744843394	CN1CCC(CN)C2=C1C=CC=C2	176,26	C11H16N2
Z818727322	NCC1CCCN(CC2=CC=CC=C2)C1	204,32	C13H20N2
Z227830236	NC1CCN(CC1)C1CC1	140,23	C8H16N2
Z1268961924	CCC1CN2CCCC2CN1S(C)(=O)=O	232,34	C10H20N2O2S
Z2327226238	CC1(C)CC(C(O)=O)C2=C(O1)C=CC=C2	206,24	C12H14O3
Z2327224817	C1CC(CO1)C1=NC2=C(N1)C=CC=C2	188,23	C11H12N2O
Z2305986609	CN1C(C)=CC2=C(C(N)=NN2)C1=O	178,20	C8H10N4O
Z1988459453	CN1N=C(C=C1C)C(O)C1=CN=CC=C1	203,25	C11H13N3O
Z2301499848	OC(=O)CC1=CC(=CC=C1)C1CC1	176,22	C11H12O2
Z31191155	CC(C)NC1=C(C=CC=N1)C#N	161,21	C9H11N3
Z54505513	NC(=O)CN1CCC(O)CC1	158,20	C7H14N2O2
Z1267773753	NC1=C(CI)C=CC(=C1)N1CCNC1=O	211,65	C9H10CIN3O
Z1267773689	CC(C)C1CCCCC1O	142,24	C9H18O
Z1267773677	NC1=C(C=C2CCCC2=N1)C#N	159,19	C9H9N3
Z1266933830	COC1=C(OC)C=C2N=C(N)NC2=C1	193,21	C9H11N3O2
Z1263714141	CCC(C)(N)C1=NC(=O)C2=C(CCC2)N1	207,28	C11H17N3O

Z33546774	NC(=O)CC1=C(CI)C=CC=C1Cl	204,05	C8H7Cl2NO
Z18083670	NC(=O)COC1=CC(=CC=C1)C#N	176,18	C9H8N2O2
Z2379767231	CC(C)C1=CSC(=N1)C1=NN=CN1	194,26	C8H10N4S
Z355729118	CC1CN(CC2=CC(C)=NO2)C(C)CO1	210,28	C11H18N2O2
Z2234866028	CCN(C)C(=O)NC1=NSN=C1	186,23	C6H10N4OS
Z286761296	CCN1CCCC1C(=O)N(C)C	170,26	C9H18N2O
Z645688832	CC1=CC=C(CNC2=NC=CN=C2)S1	205,28	C10H11N3S
Z1101640411	CC1CN(C(C)CO1)C(=O)C1=CSC=N1	226,29	C10H14N2O2S
Z1029460366	COC1=CC(CC2CCCN2)=CC=C1	191,27	C12H17NO
Z216242078	CC1CN(CC2=CC(C)=NO2)CCO1	196,25	C10H16N2O2
Z2010010168	CN1N=CC=C1C1CC2CCC(C1)N2	191,28	C11H17N3
Z1250132610	NC1=CC(=CC=C1)N1CCCCC1	190,29	C12H18N2
Z1401333862	CN1C=CC(NCC2=CC=CC=C2)=N1	187,25	C11H13N3
Z275730348	CC(N1CCC(O)CC1)C1=NC(C)=NO1	211,27	C10H17N3O2
Z2352608837		213,28	C11H19NO3
Z2434504713	CC1CC(CO1)NC1=C(F)C=CC=N1	196,23	C10H13FN2O
Z1102068247	CC(C)(C(N)=O)C1=CC=C(F)C=C1	181,21	C10H12FNO
Z2093301849	C[C@H](CO)N(C)C1=NC=C(F)C=C1	184,21	C9H13FN2O
Z2285175561	CCN(C1COC1)C(=O)C1=C(F)C=CS1	229,27	C10H12FNO2S
Z1983897532	CC1=NC=C(CNC2=CC(F)=CN=C2)S1	223,27	C10H10FN3S
Z1855969199	FC1=CCCN(C1)S(=O)(=O)C1COC1	221,25	C8H12FNO3S
Z1779277596	OC1CCN(CC2=CC(F)=CC(F)=C2)C1	213,23	C11H13F2NO
Z2379564100	CC(=O)N1CC(C1)NC1=NC(C)=NS1	212,27	C8H12N4OS
Z279623012	CN(C)S(=O)(=O)N1CCCC1	178,25	C6H14N2O2S
Z2234185613	CC1=CC2=C(C=C1)C(=O)C(=CN2)C(O)=O	203,20	C11H9NO3
Z2010655200	CC(C)CCN1C=C(C=N1)C#N	163,22	C9H13N3
Z2055186690	CC(C)CC(=O)N1C[C@H](C)[C@H](C1)C(N)=O	212,29	C11H20N2O2
Z1642373092	COC1=C2NC=CC2=CC=C1	147,18	C9H9NO
Z2301499695	CN1N=C(C=C1C)C(O)C1CC1	166,22	C9H14N2O
Z1103241017	CN1C=C(C=N1)C1CCCN1CC(C)=C	205,31	C12H19N3
Z2240988426	CC(N)(CC1=CC=CC=C1)C1CC1	175,28	C12H17N
Z103740620	CC(C)N1CCCC(CO)C1	157,26	C9H19NO
Z57033899	COC1=CC=C(C=C1)C1CCCN1	177,25	C11H15NO
Z57987855	NC1=CC=NN1CC1=CC=C(Br)S1	258,14	C8H8BrN3S
Z19735578	CC(OC1=CC=CC=C1)C(N)=O	165,19	C9H11NO2
Z803145422	CC(C)C1=C(SC=C1)C(O)=O	170,23	C8H10O2S
Z215640462	CCN1N=NN(C1=O)C1=CC=CS1	196,23	C7H8N4OS
Z228464414	O=C(CN1C=NC(=N1)C#N)N1CCCC1	205,22	C9H11N5O
Z763030026	NCC1=C(CO)C=CC=C1	137,18	C8H11NO
Z752989144	NC(=O)CN1C=CC(N)=N1	140,15	C5H8N4O
Z111834298	OC(=O)COC1=C(Br)C=CC=C1	231,05	C8H7BrO3
Z90423275	OC1CCN(CC1)C(=O)CCC(O)=O	201,22	C9H15NO4
Z235354749	Cl.CN1N=C(C)C2=C1N=CC(=C2)C(O)=O	227,65	C9H10ClN3O2
Z235354601	CN1C=CC(=C1)S(=O)(=O)N1CCNCC1	229,30	C9H15N3O2S
Z235354543	CN1N=CC(C(O)=O)=C1N1C=CC=C1	191,19	C9H9N3O2
Z85895203	CN(CC(O)=O)C(=O)C1=CC=CO1	183,16	C8H9NO4
Z56792417	NC1=CC(=CC=C1)S(=O)(=O)N1CCCC1	226,29	C10H14N2O2S
Z57455032	OC(=O)COC1=C(CI)C=CC(CI)=C1	221,03	C8H6Cl2O3
Z32013668	CN(C)C(=O)C1=CC=C(C=C1)S(C)(=O)=O	227,28	C10H13NO3S
Z332685442	CNC(=O)CNC(=O)C1=COC(Br)=C1	261,08	C8H9BrN2O3
Z212182648	CC(C)NC(=O)C1=CC=C(C(NC(C)=O)S1	226,29	C10H14N2O2S
Z57472940	OC(=O)C1CN(C(=O)C1)C1=CC=CC=C1	205,21	C11H11NO3
Z367450878	CC1=CC(C(O)=O)=C(C)N1	139,15	C7H9NO2
Z30533876	CC(=O)NC1=CC=C(OC(F)(F)F)C=C1	219,16	C9H8F3NO2
Z31408124	O=C(NCC1=CC=CO1)C1=NC=CN=C1	203,20	C10H9N3O2
Z1747218443	CNC1CCC(CC1)NC(C)=O	170,26	C9H18N2O
Z2470036257	CC1(C)CCC2=C(O1)C=CC(N)=C2	177,25	C11H15NO
Z1429867185	COC1=C2C=CNC2=CC=C1	147,18	C9H9NO
Z2467454495	CC(C)(CO)N1C=CN=C1	140,19	C7H12N2O
Z2467454603	CN1N=CC=C1C1COCCN1	167,21	C8H13N3O
Z2466617812	FC1=CC2=C(OCN2)C(F)=C1	171,15	C8H7F2NO
Z2465620036	CS(=O)(=O)C1=C2C=CN=CC2=C(N)C=C1	222,26	C10H10N2O2S
Z2465619816	CCC1=CC=C(C=C1)C1=CNC(N)=N1	187,25	C11H13N3
Z2442102917	OC(=O)CN1N=C2CCCN2C1=O	197,19	C8H11N3O3
Z228588628	OC(=O)C1(CCC1)C1=CC(F)=CC=C1	194,21	C11H11FO2
Z2418615685	NC(=O)CN1C=C(N)C=CC1=O	167,17	C7H9N3O2
Z2418193688	O=C1NC=NC2=C1COCC2	152,15	C7H8N2O2

Z2418193668	CC1=CC2=C(C=C1)N=NNC2=O	161,16	C8H7N3O
Z1263811695	CC1COCCN1CCN	144,22	C7H16N2O
Z1359429532	NCC(N1C=CC=N1)C1=CC=C(Cl)C=C1	221,69	C11H12ClN3
Z1263811762	NCC1=C(F)C=CC(F)=C1	143,14	C7H7F2N
Z1267882038	NCC1=CC(OC2CCOCC2)=NC=C1	208,26	C11H16N2O2
Z1245664663	COCC1=CC(=CC=C1)C#N	147,18	C9H9NO
Z360056084	C[C@H](O)C1=CC2=C(CCC2)C=C1	162,23	C11H14O
Z1263529837	CC(N)C1=CC(C)=C(F)C(C)=C1	167,23	C10H14FN
Z1350618224	CN(C)C1CCCC(N)C1	142,25	C8H18N2
Z1416200823	CNC1CCC(CO)CC1	143,23	C8H17NO
Z1318268746	NCCC1=C(F)C=CC(F)=C1	157,16	C8H9F2N
Z235338177	OC(=O)CC1=CN(N=C1)C1=CC=CC=C1	202,21	C11H10N2O2
Z56899122	NC(CC(O)=O)C1=CC=C(Cl)C=C1	199,63	C9H10ClNO2
Z56895681	OC(=O)CN1C=NC2=C(C=CC=C2)C1=O	204,19	C10H8N2O3
Z212045094	CS(=O)(=O)NC1CCNCC1	178,25	C6H14N2O2S
Z104343432	CC1=C(Cl)C=CC(C(O)=O)=C1N	185,61	C8H8ClNO2
Z235362573	NC1=CC=C(C=C1)C1=CN2CCCC2=N1	199,26	C12H13N3
Z235362259	N#CC1=CC=C(C(N2C=NC=N2)C=C1	184,20	C10H8N4
Z235362689	CC1=C(C=CO1)C1=NN=C(N)O1	165,15	C7H7N3O2
Z1250080886	CC1=NN(C(C)=C1)C1=NC=C(N)C=C1	188,23	C10H12N4
Z1222331415	OC(=O)C1=CC2=C(OCO2)C(Br)=C1	259,06	C9H7BrO4
Z2255112549	OC1C(=O)NCC11CCOCC1	171,20	C8H13NO3
Z2216303314	CC1=C(CCO)N=CC=N1	138,17	C7H10N2O
Z1416200822	FC1=C2NCCOC2=CC=C1	153,16	C8H8FNO
Z1269702389	CC1CC(N)CN1C1=CC=CC=C1	176,26	C11H16N2
Z1346370640	CC(C)C1=NC(=NO1)C1CCCN1	181,24	C9H15N3O
Z1357827251	NC1CCN(C1)C1=CC(Cl)=CC=C1	196,68	C10H13ClN2
Z1626920982	CN1CCC(C)(CO)CC1	143,23	C8H17NO
Z1262252914	CC1=C(SC=C1)C1=NNC(N)=C1	179,24	C8H9N3S
Z183726212	CC1CCCCN1C(=O)C1CCC=CC1	207,32	C13H21NO
Z1259339735	CN(C)CC1=NC(=NO1)C1(N)CCCC1	210,28	C10H18N4O
Z1492980784	CC(C)N1C=NN=C1C1=C(Cl)C=CC=C1	221,69	C11H12ClN3
Z2240999284	FC(F)(F)C1=CC=C(N1)C#N	160,10	C6H3F3N2
Z2240999254	CC(CO)N1C(C)=NC2=C1C=CC(N)=C2	205,26	C11H15N3O
Z2238897966	CN1CCN(CC1)C1=CC=C(S1)C(O)=O	226,29	C10H14N2O2S
Z1255452173	COC1=C2C=CC(N)=CC2=CC=N1	174,20	C10H10N2O
Z2238508600	O=C1NCC2=C1N=CC=C2	134,14	C7H6N2O
Z2236664125	CC1(CCC=CC1)C(O)=O	140,18	C8H12O2
Z1269232519	CC1=CC(Br)=C(CC(O)=O)C=C1	229,07	C9H9BrO2
Z1416201130	C[C@H](N)1CNCC(O1)C(N)=O	144,17	C6H12N2O2
Z1333717732	OC(=O)C1CC11CCCC1	140,18	C8H12O2
Z1077667680	CN1C=C(NCC2=CC=CC(C)=C2)C=N1	201,27	C12H15N3
Z823455846	FC1=C(CNC2CCOCC2)C=CC=C1	209,26	C12H16FNO
Z1142870735	O=S1(=O)CCC(C1)N1CCCNCC1	218,32	C9H18N2O2S
Z2255112034		165,19	C9H11NO2
Z2255110079	CC(C1CCC(=O)N1)C(O)=O	157,17	C7H11NO3
Z1993523194	NC1CCCC11CCOCC1	155,24	C9H17NO
Z1250089980	NC1=NC(CO)=C(Cl)C=C1	158,59	C6H7ClN2O
Z1245646686	CC1=C(C)C(=O)C2=C(N1)C(F)=CC=C2F	209,20	C11H9F2NO
Z1992316287	CCNC1=C(C)C=CC=N1	136,20	C8H12N2
Z1925961476	CC(C)C1CC(O)C2=C1C=CC=C2	176,26	C12H16O
Z1255634499	CC1CCC(CC1)N(C)S(=O)(=O)C1CC1	231,35	C11H21N2O2S
Z1820007572	CCC1=C(N)C=NN1CC(C)C	167,26	C9H17N3
Z927402744	NC1(CCCCC1)C(=O)NCC=C	182,27	C10H18N2O
Z1601554890	CCS(=O)(=O)C1=CC=C(CN)C=C1	199,27	C9H13NO2S
Z1796855094	CC1CCCN1S(=O)(=O)NC1(C)CCC1	232,34	C10H20N2O2S
Z1618272617	C1CN(CC=C1)C1=C2NC=NC2=NC=N1	201,23	C10H11N5
Z1649893125	CCC1CC(CC(=O)N1)C(O)=O	171,20	C8H13NO3
Z1649677765	N#CC1=C(N=CC=C1)C1CC1	144,18	C9H8N2
Z1708089989	CC(C)S(=O)(=O)C1=CC(=CC=C1)C(O)=O	228,26	C10H12O4S
Z1704732763	CN(C)C1=NC=C(O1)C(O)=O	156,14	C6H8N2O3
Z1704732444	COC1=C(C=NC=C1)C#N	134,14	C7H6N2O
Z85923433	CC1=NC2=C(C(=O)NN2)C(C)=C1	163,18	C8H9N3O
Z1696861466	CN1C=C(C=N1)C1NC(=O)CCC1N	194,24	C9H14N4O
Z1696844698	CC1=NN2C(N=C(C)C=C2C(O)=O)=C1Cl	225,63	C9H8ClN3O2
Z1998636703	NC1=CC(OCO2=CC=CC=C2)=NC=C1	200,24	C12H12N2O
Z1998636256	CCC(O)(C(O)=O)C1=CC(Cl)=CC=C1	214,65	C10H11ClO3

Z1993522714	CC1(CCCO1)C1=NOC(N)=C1	168,20	C8H12N2O2
Z2028214403	CN(CC(N)=O)C(=O)C1=CC(N)=CC=C1	207,23	C10H13N3O2
Z2010051560	COC1(CCOCC1)C(O)=O	160,17	C7H12O4
Z2009848113	CCC1=C(C=NO1)C(O)=O	141,13	C6H7NO3
Z1626921298	NC1=NN=C2CCCCN12	138,17	C6H10N4
Z1622825203	CN1C=NC2=C1N=CC(=C2)C(O)=O	177,16	C8H7N3O2
Z1582262995	OCCOC1CCNCC1	145,20	C7H15NO2
Z458890528	NC(=O)C1CCC(=O)NC1	142,16	C6H10N2O2
Z1575304399	CC1=CC2=C(NC=C2)C(=O)N1	148,17	C8H8N2O
Z1420098164	NC(=O)C1CCN(C1)C(=O)C1=CCCC1	208,26	C11H16N2O2
Z402607752	O=C(CN1CCCN1=O)N1CCCC1	211,27	C10H17N3O2
Z1230587767	CCN1CCCN(C1)C(=O)NCC=C	211,31	C11H21N3O
Z253340200	CCN1N=CC=C1NC(=O)C1CCCC1	207,28	C11H17N3O
Z254451326	O=C(C1CC1)N1CCCC2=C1C=CC=N2	202,26	C12H14N2O
Z364579532	CC1COCCN1C(=O)C1=NC=CN=C1	207,23	C10H13N3O2
Z1313483439	CC1=CC=C(C=C1)C1=NC(CN)=CO1	188,23	C11H12N2O
Z1164527757	CN1C=C(NCC2=CC=CS2)C=N1	193,27	C9H11N3S
Z1267882019	NCCC1=CC2=C(OCC2)C=C1	163,22	C10H13NO
Z1267882022	CC(C)C1=NOC(CN)=C1	140,19	C7H12N2O
Z2510258284	CC1COC2=C(C=CC=C12)C(O)=O	178,19	C10H10O3
Z1685775949	CCC1(CC)CCNC1=O	141,21	C8H15NO
Z1675167167	CN(C)C1=CN=C(C=C1)C(O)=O	166,18	C8H10N2O2
Z1675167132	CC1=C(C(O)=O)C(N)=CC(Cl)=C1	185,61	C8H8ClNO2
Z2235810234	OC(=O)CC1=C(N=CS1)C1=CC=CC=C1	219,26	C11H9NO2S
Z2235810230	CN1C=NC2=C1C(CC(=O)N2)C(O)=O	195,18	C8H9N3O3
Z2235790652	COC1=CC(=CC=C1)N1C=C(N)N=N1	190,21	C9H10N4O
Z2235386876	COC1=C(C=CC=C1)C1=NN=C(N)S1	207,25	C9H9N3OS
Z2230911478	OCC1CCNC(=O)CC1	143,19	C7H13NO2
Z2230911328	CC1CC2=C(C(C1)N)CN2	150,23	C9H14N2
Z2218556094	CCN1CC(O)CNC1=O	144,17	C6H12N2O2
Z2217033031	OC(=O)C1=CC(F)=C(OC(F)F)C=C1	206,12	C8H5F3O3
Z2106594212	OC(=O)C1=NN(C=C1Br)C1CCCC1	259,10	C9H11BrN2O2
Z2216711597	OC(=O)C1=C(OC=N1)C1CC1	153,14	C7H7NO3
Z2216711606	CCN1N=CC(=N1)C(O)=O	141,13	C5H7N3O2
Z2216711604	CC1=CC2=C(C=C1)N=C(C=C2)C(O)=O	187,20	C11H9NO2
Z57352018	OC(=O)C1=CC(=CC=C1)N1CCCC1	191,23	C11H13NO2
Z2568757981	CN1C=C(N=N1)C(C)C(O)	141,17	C6H11N3O
Z2568751883		191,27	C12H17NO
Z2568751838	COC1=C(OC)C=C2C(=O)NC=CC2=C1	205,21	C11H11NO3
Z2523459919	COCC1=NC(N)=CC=N1	139,16	C6H9N3O
Z2521982363	CC1=CC(C(O)=O)=C(C)N1C1=NOC=C1	206,20	C10H10N2O3
Z1741972881	CC1=CC(F)=CC(C)=C1C(O)=O	168,17	C9H9FO2
Z2513335975	CC(CC(O)=O)N1CCCC1=O	171,20	C8H13NO3
Z2512942961	O=C1NCCCC1CCCCC1	167,25	C10H17NO
Z1255450742	OC(=O)C1CCN1C1CCCC1	169,22	C9H15NO2
Z733898624	CC(C)NC(=O)C1=CC(C)=NN1C	181,24	C9H15N3O
Z104378222	CC1=NC2=C(C(N)=C(S2)C(N)=O)C(C)=C1	221,28	C10H11N3OS
Z94599194	OC(=O)CC1=CSC(=N1)C1=CN=CC=C1	220,25	C10H8N2O2S
Z96091883	OCC1=CC=C(C=C1)N1C=CC=N1	174,20	C10H10N2O
Z208331700	CC1=C(F)C=C(C=C1)C(O)=O	154,14	C8H7FO2
Z234898195	NC(=O)N1CCCNCC1	143,19	C6H13N3O
Z33546529	CN(C)S(=O)(=O)C1=CC(=CC=C1)C(N)=O	228,27	C9H12N2O3S
Z30271161	CNC(=O)COC1=C(C)C=C(Cl)C=C1C	227,69	C11H14ClNO2
Z53834531	COC1=CC=C(C=C1)C#N	133,15	C8H7NO
Z46191128	CNCC(=O)NC1=CC=C(C)C=C1	178,24	C10H14N2O
Z56881200	OC(=O)CNC(=O)C1=CC(F)=CC=C1	197,17	C9H8FNO3
Z56839661	OC(=O)C1=CC2=C(OCCO2)C=C1	180,16	C9H8O4
Z56756098	[NH4+].COC1=C(Cl)C=CC(=C1)C([O-])=O	203,62	C8H10ClNO3
Z56762560	CC1(O)C2CC3CC(C2)CC1C3	166,26	C11H18O
Z414477942	CN(C)S(=O)(=O)NC1CCCN1=O	235,30	C8H17N3O3S
Z1403325251	CNC1=C(C=CC(Cl)=C1)C(=O)N(C)C	212,68	C10H13ClN2O
Z1407672962	OC(=O)C1CCCC2=C1C=NN2	166,18	C8H10N2O2
Z1407007551	C1CNC2=C(NC1)C=NC=C2	149,20	C8H11N3
Z975826158	NC1=NC(CN=C1)N1CCCC1	164,21	C8H12N4
Z1405445662	CC1=NNC(CC(O)=O)=C1	140,14	C6H8N2O2
Z1374778829	CC1CCN(C1)C1=NC=CC(=C1)C(O)=O	206,25	C11H14N2O2
Z1365534328	CCN1N=NC(C(O)=O)=C1C(F)(F)F	209,13	C6H6F3N3O2

Z411697334	CCN1C=C(NC(=O)N2CCCC2)C=N1	208,27	C10H16N4O
Z162834430	CNC(C)C1=CC2=C(O1)C=CC=C2	175,23	C11H13NO
Z1222285094	COC1=C(C=CC=C1)N1CCC(CN)C1	206,29	C12H18N2O
Z1238477897	COCC1=C(C=CC=C1)C#N	147,18	C9H9NO
Z1250132474	CC(CC1=C(F)C=CC=C1)C(O)=O	182,19	C10H11FO2
Z993967038	CC(C)NC1CCNCC1	142,25	C8H18N2
Z90530641	CC1CCCC1NCC1=NC=CC=C1	204,32	C13H20N2
Z1171716843	CN(C)C1CCCCC1N	142,25	C8H18N2
Z2143644460	C1CC(CN1)C1=CC=CO1	137,18	C8H11NO
Z1918541965	CCC1(O)CN(C1)C1=C(Cl)C=NC=N1	213,67	C9H12ClN3O
Z1878647755	CC1CC(C)(C)CC1NCC1=NC=CS1	224,37	C12H20N2S
Z90503761	CC1=C(CNC2CCCCC2)C(C)=NO1	208,31	C12H20N2O
Z1815903106	CC1=C(Br)C(CNC2CCOC2)=CC=C1	270,17	C12H16BrNO
Z1415893880	COCC1=NC2=C(O1)C=CC(N)=C2	192,22	C10H12N2O2
Z1918541761	CCC1(O)CN(C1)C1=NC(=CC=C1)C#N	203,25	C11H13N3O
Z1263811691	CC(C)(N)C1=CC=C(F)C=C1	153,20	C9H12FN
Z1817978303	CC(=O)N1CCCC2(CCCCC2)CC1	209,33	C13H23NO
Z599664892	BrC1=CN(CC(=O)N2CCCC2)N=C1	272,15	C10H14BrN3O
Z1127236484	C(NC1=CN=CC=C1)C1=CSN=N1	192,24	C8H8N4S
Z984691402	CC(=O)NC1=CC(=NN1)C1=C(C)C=CS1	221,28	C10H11N3OS
Z30847309	FC1=C(F)C=C(NC(=O)C2CCC2)C=C1	211,21	C11H11F2NO
Z20272492	CNC(=O)C(C)OC1=CC=C(Cl)C=C1	213,66	C10H12ClNO2
Z409533506	BrC1=C(C(NC(=O)N2CCCC2)C=CC=C1	269,14	C11H13BrN2O
Z1024440952	C1CC1NC1=NC(=NO1)C1=CC=CC=C1	201,23	C11H11N3O
Z239173696	CNC(=O)C1=CC2=C(N=C1)N(C)N=C2C	204,23	C10H12N4O
Z1126744743	CC1=NN(C(N)=C1)S(=O)(=O)C1=CC=CS1	243,30	C8H9N3O2S2
Z33546775	NC(=O)CC1=CC(=CC=C1)C(F)(F)F	203,16	C9H8F3NO
Z994937532	CC1=CC(NC(=O)N2CCC2)=NO1	181,20	C8H11N3O2
Z1318516263	CC1=CC=C(O1)C1CS(=O)(=O)CCN1	215,27	C9H13NO3S
Z1318515156	CNC(C)C1=CC=C(C=C1)S(C)=O	197,30	C10H15NOS
Z991556972	OC(=O)C1CCCN2C=CN=C12	166,18	C8H10N2O2
Z1318147519	CNC(C(O)=O)C1=C(F)C=C(F)C=C1	201,17	C9H9F2NO2
Z1318147455	CC1=NC(C(O)=O)=C2CCCCN12	180,21	C9H12N2O2
Z1318147452	CC1=C(C(O)=O)C(C)=CC(=O)N1	167,16	C8H9NO3
Z29693728	O=C(NCC1=CC=CS1)C1=CC=CO1	207,25	C10H9NO2S
Z1295543903	CC1=CC2=C(C=C1)C(CCC(O)=O)=CN2	203,24	C12H13NO2
Z208333304	O=C(N1CCCCC1)N1CCOCC1	198,27	C10H18N2O2
Z177087780	CN1CCN(CC1)C(=O)N1CCOCC1	213,28	C10H19N3O2
Z1274167323	CC(C(C)C(O)=O)N1N=C(C)C=C1C	196,25	C10H16N2O2
Z1984960549	COC(C)(C)C(=O)NC1=CC(F)=CN=C1	212,22	C10H13FN2O2
Z2219509018	CC1CN(CC2=CC(=CC=C2)C#N)C1C	200,29	C13H16N2
Z1258578173	COC1=C(C)C=CC(CCN)=C1	165,24	C10H15NO
Z279819030	CN(CC1=CC=NC=C1)C1=NC=CN=C1	200,25	C11H12N4
Z1415893978	C(NC1CCCN1)C1=CC=CC=C1	190,29	C12H18N2
Z1416282822	COCC1=NN2CCCC(N)C2=N1	182,23	C8H14N4O
Z2034464797	CN(CC1CCCO1)C1=NC=C(F)C=C1	210,25	C11H15FN2O
Z1166114668	C1CCC(C1)NC1CCNCC1	168,28	C10H20N2
Z32014663	CN(C)C(=O)C1=C(C)C(C)=CC=C1	177,25	C11H15NO
Z2177153690	OCC1=CC(F)=C(OC(F)F)C=C1	192,14	C8H7F3O2
Z1838500084	CC1OCCCC1C(=O)NC1=CCN=C1	209,25	C10H15N3O2
Z1267773819	OCCNC1CCC2=C1C=CC=C2	177,25	C11H15NO
Z1791178849	O=C(CC1=CCCCC1)NC1=CN=NS1	223,29	C10H13N3OS
Z2065788086	COC1=C2N=CNC2=CC(Br)=C1	227,06	C8H7BrN2O
Z2065788380	CCC1=NC(C(O)=O)=C(C)O1	155,15	C7H9NO3
Z1260623529	FC1=CC(F)=C(C(=O)NC2CC2)C(F)=C1	215,18	C10H8F3NO
Z2039477470	BrC1=C2C(=O)NCC2=CC=C1	212,05	C8H6BrNO
Z2033454315	COC1=C(C=C(Cl)C=C1N)C(N)=O	200,62	C8H9ClN2O2
Z1270640437	O=C1CC2(CN1)CCCN2	154,21	C8H14N2O
Z1270210792	NC1=NN=C(CC2CC2)O1	139,16	C6H9N3O
Z1270210778	NC(=O)CCN1C=CC(N)=N1	154,17	C6H10N4O
Z57173821	CC(NC(=O)C1=C(Cl)C=CC=C1)C(O)=O	227,64	C10H10ClNO3
Z1269638510	NC1=NNC(=C1)C1CCOCC1	167,21	C8H13N3O
Z1269638437	NC1=NN(CC(=O)N2CCOCC2)C=C1	210,24	C9H14N4O2
Z1268152423	CC(C)NC(=O)C1CCCC(N)C1	184,28	C10H20N2O
Z666291262	CC1=CN2C=CC=NC2=N1	133,15	C7H7N3
Z1262254283	NCC1=CN=C(C=C1)N1CCCC1	177,25	C10H15N3
Z1262250860	NC1=NN(CC2=CN=CC=C2)C=N1	175,20	C8H9N5

Z1262246150	COC1=C(C=CC=C1)C1=NNC(N)=C1	189,22	C10H11N3O
Z1262246109	OCC1=CN=C(O1)C1=CC=CO1	165,15	C8H7NO3
Z2658864411	CC1=CN2C=CN=C2C(=C1)C(O)=O	176,18	C9H8N2O2
Z2658864334	CC1(C)C(=O)NC2=C1C=C(CO)C=C2	191,23	C11H13NO2
Z2630874436	OC(=O)CC1CCCS1(=O)=O	178,20	C6H10O4S
Z2588063790	OC(=O)C1=CC(=CNC1=O)C(F)(F)F	207,11	C7H4F3NO3
Z680888866	CC1=NOC2=C1C=C(Br)C=N2	213,03	C7H5BrN2O
Z2574917679	CN1C(=O)SC2=CC(N)=C(C)C=C12	194,25	C9H10N2OS
Z2522871853	OC(=O)CN1C=C(C=N1)C1CC1	166,18	C8H10N2O2
Z275169912	CCN1C=C(C(O)=O)C(C)=N1	154,17	C7H10N2O2
Z1741969315	CN1C=CC2=C1C=CC(=C2)C(O)=O	175,19	C10H9NO2
Z1741967210	COC1=CC(C(O)=O)=C(Cl)C=C1	186,59	C8H7ClO3
Z275169940	CN1C=C(Cl)C(=N1)C(O)=O	160,56	C5H5ClN2O2
Z2510259389	OC(=O)C(C1CC1)C1=CC=C(Cl)C=C1	210,66	C11H11ClO2
Z2301685460		157,17	C7H11NO3
Z2510258318	OC(=O)C1=C2NCCN2N=C1	153,14	C6H7N3O2
Z1891772637	CC1(CNC(=O)C1)C(O)=O	143,14	C6H9NO3
Z2510258100	NC1=NC=CC(C(O)=O)=C1	152,15	C7H8N2O2
Z1741959630	NC1=NC=CC(=C1)C(F)(F)F	162,12	C6H5F3N2
Z1255375308	OC(=O)C1=NN2CCOCC2=C1	168,15	C7H8N2O3
Z2380439330	CN1N=C(C=C1C)C(O)C1=CSC(C)=C1	222,31	C11H14N2OS
Z274502046	OC(=O)C1CCC(C1)C(O)=O	158,15	C7H10O4
Z2379802697	CS(=O)(=O)C1=CC=C(CO)S1	192,25	C6H8O3S2
Z2379087743	CC1=NN(C(C)=C1)C1=CN=C(C=C1)C#N	198,23	C11H10N4
Z2379087665	COC1=CC2=NC=C(N2C=C1)C(O)=O	192,17	C9H8N2O3
Z2379087811	COC1=C(Br)C=C2C(=O)NC=NC2=C1	255,07	C9H7BrN2O2
Z2372279536	CC1=C2C(O)C(=O)NC2=CC=C1	163,18	C9H9NO2
Z2327883947	CC1=CC(=O)NC(=N1)C1=CC=CS1	192,24	C9H8N2OS
Z2327883709	CN1C=CC(CCC(O)=O)=C1	153,18	C8H11NO2
Z1263529650	CNS(=O)(=O)C1=CC(=CC=C1)C(C)N	214,28	C9H14N2O2S
Z1263529614	NC1CCN(CC1)C1=NC=C(C=C1)C#N	202,26	C11H14N4
Z1080986230	CCC1=NON=C1NC(=O)C1=CC=CS1	223,25	C9H9N3O2S
Z1134990241	CC1=NC(CN2C=CC(C)=CC2=O)=CS1	220,29	C11H12N2OS
Z2679906873	CC1=CC(=NN1C1CCOCC1)C(O)=O	210,23	C10H14N2O3
Z2658864472	OCC1=CN=NN1C1=C(Cl)C=CC=C1	209,63	C9H8ClN3O
Z90526999	CC(O)CNC1CCCCC1	157,26	C9H19NO
Z1262327442	CC1=CSC(=N1)C1=CC(N)=CC=C1	190,26	C10H10N2S
Z1889909940	NC1CCN(C1)C1=CC(Br)=CC=C1	241,13	C10H13BrN2
Z1889909876	CC(N1CCNCC1)C1=NC(C)=CS1	211,33	C10H17N3S
Z1889709955	NC1=CN=C(OC2CCCC2)C=C1	178,24	C10H14N2O
Z1881620500	OCC1CC2=C(C1)C=CC=C2	148,21	C10H12O
Z1869852043	NCC1CCCCN1C1CC1	154,26	C9H18N2
Z1860991704	NCCC(O)C1=CC(Cl)=C(Cl)C=C1	220,09	C9H11Cl2NO
Z1860991707	COC1(CO)CCOCC1	146,19	C7H14O3
Z1849039889	CCC1=C(CC)C(N)=CC=C1	149,24	C10H15N
Z1839486549	CCC1=C(N)C=NN1C1=C(C)C=CC=C1	201,27	C12H15N3
Z1836338703	COC1=C(CN)C(Cl)=CC=C1	171,62	C8H10ClNO
Z1827898537	C(NC1CCNC1)C1=CC=CC=C1	176,26	C11H16N2
Z1258578979	CC(CC1=CC=CS1)C(O)=O	170,23	C8H10O2S
Z1720603241	CCS(=O)(=O)C1=C(C)OC=C1	174,21	C7H10O3S
Z296139642	CN(C)C(=O)C1=CSC(=N1)C1=CC=CO1	222,26	C10H10N2O2S
Z2238508578	OC(=O)C1(CC2=CC(Cl)=CC=C2)CC1	210,66	C11H11ClO2
Z2327131593	CN1N=CC=C1C1=CC(N)=C(C)C=C1	187,25	C11H13N3
Z2469657408	CN1C=C(C=N1)C1=CNC=C1	147,18	C8H9N3
Z2160887425	CC1=CC=C(C=C1)C1=NNC(=O)C=C1C	200,24	C12H12N2O
Z1020680398	CC1=CC(=CC(C)=C1)C(O)CN	165,24	C10H15NO
Z1874937351	CN1N=CC=C1CC(O)=O	140,14	C6H8N2O2
Z1837073433	COC1=C2N=CC(C)=C(N)C2=CC=C1	188,23	C11H12N2O
Z1137725943	CCNCC1=C2C=CNC2=CC=C1	174,25	C11H14N2
Z1795818230	CN1CC(=O)NC2=C1C=CC(Br)=C2	241,09	C9H9BrN2O
Z1762997349	CN1C=C(C=N1)C1=NN(C)C=C1C(O)=O	206,21	C9H10N4O2
Z1737940727	CN1C=C(C=N1)C1=CNC=C1C(O)=O	191,19	C9H9N3O2
Z2206895891	CC1=NC=NC(CN2CCC=C(F)C2)=C1	207,25	C11H14FN3
Z2234186172	C1CC(CN1)C1=NC2=C(O1)C=CC=C2	188,23	C11H12N2O
Z940781212	BrC1=C(CNC2=NC=CN=C2)SC=C1	270,15	C9H8BrN3S
Z56120255	CNS(=O)(=O)C1=CC2=C(NC(=O)N2)C=C1	227,24	C8H9N3O3S
Z1483950793	NCC1CN2CCN1CC2	141,22	C7H15N3

Z1266854884	NCC1(O)CCCC2=C1C=CC=C2	177,25	C11H15NO
Z2471986955	CC1OC2(CC1=C)CCNCC2	167,25	C10H17NO
Z1549154938	CC#CCNC1=NC2=C(C=C1)N=CC=N2	198,23	C11H10N4
Z1520646254	OC(=O)C1CCC2=C(C1)C=NN2	166,18	C8H10N2O2
Z1561856325	C=CCOC1=CC2=C(NC=C2)C=C1	173,22	C11H11NO
Z1259339741	CC(C)CC1=NNC(N)=C1	139,20	C7H13N3
Z1460224226	FC1=C(CI)C=CC(NC2CCNC2=O)=C1	228,65	C10H10ClFN2O
Z1480642716	N#CC1=CC2=C(OCC2)C=C1	145,16	C9H7NO
Z1465461251	CNS(=O)(=O)C1=C(C)C(N)=CC=C1	200,26	C8H12N2O2S
Z1454649804	CC1=C(C=CC=C1N)C1=NN=CO1	175,19	C9H9N3O
Z1436473077	CN(C)C1=NN=C(O1)C1=CC=C(N)C=C1	204,23	C10H12N4O
Z99598966	COC1=CC(OC)=C(C=C1)C1CCCN1	207,27	C12H17NO2
Z1168422782	C1CC1C1=CSC(=N1)C1=NC=CN=C1	203,26	C10H9N3S
Z1267773594	CCOC1=C(C)C=C(CN)C=C1	165,24	C10H15NO
Z90515731	CC1=C(CNC2CCCC2)C(C)=NO1	194,28	C11H18N2O
Z1245735294	CN(C)C1=C(CO)C=CC=C1	151,21	C9H13NO
Z2199779515	CC1=NSC(=N1)N1CCC(CC1)C1CC1	223,34	C11H17N3S
Z1333173543	CC1=NC(N[C@H]2C[C@H](CO)C=C2)=NC=C1	205,26	C11H15N3O
Z1957730368	CC1CN(CCCO1)C1=C(C)C=NC=C1	206,29	C12H18N2O
Z1266823301	CC(N)C(C)N1C=NC=N1	140,19	C6H12N4
Z32968167	CC1CCCCN1C(=O)C1=CC=CO1	193,25	C11H15NO2
Z1268152349		205,31	C12H19N3
Z1262396021	CC1=CSC(=N1)C1(N)CCC1	168,26	C8H12N2S
Z1272494722	CC1=NSC(NC2CCCC2CO)=N1	213,30	C9H15N3OS
Z1925930296	NC1=CC2=C(CC(O)C2)C=C1	149,19	C9H11NO
Z133716556	CS(=O)(=O)NC1CCOC2=C1C=CC=C2	227,28	C10H13NO3S
Z1699554564	CN1N=C(C)N=C1NCC1=CC(Br)=CS1	287,18	C9H11BrN4S
Z1729206226	CC(C)C1=CC=C(CN2C=CN=N2)C=C1	201,27	C12H15N3
Z85878070	OC(=O)C1=CC(NC(=O)C2CC2)=CC=C1	205,21	C11H11NO3
Z600428392	CC1=NOC(=N1)C1=CC(N)=C(C)C=C1	189,22	C10H11N3O
Z317476482	CC(C)NC(=O)C1=CC(=CC=C1)C(N)=O	206,25	C11H14N2O2
Z373775660	CN1C=C(NC(=O)C2=NC=CN=C2)C=N1	203,21	C9H9N5O
Z373775574	CN1C=C(NC(=O)C2=CC=CS2)C=N1	207,25	C9H9N3OS
Z219186376	O=C1CN(CCN1)C1=NC=C(C=C1)C#N	202,22	C10H10N4O
Z136725178	CC1=NOC(=C1)C(=O)NC1=NC=CC=C1	203,20	C10H9N3O2
Z167942650	COCCN1N=C(C)C(C)=C(C#N)C1=O	207,23	C10H13N3O2
Z1259341087	N[C@H]1[C@@H](O)CC2=C1C=CC=C2	149,19	C9H11NO
Z1259273299	OC(=O)CC1CCC2=C1C=CC=C2	190,24	C12H14O2
Z1238477764	NC1=CC2=C(OC(=N2)C2CC2)C=C1	174,20	C10H10N2O
Z1030080890	CC1=CC(=CC=C1)C1(CCCC1)C(N)=O	203,29	C13H17NO
Z1127124401	O[C@H]1CCN(C1)C1=NC2=C(O1)C=CC=C2	204,23	C11H12N2O2
Z728939692	CN(C)C1=NC2=C(C=CC=C2)N=C1	173,22	C10H11N3
Z1171978873	CC1=CC2=C(NN=C2)C(=C1)C(O)=O	176,18	C9H8N2O2
Z1162470564	CCC1CCC2=C(C1)C=C(C#N)C(=O)N2	202,26	C12H14N2O
Z68248958	CNC(=O)C1=CC2=C(CCCC2)S1	195,28	C10H13NOS
Z955526728	CNC(=O)C1CC1C1=CC(Br)=CC=C1	254,13	C11H12BrNO
Z54747399	CN(C)C(=O)CN1CCC(CC1)C(N)=O	213,28	C10H19N3O2
Z425387838	CC1=CC=C(C=C1)C1=CSC(CN)=N1	204,29	C11H12N2S
Z234895123	CNC(=O)C1CCCCN1	142,20	C7H14N2O
Z2678251704	CC(CC1=C(C)C=CC=C1)C(O)=O	178,23	C11H14O2
Z2678251689	CC(C)COC1=CN=CC=C1	151,21	C9H13NO
Z1373430305	FC1=C(NCC2CCOCC2)N=CC=C1	210,25	C11H15FN2O
Z1601231985	FC1=C(F)C=C(NCC2=NNC=C2)C=C1	209,20	C10H9F2N3
Z1373427763	CC1=NOC(NC2=C(F)C=CC=N2)=C1	207,21	C10H10FN3O
Z1973746834	CC1=CCCN(C1)C1=NC(C)=CC(C)=N1	203,29	C12H17N3
Z1573518667	CC1=C(NCC2=CSN=N2)C=CC=C1F	223,27	C10H10FN3S
Z1613960888	CC(=O)NCC1=CC=NO1	140,14	C6H8N2O2
Z2216303543	OC(=O)C1CCC(C1)C1=CC=CC=C1	190,24	C12H14O2
Z2197159967	NC1=C(OCC2CCOCC2)C=CC(Br)=C1	272,14	C11H14BrNO2
Z1407004013	CC(N)C1=CC(F)=C(C)C=C1	153,20	C9H12FN
Z2584255713	COC1=C(C=CC=C1)C1=NOC(Cl)=C1	209,63	C10H8ClNO2
Z2442592378	CCC1=NOC(CC2CCNCC2)=N1	195,27	C10H17N3O
Z1889975637	CC1(C)CCC(O1)C(O)=O	144,17	C7H12O3
Z2216523547		209,22	C11H12FNO2
Z2216303101	CN1C=NN(CCC(O)=O)C1=O	171,16	C6H9N3O3
Z2216302968	NC1=CC=C(C=C1)C1CCOC1	163,22	C10H13NO
Z2213893377	CN(C)C1=CC=C(C=C1)C1(CC1)C(O)=O	205,26	C12H15NO2

Z31725206	OCCNC(=O)C1=CC=C(Cl)C=C1	199,63	C9H10ClNO2
Z94832620	NC(=O)CNC1=C2C=CSC2=NC=N1	208,24	C8H8N4O5
Z1891776008	CN1CC(CN)CC2=C1C=CC=C2	176,26	C11H16N2
Z2182155697		176,22	C11H12O2
Z2177031159	NC1=NC=C2CCCCC2=C1	148,21	C9H12N2
Z359419600	CN1N=C(C)C2=C1N=C(C)C(=C2)C(O)=O	205,22	C10H11N3O2
Z281802052	CN(C)C1=NC=C(C=C1)C#N	147,18	C8H9N3
Z327224228	CN(C)C1=C(C=C2CCCCC2=N1)C#N	201,27	C12H15N3
Z30281273	CCNC(=O)C1=CC(Br)=CN=C1	229,08	C8H9BrN2O
Z85886818	CC1CC1C(=O)NCC(O)=O	157,17	C7H11NO3
Z57728694	CC1=CC2=C(OC(=O)N2CC(O)=O)C=C1	207,19	C10H9NO4
Z188924172	OC(=O)CCC1=CC2=C(OCOC2)C=C1	208,21	C11H12O4
Z256708392	COC1=C(OC)C(=CC=C1)C(O)=O	182,18	C9H10O4
Z1203890368	OC1CCCCC1NCC1=CC=C(Cl)S1	245,77	C11H16ClNOS
Z416879296	OCC1CCN(CC2=CC=C(Cl)S2)CC1	245,77	C11H16ClNOS
Z1555979444	CC(C)=C(F)C1=NC(=NO1)C1CCOC1	212,22	C10H13FN2O2
Z1657807341	CN1C(C)=NN=C1NC(=O)C1CCCC1	208,27	C10H16N4O
Z1354416046	CCC1=NOC(=N1)C1=CC(N)=C(C)C=C1	203,25	C11H13N3O
Z1347206048	CNS(=O)(=O)C1=C(OC)C=C(C)C(C)=C1	229,29	C10H15NO3S
Z1347206039	CNS(=O)(=O)C1=CC(C)=C(Cl)C=C1	219,68	C8H10ClNO2S
Z905065926	CC(C)N1C2CCC1CC(C2)C(O)=O	197,28	C11H19NO2
Z1335657824	CC(C)C(O)C(O)=O)C1=CC=CC=C1	194,23	C11H14O3
Z1335657800	COC1=C(OC)C=C(Cl)C=C1	172,61	C8H9ClO2
Z1333043358	COC1=C(N)N=C(C)C=C1	138,17	C7H10N2O
Z1324054916	CN1N=CC2=C1N=CC(=C2)C(O)=O	177,16	C8H7N3O2
Z729603782	OC(=O)C1CN(C(=O)C1)C1=NC=CS1	212,22	C8H8N2O3S
Z857666962	OC(=O)C1=C(Br)C(=NN1)C1CC1	231,05	C7H7BrN2O2
Z1614607167	OC(=O)C1(CC1)C(=O)N1CCCC1	183,21	C9H13NO3
Z1815156923	COC1=C(C=C(Br)C(C)=N1)C(O)=O	246,06	C8H8BrNO3
Z1815155511	COC1=C(C(O)=O)C(N)=C(Br)C=C1	246,06	C8H8BrNO3
Z1815155451	CN1N=CC=C1C(O)C1=CC=CC=C1	188,23	C11H12N2O
Z1815155461	OC(=O)CC1=CC=C(Cl)S1	176,61	C6H5ClO2S
Z1147473989	NC(=O)C1NCCC2=C1C=CC=C2N	191,23	C10H13N3O
Z1741970419	COC1=CN=C(C=C1)C(O)=O	153,14	C7H7NO3
Z1381299162	CN(C(N)=O)C1=CN=CC=C1	151,17	C7H9N3O
Z1067997558	BrC1=CN=C(C=C1)C(=O)N1CCCC1	255,12	C10H11BrN2O
Z90667799	OC(=O)C1=NC=CC(=C1)N1CCCC1	192,22	C10H12N2O2
Z1741962447	CC1=CSC2=C1N=CNC2=O	166,20	C7H6N2OS
Z1787158566	O=C1NCCN1CCN1CCNCC1	198,27	C9H18N4O
Z127111070	COC1=NC(NC2CCCC2)=NC=C1	193,25	C10H15N3O
Z1696946301	CC1OCCC1C(=O)NC1=NC=CN=C1	207,23	C10H13N3O2
Z1778350604	CC1=C(Br)C=C(CC(O)=O)C=C1	229,07	C9H9BrO2
Z409308414	CC1CC1CNC(=O)C1=C(N)N=CC=N1	206,25	C10H14N4O
Z451350338	CN1C=C(C=N1)C1=NC(=CS1)C(O)=O	209,22	C8H7N3O2S
Z332625816	BrC1=CC(=CS1)C(=O)N1CCOCC1	276,15	C9H10BrNO2S
Z57985394	CC1=C(CCC(O)=O)C(C)=NN1	168,20	C8H12N2O2
Z274538288	COC1=CC=C(C=C1)C1=C(N)NN=C1C	203,25	C11H13N3O
Z425389704	CC(C)C1=CC(=NN1)C(O)=O	154,17	C7H10N2O2
Z398513274	CC(C)OC1=NC=C(C=C1)C(O)=O	181,19	C9H11NO3
Z19739447	CNC(=O)COC1=CC=C(C=C1)C#N	190,20	C10H10N2O2
Z405825414	CCC(=O)N1CCCC(C1)NS(C)(=O)=O	234,31	C9H18N2O3S
Z394174378	CC1=CC(=NO1)C(=O)NCC1CCOC1	210,23	C10H14N2O3
Z992716900	CC1=NN2C=C(C(O)=O)C(=O)NC2=C1	193,16	C8H7N3O3
Z226499634	NC(=O)CCN1C=NC2=C(SC=C2)C1=O	223,25	C9H9N3O2S
Z396112684	CN1C=C(NC(=O)C2=CC=C(Br)S2)C=N1	286,15	C9H8BrN3O5
Z216237334	CNC(=O)CN1CCC(CC1)C(=O)NC	213,28	C10H19N3O2
Z1868316890	OC(=O)C1=NN2CCCOC2=C1	168,15	C7H8N2O3
Z2106601577	CC(C)C(N1N=C(C)C=C1)C(O)=O	196,25	C10H16N2O2
Z2418194250	CN1N=C(N=C1CC(O)=O)C1CC1	181,20	C8H11N3O2
Z444349634	CC(N)C1=CC2=C(NC(=O)N2)C=C1	177,21	C9H11N3O
Z2235390200		190,25	C11H14N2O
Z1070938482	C(NC1CCOC2=C1C=CC=C2)C1CC1	203,29	C13H17NO
Z2053696021	C[C@@H]1CN(C[C@H]1C(N)=O)C1=NC=CC=N1	206,25	C10H14N4O
Z1184890099	NC1=NC=C(C=C1)N1CCCCC1	177,25	C10H15N3
Z159528224	CNC(C)C1=C(F)C=CC=C1	153,20	C9H12FN
Z2327131645	OC(=O)C1(O)CCC2=C(C1)C=CC=C2	192,21	C11H12O3
Z1245537943	CCC(=O)NC1=CC=C(C=C1)C(C)N	192,26	C11H16N2O

Z31255646	FC1=CC=C(CNC2=NC=CC=N2)C=C1	203,22	C11H10FN3
Z1262252950	NCC1=CC2=C(CCCCC2)S1	181,30	C10H15NS
Z1407654394	OCC1CC11CCOCC1	142,20	C8H14O2
Z1266823139	NC(=O)C1NCCC2=C1C=CC=C2	176,22	C10H12N2O
Z56791573	CC(C)CC1=NN=C(N)S1	157,24	C6H11N3S
Z2211231470	O=C1NCCN1CC1=CN=CC=C1	177,21	C9H11N3O
Z1713595338	CS(=O)(=O)N1CCC[C@@H]1CN	178,25	C6H14N2O2S
Z1893225335	NCC1=CC=C(C=C1)N1CCNC1=O	191,23	C10H13N3O
Z1269638430	CC(=O)NCC1CNCCO1	158,20	C7H14N2O2
Z32016429	CNC(=O)CNC(=O)C1=CC=CC=C1	192,22	C10H12N2O2
Z104829962	NC(=O)CNC1=C(F)C=C(Cl)C=C1	202,61	C8H8ClFN2O
Z26743795	COC1=C(Cl)C=C(NC(=O)C(C)C)C=C1	227,69	C11H14ClNO2
Z221429956	OC(=O)C1=CC=C(CN2C=NC=N2)C=C1	203,20	C10H9N3O2
Z57070418	CN1C(=O)NC2=C1C=CC=C2	148,17	C8H8N2O
Z212063048	NC1=CC2=C(C=C1)N=C(S2)N1CCCC1	219,31	C11H13N3S
Z217102760	COC1=NC=C(C=C1)C#N	134,14	C7H6N2O
Z30272262	CNC(=O)C1=CC=C(Br)C=C1	214,06	C8H8BrNO
Z32015103	CN(C)C(=O)C1=CC(NC(C)=O)=CC=C1	206,25	C11H14N2O2
Z740994328	O=C(NCC1=CC=CC=C1)C1=CSN=N1	219,26	C10H9N3OS
Z1863617864	NC1CCN(CC1)C1=NN=CC=C1	178,24	C9H14N4
Z111634612	CC(C)C1=CC(=O)N2N=C(C)N=C2N1	192,22	C9H12N4O
Z1860974908	CN1C=CC(=O)C(=C1)C(N)=O	152,15	C7H8N2O2
Z1849011119	COC1=C(N=CC(C)=C1)C(O)=O	167,16	C8H9NO3
Z1889710290	CC1=CSC(CCC(O)=O)=N1	171,21	C7H9NO2S
Z1713446741	CN1C=NN=C1NC(=O)C1=CSC=C1C	222,27	C9H10N4OS
Z1868431117	CC1(CCCOC1)C(O)=O	144,17	C7H12O3
Z1868430495	CC(C)(C(O)=O)C1=CN=C1	154,17	C7H10N2O2
Z1222283865	COC1=C(C)C=CC(=C1)C1(CC1)C(O)=O	206,24	C12H14O3
Z1124405402	O=C(NCC1CC1)N1CCS(=O)(=O)CC1	232,30	C9H16N2O3S
Z997948620	NC(=O)CCC1=CC(Cl)=C(Cl)C=C1	218,08	C9H9Cl2NO
Z1229682715	CC1(COC2=C(C=CC=C2)C#N)COC1	203,24	C12H13NO2
Z238708260	COC1=C(C=C(F)C=C1)C(N)=O	169,16	C8H8FNO2
Z56851231	CC1=NC2=C(C=CC=C2)C(N)=C1	158,20	C10H10N2
Z216238752	CNC(=O)C1CCN(CC(C)=O)CC1	196,29	C11H20N2O
Z1184882872	CN1CCC(O)(CC1)C1=CC=CC=C1	191,27	C12H17NO
Z1722750874	CN(CC1=NC=CS1)C1=NC(C)=CC=C1	219,31	C11H13N3S
Z1245633080	NC1=C(CN2CCCC2)C=CC=C1	176,26	C11H16N2
Z154053600	CC(=C)CN1N=C(C)C(C)=C(C#N)C1=O	203,25	C11H13N3O
Z1267882017	NCC1CCCNC1CC1=CC=CC=C1	190,29	C12H18N2
Z1495385325	C1CC(CN1)C1CCOC1	141,21	C8H15NO
Z30718674	CN(CC1=CC=CS1)C(=O)C1CCC1	209,31	C11H15NOS
Z374427992	CN(C)C1=NC=CC(CNC(C)=O)=C1	193,25	C10H15N3O
Z87002128	COC1=CC2=C(OC(C)=C2C(O)=O)C=C1	206,20	C11H10O4
Z1439422127	CC1OCCN(C1C)C1=NC(C)=NS1	213,30	C9H15N3OS
Z1331054519	CC(C(O)=O)C1=CC=C(C)S1	170,23	C8H10O2S
Z373768900	CCN1C=C(NC(=O)C2CCC2)C=N1	193,25	C10H15N3O
Z1266823336	CN(CCN)C1CCCC1	142,25	C8H18N2
Z1188324959	CCN(C)C(=O)NCC1=CC(Cl)=CC=C1	226,70	C11H15ClN2O
Z1250132786	NC1CCN(CC1)C1=CC(F)=CC=C1	194,25	C11H15FN2
Z224449904	C1C1=CC=C(O1)C(=O)N1CCCCC1	227,69	C11H14ClNO2
Z2509351076	CNS(=O)(=O)C1=C(N)C=CC=N1	187,22	C6H9N3O2S
Z2492800177	COC1=CC2=C(CCCC2C(O)=O)C=C1	206,24	C12H14O3
Z2492774599	COC1=CN2N=CC(C(O)=O)=C2C=C1	192,17	C9H8N2O3
Z963502702	OC(=O)C1=C2OCCOC2=CS1	186,18	C7H6O4S
Z2471262567	COC1=C2C(O)=NC=NC2=CC=C1	176,18	C9H8N2O2
Z2510258230	OC(=O)C1=CN(N=N1)C1CC1	153,14	C6H7N3O2
Z2510258122	OC(=O)CN1NC2=C(C=CC=C2)C1=O	192,17	C9H8N2O3
Z1982493921	NCCC1=NC(=CC=C1)C(O)=O	166,18	C8H10N2O2
Z353243890	CC(CO)NC(=O)C1=C(Br)C=C(F)C=C1	276,11	C10H11BrFNO2
Z1966567481	CN(C)C(=O)C1=CC(N)=CC(C)=C1	178,24	C10H14N2O
Z1948933405	NC1=NC=CC(=C1)S(=O)(=O)N1CCCCC1	227,28	C9H13N3O2S
Z1946684528	NC1(CCC2=C(C1)C=CC=C2)C(O)=O	191,23	C11H13NO2
Z1729209128	COC1=C(CN2C=CN=N2)C=C(Cl)C=C1	223,66	C10H10ClN3O
Z1983079741	COC1=CC2=C(OC=C2C(O)=O)C=C1	192,17	C10H8O4
Z68590139	NC(=O)C1=C(C=CC=C1)C(F)(F)F	189,14	C8H6F3NO
Z827056754	CN(C(C)=O)C1=NC(CS(C)=O)=O)=CS1	248,32	C8H12N2O3S2
Z992717056	CC1=CSC(=N1)C1=CC=C(C=C1)C(O)=O	219,26	C11H9NO2S

Z744930860	CCC(C)(C)NC(=O)C1=CC(C)=NN1	195,27	C10H17N3O
Z56760747	COCC1=C(N)N=C(C)N=C1	153,19	C7H11N3O
Z2408594799	CNC1=NN=C(O1)C1=CC=CC=C1	175,19	C9H9N3O
Z2692095125	CN1CC(=O)NC2=C1C=C(Cl)C=C2	196,63	C9H9ClN2O
Z2692093683	NC1=CC(=CC=C1)C1CCOCC1	177,25	C11H15NO
Z274538286	CC1=NNC(N)=C1C1=CC=C(F)C=C1	191,21	C10H10FN3
Z1820178775	COC1=C(N)C2=C(NC=C2)C=C1	162,19	C9H10N2O
Z1716711716	CN(C)C1=C(F)C=C(C=C1)C(O)=O	183,18	C9H10FNO2
Z1816507484	OC(=O)C1=COC(=N1)C1CCC1	167,16	C8H9NO3
Z1695756662	CN1C=NN=C1NC(=O)C1=COC(Br)=C1	271,07	C8H7BrN4O2
Z1836338827	NC1=NN=C(NCC2=CC=CC=C2)O1	190,21	C9H10N4O
Z1653345844	CCC(=O)N(C)C1=C(Br)C=CC=N1	243,10	C9H11BrN2O
Z118458694	COC1=C(C=CC(Cl)=C1)C(O)=O	186,59	C8H7ClO3
Z1258992647	COC1=CC(CO)=NC=C1	139,15	C7H9NO2
Z56820874	CC1=C(C)C=C(OCC(O)=O)C=C1	180,20	C10H12O3
Z1258943242	CN1C(=O)NC2=C1C=CN=C2	149,15	C7H7N3O
Z224746000	CNC(=O)C1=CC=C(C=C1)N1C=NC=N1	202,22	C10H10N4O
Z1258578343	NCC1(CC(O)=O)CCCCC1	171,24	C9H17NO2
Z1255523357	CC1=CN=C(C=C1)N1CCC(N)CC1	191,28	C11H17N3
Z1250208655	CC1CCCC(N)(Cl)C(O)=O	157,21	C8H15NO2
Z1238835893	NCC(O)C1=CC2=C(OCCO2)C(Cl)=C1	229,66	C10H12ClNO3
Z927405036	NC1=C(C=C(Cl)C=C1)C(=O)NC1CC1	210,66	C10H11ClN2O
Z1259340984	NC(C(O)=O)C1=CC(F)=CC=C1	169,16	C8H8FNO2
Z1259339927	CN(C)C1=C(C=C(Br)C=N1)C(O)=O	245,08	C8H9BrN2O2
Z1259335906	CC(C)C1=C(N=CO1)C(O)=O	155,15	C7H9NO3
Z1259335908	CC1=NC(=NN1C1=CC=CC=C1)C(O)=O	203,20	C10H9N3O2
Z360882520	OC(=O)CCN1N=C2C=CC=CN2C1=O	207,19	C9H9N3O3
Z1259335818	OC(=O)CC1=NOC(=C1)C1=CC=CC=C1	203,20	C11H9NO3
Z228584328	OC(=O)CCC1=NC2=C(S1)C=CC(Cl)=C2	241,69	C10H8ClNO2S
Z1259273127	OC(=O)C1CNC2=C1C=CC=C2	163,18	C9H9NO2
Z1259162083	Cl.CC(N)C1=C(C=CC=C1)C(F)(F)F	225,64	C9H11ClF3N
Z57915930	COC1=C(C=C(Br)C=C1)C(O)=O	231,05	C8H7BrO3
Z1741977234	COC1=NC2=C(NC=C2)C=C1	148,17	C8H8N2O
Z2689031548	COC1=CC(=CC=C1)C(O)CO	168,19	C9H12O3
Z1974213299	CC1=C(NC=C1)C(=O)N1CCC=C(F)C1	208,24	C11H13FN2O
Z1267773497	CN1N=C(C)C=C1N1CCC(N)C1=O	194,24	C9H14N4O
Z1263529814	CC(CN)OC1=CC(C)=CC=C1	165,24	C10H15NO
Z2687203880	COCC1CCNC(=O)C1	143,19	C7H13NO2
Z1724883809	CNS(=O)(=O)C1=C(F)C=CC=C1C	203,23	C8H10FNO2S
Z1741958230	OC(=O)CC1=CC(Cl)=C(F)C=C1	188,58	C8H6ClFO2
Z2684296842	OC(=O)C1=CC=C(CN2C=CN=N2)C=C1	203,20	C10H9N3O2
Z1530133038	CS(=O)(=O)NCC1=NC=CN1	175,21	C5H9N3O2S
Z2680629434	CC1=CC(F)=C(C(O)=O)C(N)=C1	169,16	C8H8FNO2
Z1171979211	CC(C)NC1=NC=C(C=C1)C(O)=O	180,21	C9H12N2O2
Z1171978798	CC1OC2=C(NC1=O)C=CC=C2C(O)=O	207,19	C10H9NO4
Z246686976	COC1=C(C=CC(Cl)=C1)S(=O)(=O)N(C)C	249,71	C9H12ClNO3S
Z1170039625	OC(=O)CN1C(=O)CCC2=C1C=CC=C2	205,21	C11H11NO3
Z1769859572	OC(=O)C1=C(Br)C=NC(=N1)C1CC1	243,06	C8H7BrN2O2
Z52584368	CNC(=O)CNC1=C2C=CSC2=NC=N1	222,27	C9H10N4OS
Z1762658221	NC(CC1=CC=CO1)C(O)=O	155,15	C7H9NO3
Z1753012806	CC1=NN2CCC(=O)N(CC(O)=O)C2=C1	209,21	C9H11N3O3
Z1751961091	Cl.Cl.CC(N)C1=C(C)N(C)N=C1	212,12	C7H15Cl2N3
Z1742055044	CNC1(CO)CCC(C)C1	143,23	C8H17NO
Z1742055041	OC(C1=CC=CO1)C1=NC=CN1	164,16	C8H8N2O2
Z929061422	CC(C)(NC(=O)C1=C(Br)C=CS1)C(O)=O	292,15	C9H10BrNO3S
Z394693484	CN(CC(O)=O)C1=NC=C(Cl)C=C1	200,62	C8H9ClN2O2
Z1603606795	CC1=C(OC=C1)C(=O)NC1(CC1)C(O)=O	209,20	C10H11NO4
Z1718361633	COC1=C(Cl)C(OC)=C(C=C1)C(O)=O	216,62	C9H9ClO4
Z1270484159	FC(F)(F)CN1CCCNCC1	182,19	C7H13F3N2
Z1398473882	CC(N)COC1CCOC1	145,20	C7H15NO2
Z1578665941	CC1=NSC(=N1)N1CCCNCC1	198,29	C8H14N4S
Z234898257	CNCC1=NN=C2C=CC=CN12	162,20	C8H10N4
Z1744662180	CC(O)CN1CCNCC1	144,22	C7H16N2O
Z2146566307	NCC1COC2=C1C=CC=C2	149,19	C9H11NO
Z2146513917	CC1=CC=C(O1)C1=CN(C=O)C=N1	176,18	C9H8N2O2
Z2111526430		158,20	C8H14O3
Z1911007933	CC1N(CCNC1=O)C1=C(Br)C=CC=N1	270,13	C10H12BrN3O

Z2092369612	OCC1=C(CC2CCNCC2)C=CC=C1	205,30	C13H19NO
Z2081962638	CNC(=O)C1=C2CNCCN2N=C1	180,21	C8H12N4O
Z1918536387	CN1C=C(OC2=NC=C(Cl)C=N2)C=N1	210,62	C8H7ClN4O
Z1839021932	CNC(=O)COC1=CC(C)=C(Br)C(C)=C1	272,14	C11H14BrNO2
Z2160914783	OC(=O)C1(CNC(=O)C1)C1=CC=CC=C1	205,21	C11H11NO3
Z1674937530	CCN1C=C(CCO)C=N1	140,19	C7H12N2O
Z1768415350	OC(=O)C1CC2(C1)CCCCC2	168,24	C10H16O2
Z1498346202	CN(CC1(O)CCCC1)C1=NC=CC=N1	207,28	C11H17N3O
Z414834692	NC1C2CCCC1CN(C2)C1CC1	180,30	C11H20N2
Z360055638	CCOC1=CC=C(C=C1)[C@H](C)O	166,22	C10H14O2
Z1431002654	NCC1(CCO)CCOC1	145,20	C7H15NO2
Z1497165919	CC1CCC(N)C2=C1C=CC=C2	161,25	C11H15N
Z1324054926	NCCC1=NC(=CS1)C1CC1	168,26	C8H12N2S
Z1324054929	C1CNCC2(C1)CCCOC2	155,24	C9H17NO
Z1522182920	CC1=C(Br)C=CC(=C1)C(=O)N1CC(O)C1	270,13	C11H12BrNO2
Z1744658498	CCN1CCNC(C)C1=O	142,20	C7H14N2O
Z1270207989	CN1C=C(C=N1)N1CCC(N)C1=O	180,21	C8H12N4O
Z56983120	CC1=C(C=CC=C1)C(=O)NCC(O)=O	193,20	C10H11NO3
Z422398218	CCC(C)(C)NC(=O)C1=C(C)N=CS1	212,31	C10H16N2OS
Z31384892	CC(C)NC(=O)CC1=CSC(C)=N1	198,28	C9H14N2OS
Z49527506	BrC1=CC=C(C=C1)C1=NNC(=O)CC1	253,10	C10H9BrN2O
Z237528064	CCC(N1C=NC2=C1C=CC=C2)C(O)=O	204,23	C11H12N2O2
Z57085731	CC(O)C1=NC2=C(C=CC=C2)N1C	176,22	C10H12N2O
Z18430744	NC(=O)COC1=CC(Cl)=C(F)C=C1	203,60	C8H7ClFNO2
Z18532934	CN(C)C(=O)COC1=C(Cl)C(Cl)=CC=C1	248,10	C10H11Cl2NO2
Z234796412	CC1=CC=C(C#N)C(=O)N1	134,14	C7H6N2O
Z29693812	O=C(NCC1=CC=CS1)C1=NC=CN=C1	219,26	C10H9N3OS
Z992422554	CC(CCN)C1=CC=CC=C1	149,24	C10H15N
Z108545254	CN1C=CC(NC(=O)C2=CC=C(C)O2)=N1	205,22	C10H11N3O2
Z729726726	CC1=NOC(NC(=O)C2=CC=CC=C2)=N1	203,20	C10H9N3O2
Z26794351	CCC(=O)NC1=CC2=C(NC(=O)N2)C=C1	205,22	C10H11N3O2
Z55928783	OC(=O)CNC(=O)C1=CC(Br)=CC=C1	258,07	C9H8BrNO3
Z1483951153	COC1(C)CC(O)C1(C)C	144,21	C8H16O2
Z90507426	C(NC1CCCCC1)C1=CC=NC=C1	204,32	C13H20N2
Z1192046301	NCC1=NC(=NC=C1)N1CCCC1	178,24	C9H14N4
Z254582744	CN(C)C(=O)C1=C(F)C=CC=C1F	185,17	C9H9F2NO
Z32455036	CN(CC1=CC=CO1)C(=O)C1CCCO1	209,25	C11H15NO3
Z969563028	NC1CCCC2=C1C=CC(OC(F)F)=C2	213,23	C11H13F2NO
Z223428262	CC1CC1C1=CC=C(CN(C)C(C)=O)O1	207,27	C12H17NO2
Z915781054	CCC(C)(C)NC(=O)C1=CC=NN1C	195,27	C10H17N3O
Z204776284	CNC(=O)CN(C)C1CCCCC1	198,31	C11H22N2O
Z265547286	CC1CCN(CC2=NC(C)=NO2)CC1	195,27	C10H17N3O
Z422522084	CN(C)C(=O)C1=C(C)N=CS1	170,23	C7H10N2OS
Z100642434	CN(C)C(=O)CCN1C(C)=CSC1=O	214,28	C9H14N2O2S
Z271004888	CNC1=NC(OC)=CC=C1	138,17	C7H10N2O
Z2235814825	CC1(CO)CCC(=O)NC1	143,19	C7H13NO2
Z2327226192	OC(=O)C1CN(C1)C1=C(C=CC=C1)C#N	202,21	C11H10N2O2
Z2327040060	COC1=CC2=C(C(=O)NC(C)=N2)C(Br)=C1	269,10	C10H9BrN2O2
Z111423554	COC1=CC(N)=C(C=C1)N1C=CC=C1	188,23	C11H12N2O
Z274764492	NC1=NN=C(COC2=CC=C(Cl)C=C2)S1	241,69	C9H8ClN3OS
Z2301438511	CC1=C(CCC(O)=O)SC=N1	171,21	C7H9NO2S
Z2284385174	CC1=NC(C)=C(Cl)C(N)=C1Cl	191,06	C7H8Cl2N2
Z736586356	CC(=O)NC1CCCN(C1)S(C)(=O)=O	220,29	C8H16N2O3S
Z1267881684	CC(C)N1C=C2C=C(N)C=CC2=N1	175,24	C10H13N3
Z1267773786	CCNC1=NN=C(C)C=C1	137,19	C7H11N3
Z1267773695	NC1=C(C=C2CCCCC2=N1)C#N	173,22	C10H11N3
Z1266933933	CCOC(C)C1=NC=CN1	140,19	C7H12N2O
Z941495390	BrC1=C(CNC(=O)C2CC2)SC=C1	260,15	C9H10BrNOS
Z1263714107	CC(C)NC1=CC(C)=C(C=C1)C(N)=O	192,26	C11H16N2O
Z1263714081	CNCC1=CC=C(O1)C(=O)NC	168,20	C8H12N2O2
Z1263602450	CNS(=O)(=O)C1=C(N)C=C(OC)C=C1	216,26	C8H12N2O3S
Z57796090	CC1=NN(C(=O)C1)C1=NC(C)=CC(C)=N1	204,23	C10H12N4O
Z1741815243	NCCN1CCC2(CCCCC2)CC1	196,34	C12H24N2
Z1675323023	C1CC1C1COCCN1C1=NC=CC=N1	205,26	C11H15N3O
Z2234185661	O=C1COCC(N1)C1=CC=CC=C1	177,20	C10H11NO2
Z416879132	CC1=CC(CN2CCC(CO)CC2)=NO1	210,28	C11H18N2O2
Z2052057458	CCS(=O)(=O)N1CCO[C@H](C)[C@H](C)1C(N)=O	236,29	C8H16N2O4S

Z354991212	CC1CN(CC2=NOC(C)=C2)C(C)CO1	210,28	C11H18N2O2
Z228570974	NCC(N1CCCC1)C1=CC(Cl)=CC=C1	224,73	C12H17ClN2
Z216450634	CN(C1CCCCC1)S(C)=O=O	205,32	C9H19NO2S
Z31152880	CN(CC1=CC=C(C)O1)C1=NC=CC=N1	203,25	C11H13N3O
Z85895292	CN(CC(O)=O)C(=O)C1=CC=C(Br)O1	262,06	C8H8BrNO4
Z1373429822	OC[C@H]1CCCN1C1=C(F)C=CC=N1	196,23	C10H13FN2O
Z2272595387	CC1=CC(=CO1)C(=O)NC(C)(C)C(O)=O	211,22	C10H13NO4
Z2017991856	CC(=O)NC1=CN=C(OC(F)F)C=C1	202,16	C8H8F2N2O2
Z2273418869	FC1=CCCN(CC2=CN=NS2)C1	199,25	C8H10FN3S
Z1460223235	FC1=C(NC2CCNC2=O)C=C(Cl)C=C1	228,65	C10H10ClFN2O
Z1796224493	CN1CCCC1C(=O)N1CCC=C(F)C1	212,27	C11H17FN2O
Z1766614316	CC1=CC(=CO1)C(=O)N1CCC=C(F)C1	209,22	C11H12FN2O
Z2274076372	CC(C)1CCN1C1=NC=C(F)C=N1	195,24	C10H14FN3
Z1481134589	FC1=CN=C(N=C1)N1CCC(=C)CC1	193,23	C10H12FN3
Z1267885776	COC1=C(N)C(C)=NN1C	141,17	C6H11N3O
Z1262396035	CCOC1=C(CN)C=CC=N1	152,20	C8H12N2O
Z2234631183	OC(=O)C1CCN(C1)C1=CC=CC=C1	191,23	C11H13NO2
Z2327224883	O[C@@H]1CC[C@H]1OCC1=CC=CC=C1	178,23	C11H14O2
Z2235790909	OCC1CN(CCO1)C1=CC=CC=C1	193,25	C11H15NO2
Z2327226290	NC1CCN(C1)C1=CC=C(F)C=C1	180,23	C10H13FN2
Z2327226304	CNC(C)(C)CN1CCOCC1	172,27	C9H20N2O
Z85919065	CC1=C(CC(O)=O)C(C)=NO1	155,15	C7H9NO3
Z57052849	OC(=O)CCN1NC(=O)C=CC1=O	184,15	C7H8N2O4
Z55928802	FC(F)OC1=CC=C(C=C1)C#N	169,13	C8H5F2NO
Z57473788	NC1=NN(CC1)C1=CC=CC=C1	161,21	C9H11N3
Z89283361	NC(C1=CC=CS1)C1=CC=CC=C1	189,28	C11H11NS
Z57042068	OC(=O)COC1=C(Cl)C=CC=C1	186,59	C8H7ClO3
Z56347545	OC(=O)CN1C(=O)C=NC2=C1C=CC=C2	204,19	C10H8N2O3
Z56347236	NC1=C(C=CC=C1)C(=O)NC1CCCC1	204,27	C12H16N2O
Z56347132	CC(C1CC1)N1N=CC=C1N	151,21	C8H13N3
Z31205964	CN(CCO)C1=C2C=CSC2=NC=N1	209,27	C9H11N3O5
Z57001599	CC1=CC(=O)NC(O)=C1C#N	150,14	C7H6N2O2
Z56973555	CCC1=C(C(O)=O)C(C)=NO1	155,15	C7H9NO3
Z29671587	CC1=CC=C(O1)C(=O)NC1=NN=C(C)S1	223,25	C9H9N3O2S
Z53038500	CCNS(=O)(=O)C1=CC2=C(OCC2)C=C1	227,28	C10H13NO3S
Z818727094	CC(C)CC1=NOC(N)=C1	140,19	C7H12N2O
Z993967022	CC1=NOC(Cl)=C1CC(O)=O	175,57	C6H6ClNO3
Z87660867	CNC(=O)CN(C)C(=O)C1=CC=C(Br)S1	291,16	C9H11BrN2O2S
Z364575442	CC1COCCN1C(=O)C1=CC(C)=NO1	210,23	C10H14N2O3
Z31407955	CC1=C(SC=C1)C(=O)NCC1=CC=CO1	221,27	C11H11NO2S
Z432742414	BrC1=CC(CN2CCNC(=O)C2)=CS1	275,16	C9H11BrN2O5
Z98655413	C[C@H](NC(=O)C1CCCCC1)C(O)=O	199,25	C10H17NO3
Z381785592	CCC1=C(C=NN1)C(O)=O	140,14	C6H8N2O2
Z55992974	COC1=C(OC)C(Cl)=CC(=C1)C(O)=O	216,62	C9H9ClO4
Z235354629	CC1=C(N=C(S1)C1=CC=CO1)C(O)=O	209,22	C9H7NO3S
Z228588958	CC1=CC(=CC=C1)C1(CCC1)C(O)=O	190,24	C12H14O2
Z32014551	CN(C)C(=O)C1=CC=C(C=C1)C#N	174,20	C10H10N2O
Z30612234	CC(C)C(=O)NC1=CC=C(C=C1)C#N	188,23	C11H12N2O
Z372854136	CC1=CC=C(C=C1)C1=NOC(=C1)C(O)=O	203,20	C11H9NO3
Z367452140	NC1=NN=C(O1)C1CCCCC1	167,21	C8H13N3O
Z2467523306	CNC(=O)C1=NN=C(N)C=C1	152,16	C6H8N4O
Z2467454517	CC(C)C1CCC2=C1NC(C)=CC2=O	205,30	C13H19NO
Z1741975083	OCCC1=NC2=C(C=CC=C2)C=C1	173,22	C11H11NO
Z1265689880	CC1=C(C=C(Br)C=C1)C(N)=O	214,06	C8H8BrNO
Z2418194164	CCN1C(=O)NN=C1CC	141,17	C6H11N3O
Z2418193660	OC(=O)C1=CN(CC=C)N=N1	153,14	C6H7N3O2
Z2418193634	C1CC2=C(C=NC2)C2(CCOCC2)N1	193,25	C10H15N3O
Z1389112660	NC(=O)CC1=C(F)C=CC=C1F	171,15	C8H7F2NO
Z2412196555	COC1=C(C(O)=O)C(F)=CC=C1Br	249,04	C8H6BrFO3
Z1266823324	COCC1=C(F)C=C(CN)C=C1	169,20	C9H12FNO
Z1266823338	CC(N)(C)N1C=C(C)C=C1	153,23	C8H15N3
Z927398482	NCCC(=O)NC1CCCCC1	170,26	C9H18N2O
Z1359429514	NC1(CCO)CCCCC1	143,23	C8H17NO
Z1359429530	CC1=CN=C(S1)C(C)C(N)	156,25	C7H12N2S
Z1436181071	CC1(C)CCC(CO)CC1	142,24	C9H18O
Z1263811673	CN1CCN(CC1)C1=C(CN)C=CC=C1	205,31	C12H19N3
Z1483951161	CN1C=C(CCN)C(C)=N1	139,20	C7H13N3

Z1263529758	CC(N)C1=CC(C)=C(C)C=C1	149,24	C10H15N
Z1335709095	CC(CN)OC1=C(Br)C=CC=C1	230,11	C9H12BrNO
Z1270312194	CC(OC1CCCCC1)C(O)=O	172,22	C9H16O3
Z1404661574	CC(C)N1CC(C)C(N)C1	142,25	C8H18N2
Z1431920316	CC(C)C1CCC(N)CC1	141,26	C9H19N
Z235336615	COC1=C(C=C(F)C=C1)C(O)=O	170,14	C8H7FO3
Z223688256	CC(=O)NC1=NC(=CC=C1)C(O)=O	180,16	C8H8N2O3
Z185578978	OC(=O)C12CC(CN1)CCC2	155,20	C8H13NO2
Z1250080944	CC1=C(N)C=C(CO)C=C1	137,18	C8H11NO
Z1250080919	CC1CCN(CC1)C1=CC(N)=CC=C1	190,29	C12H18N2
Z1342206615	CC(C)S(=O)(=O)N1CCC(N)C(C)C1	220,33	C9H20N2O2S
Z2218586413	CCOC1=C(N)C=C(C)C=N1	152,20	C8H12N2O
Z1245735228	COC1=C(Cl)C=C(C=C1)C(C)O	186,64	C9H11ClO2
Z1263529766	CCOC1=C(N)C=C(F)C=C1	155,17	C8H10FNO
Z1267773652	CN(C)C1=NC(C)=C(CCN)S1	185,29	C8H15N3S
Z2240989990	CN1C=C(C=N1)C1=CC=C(O1)C(O)=O	192,17	C9H8N2O3
Z27769921	CC(=O)N1CCN(CC1)C1=CC=CC=C1	204,27	C12H16N2O
Z2238508666	N#CC1=NC(=NN1)C1CC1	134,14	C6H6N4
Z1504688330	COCC1=NN(C)C=C1C(O)=O	170,17	C7H10N2O3
Z788000702	OC(C(O)=O)C1=CC(Cl)=C(Cl)C=C1	221,03	C8H6Cl2O3
Z1201620504	COC1=C2C=CNC(=O)C2=CC=C1	175,19	C10H9NO2
Z1157836416	CC1=NC2=CC=NN2C=C1C(O)=O	177,16	C8H7N3O2
Z1101435035	OC(=O)C1CCC2=C1C=CC=C2	162,19	C10H10O2
Z1416200845	CC1CCC(CC(O)=O)C1	142,20	C8H14O2
Z1359429533	NC1CCC(CC1)N1CCCCC1	182,31	C11H22N2
Z1259339846	NC1=C2OCCOC2=CC=C1	151,17	C8H9NO2
Z1245664685	CC(N)C1=C(C)SC(C)=C1	155,26	C8H13NS
Z50145861	CC1=NN(C(=O)C1)C1=CC=CC=C1	174,20	C10H10N2O
Z1245635810	OC(C1=CC=NC=C1)C1=CC=C(F)C=C1	203,22	C12H10FNO
Z1245635739	NC1=CC=C(C(Cl)C=C1)C(F)(F)F	195,57	C7H5ClF3N
Z751810922	O=S(=O)(N1CCOCC1)C1=CN=CC=C1	228,27	C9H12N2O3S
Z1245633364	COC1=C(C=CC=C1)C1=CSC(=O)N1	207,25	C10H9NO2S
Z1575325613	CC(N)C1=C(C)ON=C1C	140,19	C7H12N2O
Z1626612682	CCOC1=NC(C)=CC=C1	137,18	C8H11NO
Z133743260	CC(NS(C)(=O)=O)C1=CC(F)=C(F)C=C1	235,25	C9H11F2NO2S
Z729353192	ClC1=CC=C(CN2CCS2(=O)=O)S1	251,74	C8H10ClNO2S2
Z1238477831	NCC1CCN(C1)C1CC1	140,23	C8H16N2
Z1020680172	NCC(O)C1=C(F)C=C(F)C=C1	173,16	C8H9F2NO
Z1127662837	O[C@H]1CCN(CC2=CC=C(F)C=C2)C1	195,24	C11H14FNO
Z1649677579	Cl.NC1(CCC2=C1C=CC=C2)C(F)(F)F	237,65	C10H11ClF3N
Z929055810	CC(C)(NC(=O)C1=COC(Br)=C1)C(O)=O	276,09	C9H10BrNO4
Z1696860273	NCC1=C(CC(O)=O)C=CC=C1	165,19	C9H11NO2
Z1312590981	NC(=O)C(O)C1CCOCC1	159,19	C7H13NO3
Z2004547966	CC1=C(C=CC=C1C#N)C(O)=O	161,16	C9H7NO2
Z1993522642	COC1=C(C=CC=C1)C1CNCCN1	192,26	C11H16N2O
Z1992316420	CC(C)(CO)N1CCNC1=O	158,20	C7H14N2O2
Z1992316412	CC1=CC(=O)C(=CN1C1CC1)C(O)=O	193,20	C10H11NO3
Z2028214428	NC1=C(CO)C=C(Cl)C(Cl)=C1	192,04	C7H7Cl2NO
Z1537047698	O=C1NC(CC2CC2)=NC2=C1C=CC=C2	200,24	C12H12N2O
Z2024187616	NCCC1=C2C=CNC2=CC=C1	160,22	C10H12N2
Z1591894147	CC(C)(CO)N1CCN(CC1)S(C)(=O)=O	236,33	C9H20N2O3S
Z1642061028	CN1N=CN=C1C1=CC=C(C=C1)C(O)=O	203,20	C10H9N3O2
Z1642061040	CNCC1=CN=C(N)C=C1	137,19	C7H11N3
Z1625822275	CC1CCCC1(N)C(N)=O	142,20	C7H14N2O
Z1582263000	CC1=CNC=C(C(O)=O)C1=O	153,14	C7H7NO3
Z1582263014	CC1=CC=CN2C(=O)C(=CN=C12)C(O)=O	204,19	C10H8N2O3
Z1575311832	COCC1=NOC(N)=C1	142,16	C6H10N2O2
Z1575304428	NC1=NN=C(CC2CCCC2)O1	167,21	C8H13N3O
Z1575143756	CC1=C(N)C=C(S1)C(N)=O	156,20	C6H8N2OS
Z1642389904	OC(=O)CN1C=NNC1=O	143,10	C4H5N3O3
Z1642389889	OCC1(CO)CCCC1	144,21	C8H16O2
Z1700091114	CC1=NC(OCC2=NC=CC=C2)=CC=C1	200,24	C12H12N2O
Z1607437929	CC1=NC(CCN2C=CN=C2C)=CS1	207,30	C10H13N3S
Z1139583522	CC(=C)CN1CCC2=C(C1)N=C(C)N=C2	203,29	C12H17N3
Z196024084	CN(C)C(=O)C1CCCN1CC=C(C)C	210,32	C12H22N2O
Z268316368	CCC1=NC(CN2C=NC(=N2)C#N)=CS1	219,27	C9H9N5S
Z236893404	CN(C1CCCC1)C(=O)C1=CC=CN1C	206,29	C12H18N2O

Z1815155563	CC(C)C(CN)C1=CC=NN1C	167,26	C9H17N3
Z1266823352	CC(N)CCN1CCCC1	142,25	C8H18N2
Z57102477	CCOC1=C(CN)C=CC=C1	151,21	C9H13NO
Z1238477832	CCC(CN)N1CCCC1	142,25	C8H18N2
Z54751796	CC1CC(C)CN(CC(=O)N(C)C)C1	198,31	C11H22N2O
Z1695797886	NC(C(O)=O)C1=C(F)C=CC(F)=C1	187,15	C8H7F2NO2
Z1692788303	COCC1=CC(=CN=C1)C(O)=O	167,16	C8H9NO3
Z1691545032	OC(=O)C1(CCC1)C(O)=O	144,13	C6H8O4
Z1474242573	CC1CCCN(CC1)C(=O)C1=NNC=N1	208,27	C10H16N4O
Z1664966434	O=S(=O)(C1CCCN1)N1CCOCC1	234,31	C9H18N2O3S
Z2235790793	CCC1=C(N)NC(C)=NC1=O	153,19	C7H11N3O
Z2235681425	CC1=C(N)C=NN1C1CCOC1	167,21	C8H13N3O
Z2235678973	CC1=C2OC(N)=NC2=CC(Cl)=C1	182,61	C8H7ClN2O
Z1983181712	CC1=NC(NC(=O)C2CC=CC2)=NC=C1	203,25	C11H13N3O
Z2235386865	OCC1(CNC(=O)C1)C1=CC=CC=C1	191,23	C11H13NO2
Z2230911760	CC1=C(C=CN=C1)C(O)C1=CC=CC=C1	199,25	C13H13NO
Z2230911737	CC1=NC(C(O)=O)=C(C)O1	141,13	C6H7NO3
Z2218556016	N#CC1=CC2=C(NCCC2)C=C1	158,20	C10H10N2
Z2218555426	CC1=C(N)C=C(C(O)=O)C(Cl)=C1	185,61	C8H8ClNO2
Z2218556033	OC(=O)CC1=CSC=C1C(O)=O	186,18	C7H6O4S
Z1891776064	OCC1=CN(N=N1)C1=CC(Cl)=C(Cl)C=C1	244,08	C9H7Cl2N3O
Z2217033016	CC1(C)C(=O)NC2=C1C=CC(=C2)C(O)=O	205,21	C11H11NO3
Z2216720825	CC(=O)NC1=C(C=CC(Br)=C1)C(O)=O	258,07	C9H8BrNO3
Z1741965319	CC1=CC=C(C=C1)S(=O)(=O)N1C=CN=C1	222,26	C10H10N2O2S
Z2568757995	CNC(C(O)=O)C1=C(Cl)C(Cl)=CC=C1	234,08	C9H9Cl2NO2
Z1129283193	CC(=O)NC1=C(C)C=CN=C1	150,18	C8H10N2O
Z2527856103	CC(C)C(O)C(N)C1=CC=CC=C1	179,26	C11H17NO
Z2526439730	CCN1C(=O)NC2=C1C=CC(=C2)C(O)=O	206,20	C10H10N2O3
Z2522503408	OC1CCNC11CCCCC1	155,24	C9H17NO
Z1891775536	CN(C)C1=NC(N)=NC=C1	138,17	C6H10N4
Z2515238980	OCC#CC1=NC=C(Br)C=C1	212,05	C8H6BrNO
Z104378280	OC(C(O)=O)C1=CC=C(F)C=C1	170,14	C8H7FO3
Z53825020	CCS(=O)(=O)N1CCC(CC1)C(O)=O	221,27	C8H15NO4S
Z96092051	OC(=O)CC1=CSC(=N1)N1CCCC1=O	226,25	C9H10N2O3S
Z203038516	OC(=O)C1=NOC(=C1)C1CC1	153,14	C7H7NO3
Z90662852	CS(=O)(=O)CC1=CC(=CC=C1)C(O)=O	214,24	C9H10O4S
Z90664673	OC(=O)C1=CC2=C(OCCC2)C(Cl)=C1	228,63	C10H9ClO4
Z57169536	COC1=C(F)C=C(C=C1)C(O)=O	170,14	C8H7FO3
Z234898245	OC(=O)CC1CCC(=O)N1	143,14	C6H9NO3
Z27797569	COC1=C(NC(=O)C2CC2)C=CC=C1	205,26	C12H15NO2
Z56960248	CNCC1COC2=C(O1)C=CC=C2	179,22	C10H13NO2
Z56936647	C[C@H](NC(=O)C1=CC=C(F)C=C1)C(O)=O	211,19	C10H10FNO3
Z54794538	CCOC1=C(OC)C=C(C=C1)C#N	177,20	C10H11NO2
Z26824672	CCC1=NN=C(NC(=O)C2CC2)S1	197,26	C8H11N3OS
Z56913174	CC1(C)NC2=C(NC1=O)C=CC=C2	176,22	C10H12N2O
Z45527666	CNS(=O)(=O)C1=CC2=C(OCCO2)C=C1	229,25	C9H11NO4S
Z56886305	CC1=C(Cl)C=C(Cl)C(N)=N1	177,03	C6H6Cl2N2
Z56869297	CN1N(C(=O)C=C1C)C1=CC=CC=C1	188,23	C11H12N2O
Z56827661	CC1=CC(=CC=C1)C(=O)NCC(O)=O	193,20	C10H11NO3
Z19629920	CN1N=C(C(O)=O)C2=C(C=CC=C2)C1=O	204,19	C10H8N2O3
Z56791215	NC1=NC2=C(CCCC2)C(N)=N1	164,21	C8H12N4
Z56822380	OC(=O)C1=CC2=C(CCC2)S1	168,21	C8H8O2S
Z56788806	O[Cl](=O)(=O)=O.CC1=NN(C(C)=C1)C1=NC=CC=C1	273,67	C10H12ClN3O4
Z56754157	CC1=NN(CCC(N)=O)C(C)=C1	167,21	C8H13N3O
Z1429378656	CC1=CC(=O)NC=C1C(O)=O	153,14	C7H7NO3
Z168552936	CCC(=O)N(C)C(C)C1=CC=CS1	197,30	C10H15NOS
Z54849993	COC1=C2N=CC=CC2=CC=C1	159,19	C10H9NO
Z1365534337	CNCC1=CC2=C(N1)C=CC=C2	160,22	C10H12N2
Z104346732	CNCC1=C(OC)C=CC(Cl)=C1	185,65	C9H12ClNO
Z314451142	CCN(C1CC1)C(=O)C1=C(C)OC=C1	193,25	C11H15NO2
Z277959532	NCC(C1CCOC1)N1CCOCC1	200,28	C10H20N2O2
Z959151572	CC(C)N1C=C(C=N1)C(C)N	153,23	C8H15N3
Z1267882046	CN(C)C1(CN)CCOCC1	158,25	C8H18N2O
Z1309496197	CC1CCC(CCC(O)=O)O1	158,20	C8H14O3
Z262221634	C1CN(CCN1)C1=NC=CC=N1	164,21	C8H12N4
Z284779336	CC(=O)N1CCC(CC1)C1=CC=CC=C1	203,29	C13H17NO
Z1267773588	CN1CCN(C)C(CN)C1	143,23	C7H17N3

Z1267773565	CC(C)C(N)C1=C(C)C=CC=C1	163,26	C11H17N
Z57036344	C1CNC(C1)C1=CC2=C(OCCO2)C=C1	205,26	C12H15NO2
Z2108806948	CC1(CC(O)=O)CCCC1	142,20	C8H14O2
Z2092396826	CN(C)C(=O)C1CCCC(N)C1	170,26	C9H18N2O
Z1881545321	CC1=CC(=NS1)C(=O)NCC1CCCO1	226,29	C10H14N2O2S
Z1723547340	COC1=C(C=CC=C1)N1C=CC=N1	174,20	C10H10N2O
Z2017694687	CCN1CCC2NCCOC2C1	170,26	C9H18N2O
Z2004563998	NCC1CN2CCN1CCC2	155,25	C8H17N3
Z422410426	CN(C)C(=O)CNC(=O)C1=C(C)N=CS1	227,28	C9H13N3O2S
Z821829386	CN(CC(N)=O)C1CC2=C(C1)C=CC=C2	204,27	C12H16N2O
Z32064555	FC1=CC=C(C=C1)C(=O)NCC=C	179,19	C10H10FNO
Z68093999	COCC(=O)NC1=NC2=C(N1)C=CC=C2	205,22	C10H11N3O2
Z168290016	CN1C(C)=CC=C1C(=O)NC1CCCC1	206,29	C12H18N2O
Z432141618	CC(N(C)S(C)(=O)=O)C1=CC=C(C)C=C1	227,32	C11H17NO2S
Z221220996	CC(=O)N1CCC(CC1)NS(C)(=O)=O	220,29	C8H16N2O3S
Z422952360	CN(CC(N)=O)C(=O)C1=CC=C(Cl)S1	232,68	C8H9ClN2O2S
Z280480820	O=C(CN1C=CC=N1)NC1=CN=CC=C1	202,22	C10H10N4O
Z1272739430	OC(CC1CCCN1)C1=CC=CC=C1	191,27	C12H17NO
Z1318516269	CN1CC(=O)NC2=C1C=CC(Cl)=C2	196,63	C9H9ClN2O
Z1318356934	O=C1CC2(CCCC2)CN1	139,20	C8H13NO
Z193095560	CS(=O)C(=O)NC1CCC2=C1C=CC=C2	211,28	C10H13NO2S
Z1318147481	CCC1=C(N)C=C(C=C1)C(O)=O	165,19	C9H11NO2
Z1313483209	COC1=C2C=CC=CC2=NC=C1C(O)=O	203,20	C11H9NO3
Z1310777667	CN1N=C(C=C1N)C1=C(C)C=CC=C1	187,25	C11H13N3
Z1297758312	OC(=O)C1=CC(=NO1)C1CCCC1	181,19	C9H11NO3
Z274553588	CC(CC(O)=O)N1N=C(C)N=C1C	183,21	C8H13N3O2
Z1295543888	CC(C)CC1CNC(=O)C1	141,21	C8H15NO
Z1278604242	COC1=NC2=C(C=CC=C2)C(=C1)C#N	184,20	C11H8N2O
Z274554372	CC1=NN(CCC(O)=O)C(C)=C1Br	247,09	C8H11BrN2O2
Z55290928	CCN(CC)C(=O)NC1=CC=C(F)C=C1	210,25	C11H15FN2O
Z1258855725	ClC1=CC(CN2C=CSC2=O)=CC=C1	225,69	C10H8ClNO5
Z733898630	CC(C)NC(=O)C1=NN(C)C(C)=C1	181,24	C9H15N3O
Z1796014543	CNC(=O)C1(CC2=C(F)C=CC=C2)CC1	207,25	C12H14FNO
Z1661748363	FC1=CC=C(CN2N=CSC2=O)C=C1	210,23	C9H7FN2O5
Z235582156	CNCC1=C(F)C=CC(=C1)C#N	164,18	C9H9FN2
Z2182115595	CCC1=NC(C)=C(CO)O1	141,17	C7H11NO2
Z32013792	CN(C)C(=O)C1=CC(=CC=C1)S(C)(=O)=O	227,28	C10H13NO3S
Z1324054938	CC1CN(CCO1)C1=NC=CC(CN)=C1	207,28	C11H17N3O
Z1318186467	NC1CCCCC1N1C=CC=N1	165,24	C9H15N3
Z2065788160	OC(=O)C1=C2CCOCC2=CO1	168,15	C8H8O4
Z2065788258	CC1=C(C(O)=O)C(=NO1)C1CC1	167,16	C8H9NO3
Z2065464360	OC1=CC(=O)N2CCNC2=N1	153,14	C6H7N3O2
Z373221060	C1CN(C1)C1=C2NC=NC2=NC=N1	175,20	C8H9N5
Z2050688057	OC(=O)C1=CN=NN1CC1=CC=CC=C1	203,20	C10H9N3O2
Z1891773873	Cl.CCOC1=CC=C(C=C1)C(C)N	201,69	C10H16ClNO
Z1791180060	CC1=NC=C(C=C1)C(=O)NC1=CN=NS1	220,25	C9H8N4O5
Z2037266949	OC(=O)CC1=C(C=CC=C1Cl)C(O)=O	214,60	C9H7ClO4
Z1822538122	FC1=CN(CC2=CSC(Br)=C2)C(=O)C=C1	288,13	C10H7BrFNOS
Z54614962	CC1(CCS(=O)(=O)C1)NC(=O)C1CCCC1	231,31	C10H17NO3S
Z1874203205	CC1CCC(C)N1C1=C(Cl)C(N)=NC=N1	226,71	C10H15ClN4
Z1270387207	CC1=CC(OC(F)F)=C(S1)C(O)=O	208,18	C7H6F2O3S
Z1270384393		198,17	C10H8F2O2
Z1270358403	CC1=C(OCC(O)=O)C(Cl)=CC=C1	200,62	C9H9ClO3
Z50146693	CC1=NN(C(=O)C1)C1=CC=C(F)C=C1	192,19	C10H9FN2O
Z1270246402	COC1=CC(=CC(OC)=C1)C(O)=O	196,20	C10H12O4
Z32368096	O=C(NC1CC1)C1=NNC2=C1C=CC=C2	201,23	C11H11N3O
Z228588366	O=S(=O)(N1CCCCC1)N1CCNCC1	233,33	C9H19N3O2S
Z1259159887	C1CC(CCN1)NC1=NN=CC=C1	178,24	C9H14N4
Z1268152412	NCC1(CCCC1)C(N)=O	142,20	C7H14N2O
Z1268152328	NCCN1N=CC2=C(C=CC=C2)C1=O	189,22	C10H11N3O
Z1267881725	O=C1CCCN1CC1=CC(=CC=C1)C#N	200,24	C12H12N2O
Z235538124	COC1=CC=C(C=C1)C1=NN=C(N)O1	191,19	C9H9N3O2
Z274575916	CC1=NC(C)=NC(=C1)N1CCNCC1	192,27	C10H16N4
Z1262246174	NC1CCN(CC1)C1=CC=C(C=C1)C#N	201,27	C12H15N3
Z1262245653	CS(=O)C(=O)CC1=C(N)C=C(Cl)C=C1	219,68	C8H10ClNO2S
Z2658866526		247,11	C8H7BrO2S
Z2658863336	OC1(CNC1)C1=CC(Br)=CC=C1	228,09	C9H10BrNO

Z2588063750	OC(=O)C1=CC=NN1C1CCOCC1	196,21	C9H12N2O3
Z2587654834	CC1=NOC(=C1)C1(CC1)C(O)=O	167,16	C8H9NO3
Z2106593039	OC(=O)CN1C=C(Br)C(=N1)C1CC1	245,08	C8H9BrN2O2
Z2583036236	NC1=NC(CC2CC2)=NS1	155,22	C6H9N3S
Z2583036218	CCOC1=C(C)N=C(N)C=C1	152,20	C8H12N2O
Z2054890075	CC(C)=CCN1CCCC(O)(C1)C(N)=O	212,29	C11H20N2O2
Z2574909701	CN1C=C(N=N1)C1=CC(N)=CC=C1	174,21	C9H10N4
Z2106593715	CC1=CN2N=CC(C(O)=O)=C2N=C1	177,16	C8H7N3O2
Z729606832	CN1C=C(C=N1)N1CC(CC1=O)C(O)=O	209,21	C9H11N3O3
Z2106598193	CCN1N=C(C=C1C(O)=O)C1CC1	180,21	C9H12N2O2
Z2167281379	CC1=C(SC(=N1)C1CCCO1)C(O)=O	213,25	C9H11NO3S
Z2106601217	CC(C)C1=C(SN=N1)C(O)=O	172,20	C6H8N2O2S
Z2510259349	CC1=C2C=C(C=CN2C=N1)C(O)=O	176,18	C9H8N2O2
Z2510259461	CCC1=C(OC=N1)C(O)=O	141,13	C6H7NO3
Z1738984510	OC(=O)C1CN(C1)S(=O)(=O)C1CC1	205,23	C7H11NO4S
Z2510258170	OCC1=C(F)C=C(C=C1)C(O)=O	170,14	C8H7FO3
Z2379087719	OCC1=CN=C(C=C1)C1=NC=CC=C1	186,21	C11H10N2O
Z1561886252	CC1=CC=C(CN2CCC(C2)C(N)=O)S1	224,32	C11H16N2O5
Z2353496673	COC1=C(Br)C=C(C=N1)C(O)=O	232,03	C7H6BrNO3
Z2346401081	COC1=CC=CN2C(=O)NN=C12	165,15	C7H7N3O2
Z594413678	OC(=O)CN1C=C(Br)C=N1	205,01	C5H5BrN2O2
Z2327893661	CS(=O)(=O)N1C=C(N)C=N1	161,18	C4H7N3O2S
Z2327883941	COC1=C(N)C=C(Br)C(F)=C1	220,04	C7H7BrFNO
Z2327883919	CC1=C(C=CC(=C1)C#N)N1C=CC=N1	183,21	C11H9N3
Z2327883382	CN1C=CC(=CC1=O)C#N	134,14	C7H6N2O
Z2327673239		191,23	C11H13NO2
Z2327531717	CC1=C(C)C(=CC=C1)C(O)C1=CNC=N1	202,26	C12H14N2O
Z960282416	CCC1=NC(C)=C(S1)C(=O)NC(C)C	212,31	C10H16N2O5
Z1262691690	CC1CC(N)C(=O)N1C1=CC=CC=C1	190,25	C11H14N2O
Z1262398489	CCC1=NC(C)=NC(N)=C1	137,19	C7H11N3
Z1262398455	CNS(=O)(=O)C1=C(OC)C=C(N)C=C1	216,26	C8H12N2O3S
Z2671044820	CC1=NN=C(C(C)C(CO)=C1	138,17	C7H10N2O
Z90519865	CC1CCC(CC1)NC1CCC(O)CC1	211,35	C13H25NO
Z1262327462	CC1=C(NC(=O)CCN)C=CC(Br)=C1	257,13	C10H13BrN2O
Z1262254308	COC1=C2CNCCC2=NC=N1	165,20	C8H11N3O
Z1881620389	CN1C=CN=C1C1CCNC1	165,24	C9H15N3
Z1849039509	COC1(CO)CCCC1	144,21	C8H16O2
Z1834223476	C(OC1=CC=CC=C1)C1CNCCO1	193,25	C11H15NO2
Z1706008539	CNCC1=NC=C(C)C=C1	136,20	C8H12N2
Z1333717726	NCC1=C(F)C=CC=C1N	140,16	C7H9FN2
Z1436311340	FC1=CC2=C(NC3(CCC3)C(=O)N2)C=C1	206,22	C11H11FN2O
Z2065464333	NC1=CC2=C(C=C1)N=C(S2)C(F)F	200,21	C8H6F2N2S
Z2017679560		190,67	C8H15ClN2O
Z1945984231	CC1=NC2=C(O1)C=CC=C2C(O)=O	177,16	C9H7NO3
Z1918018570	OC1CNC2=C(C1)C=CC=C2	149,19	C9H11NO
Z1913660888	NC(=O)CN1CCC2=C(C1)C=C(N)C=C2	205,26	C11H15N3O
Z1889706359	CN1C=C(C=N1)C1=NN(C)C(N)=C1	177,21	C8H11N5
Z1839480878	COC1=C(OC)C=C2C(=O)C=CNC2=C1	205,21	C11H11NO3
Z1837073451	CC1=C(C=CC(=C1)N1C=CN=C1)C(O)=O	202,21	C11H10N2O2
Z1401276297	C1CC2(CCN(C2)C2=NC=CN=C2)CO1	205,26	C11H15N3O
Z57186564	COC1=CC=C(NC2=NCCN2)C=C1	191,23	C10H13N3O
Z2217052350	CC(C)C1CNCCC1	143,23	C8H17NO
Z56347426	CC(N)C1=C(F)C=CC=C1	139,17	C8H10FN
Z1954439425	CC1CCC(CNC(=O)C2=CN=C2)C1	207,28	C11H17N3O
Z1515773863	CC1=CC(Br)=C(C=C1)C(=O)N1CC(O)C1	270,13	C11H12BrNO2
Z1454840342	CC(=O)N1CCOC(CO)C1	159,19	C7H13NO3
Z46280391	NCC(=O)NC1=CC2=C(OCO2)C=C1	208,22	C10H12N2O3
Z1891776561	CN1CCN(CCC(C)C)N)CC1	185,32	C10H23N3
Z1079003794	CN1N=CC=C1CNC1CC1	151,21	C8H13N3
Z1552026873	OCCN1CCCCC1=O	143,19	C7H13NO2
Z1552027610	CCN1C(N)=NC2=C1C=CC(=C2)C(O)=O	205,22	C10H11N3O2
Z1532540940	CC1=NC2=CC=NN2C(C)=C1C(O)=O	191,19	C9H9N3O2
Z1532540939	COC1=CC2=C(C=C1)C(CC(O)=O)CO2	208,21	C11H12O4
Z1444783243	CC(=O)NC1=C(CC(O)=O)C=CC=C1	193,20	C10H11NO3
Z1516394657	CC(C)OC1=NC(=CC=C1)C(O)=O	181,19	C9H11NO3
Z755016692	O=C(N1CCCCC1)C1=NC(=O)NN1	210,24	C9H14N4O2
Z1511494958	NC1=NC=C(CCC(O)=O)C=C1	166,18	C8H10N2O2

Z1501469871	CN(C)C1=NC=C(N)C=N1	138,17	C6H10N4
Z1495385201	CN1C(=O)NC2=C1C=C(C=C2)C(O)=O	192,17	C9H8N2O3
Z2405062308	CN1C=CN=C1C(N)C1CC1	151,21	C8H13N3
Z2469698599	CS(=O)(=O)C1=CNC2=C1C=CC=C2	195,24	C9H9NO2S
Z220356550	Cl.CNCC1=NN=C2CCCCCN12	216,71	C9H17ClN4
Z979897846	N#CC1=NN(CCC2=CC=CS2)C=N1	204,25	C9H8N4S
Z803153228	COC1=C(CN)C=CC(C)=N1	152,20	C8H12N2O
Z1436473525	COC1=CC=C(C=C1)C1CC(C)CN1	191,27	C12H17NO
Z1250132763	OCC1CC2=C(O1)C=CC(F)=C2	168,17	C9H9FO2
Z1257966114	CNC(=O)N1CC(CCC1C)C1=CC=CS1	224,32	C11H16N2OS
Z1266823302	NCCC1=C(F)C=C(Br)C=C1	218,07	C8H9BrFN
Z1259086951	OC1CCC2=C(C1)C=CC=C2	148,21	C10H12O
Z1649880140	CCC1=NOC(C)=C1C#N	136,15	C7H8N2O
Z1245633276	O=C(CC1=CC=CC=C1)N1CCNCC1	204,27	C12H16N2O
Z228572562	CC(CN)N(C)C1=CC=CC=C1	164,25	C10H16N2
Z1263714192	OCCN1CCCC2=C1C=CC=C2	177,25	C11H15NO
Z67735551	COC1=C(F)C=C(CN(C)C(C)=O)C=C1	211,24	C11H14FN2O2
Z1483947758	OC1CCC2=C(F)C=CC(F)=C12	170,16	C9H8F2O
Z268462794	CN(CC1=NC(C)=NO1)C1CCCC1	195,27	C10H17N3O
Z220654802	O=C(CCN1C=CC=N1)N1CCOCC1	209,25	C10H15N3O2
Z1945707500	NC1=CC(CCC2=CC=CO2)=NO1	178,19	C9H10N2O2
Z1945695967	NC1=NN2C(C=C1)=NN=C2C(F)(F)F	203,13	C6H4F3N5
Z1898727512	NC1=C(CN2C=CSC2=O)C=C(F)C=C1	224,25	C10H9FN2OS
Z1763483008	CN1N=CC(CI)=C1C=CC1=NC=NC=C1	220,66	C10H9ClN4
Z1895741719	CCOC1=NC=C(N=C1)C#N	149,15	C7H7N3O
Z1702887695	CC1CN(C1)C(=O)C1=CNC(=C1)C#N	189,22	C10H11N3O
Z432840754	BrC1=C(SC=C1)C(=O)N1CCNC(=O)C1	289,15	C9H9BrN2O2S
Z138863066	CC1CCCCN1CC1=C(CI)SN=N1	231,74	C9H14ClN3S
Z600428468	CC1=NOC(=N1)C1=CC(C)=C(N)C=C1	189,22	C10H11N3O
Z225891644	CC1=CSC(CNC(=O)C2=CC=CO2)=N1	222,26	C10H10N2O2S
Z372500342	CC1=CC=C(S1)C(=O)NC1=CN=C1	207,25	C9H9N3OS
Z372501562	CC1=C(C=CO1)C(=O)NC1=CN=C1	191,19	C9H9N3O2
Z183987204	O=C(CC1=CC=CS1)NC1=NC=CC=C1	218,27	C11H10N2OS
Z31067607	CN(C)C(=O)CN(C)C1=NC=CN=C1	194,24	C9H14N4O
Z31721308	ClC1=CC=C(S1)C(=O)N1CCOCC1	231,69	C9H10ClNO2S
Z332685420	CNC(=O)CNC(=O)C1=CSC(Br)=C1	277,14	C8H9BrN2O2S
Z271188802	CCC1=NC(CN2CCNC(=O)C2)=CS1	225,31	C10H15N3OS
Z220784562	ClC1=CC=C(O1)C(=O)N1CCNC(=O)C1	228,63	C9H9ClN2O3
Z1258992664	OC1(CC2=CC=CC=C2)CCCC1	176,26	C12H16O
Z1225460101	OC1CN(C1)C1=NC=C(C=C1)C(F)(F)F	218,18	C9H9F3N2O
Z409524162	CN(C(N)=O)C1=CC=CC=C1	150,18	C8H10N2O
Z1222423417	CN(C)C1=NC2=C(C=C1)C=C(N)C=C2	187,25	C11H13N3
Z230671654	O=C(NC1CC1)N1CCC2=C(C1)C=CS2	222,31	C11H14N2OS
Z285642082	O=C(NC1CC1)C1=C2N=CC=CN2N=C1	202,22	C10H10N4O
Z197276438	OCCN1CCCC(O)C1	145,20	C7H15NO2
Z239533106	CN1N=C(C)C2=C1N=CC(NC(C)=O)=C2	204,23	C10H12N4O
Z2678251679	OCCC1=CC2=C(CCC2)C=C1	162,23	C11H14O
Z137630580	CN1C=C(CNC2=CC=C(F)C=C2)C=N1	205,24	C11H12FN3
Z68247201	CN(C)C(=O)C1=C(C=CC=C1)C(F)(F)F	217,19	C10H10F3NO
Z1699556036	CN1N=C(C)N=C1NCC1=C(C)N=CS1	223,30	C9H13N5S
Z1562812679	CN(CC1=CSN=N1)C1CCCC1	197,30	C9H15N3S
Z274787914	CC1(C)CC2=C(O1)C=CC(CO)=C2	178,23	C11H14O2
Z2379767449	CC(C)CC1=CSC(=N1)C1=C(N)SN=N1	240,34	C9H12N4S2
Z2002368339	CCC(C)N1CCS(=O)(=O)CC(C)C1	219,34	C10H21NO2S
Z1747823555	CC(C)CC(=O)N1CCCC1CO	185,27	C10H19NO2
Z992717128	NC(C(O)=O)C1=CC=C(Br)C=C1	230,06	C8H8BrNO2
Z2216314212		205,26	C12H15NO2
Z2213893364	CC1=NC2=C(CCCC2)N1	136,20	C8H12N2
Z2213893403	CC1(C)CCCC1(O)CN	143,23	C8H17NO
Z1273312153	CNC(=O)C1=C2NC=CC2=CC=C1	174,20	C10H10N2O
Z2211231211	CCC1=NC(C)=C(O1)C(O)=O	155,15	C7H9NO3
Z85878916	CCC(=O)NC1=C(C=CC=C1)C(O)=O	193,20	C10H11NO3
Z2182115458	CC1=C(C(O)=O)C(C)=NS1	157,19	C6H7NO2S
Z1988116721	OCC(=O)NC1CC(C1)C1=CC=CC=C1	205,26	C12H15NO2
Z285707260	CNC(=O)CN(C)C1=NC(C)=CC(C)=N1	208,27	C10H16N4O
Z336481640	Cl.CCNCC1=NC2=C(C=CC=C2)C(=O)N1	239,70	C11H14ClN3O
Z55149005	CC1=CSC(=N1)N1CCCC1=O	182,24	C8H10N2OS

Z57101192	CN(C)C1=C2C=NN(C)C2=NC=N1	177,21	C8H11N5
Z278101784	N[C@H](C(O)=O)C1=CC=CC=C1	151,17	C8H9NO2
Z118458680	COC1=C(C=C(C)C)C=C1)C(O)=O	186,59	C8H7ClO3
Z57790409	CCN1C(O)=CC(C)=C(C#N)C1=O	178,19	C9H10N2O2
Z256709352	CN1C=C(C)C(C(O)=O)=C1CC(O)=O	197,19	C9H11NO4
Z149205804	COC1=CC(OC)=C(C=C1)C(O)=O	182,18	C9H10O4
Z57127001	CC1=C(N)C=C(C=C1)C(O)=O	151,17	C8H9NO2
Z234895245	OC(=O)C1CCCN(C1)C1=NC=CC=C1	206,25	C11H14N2O2
Z1357827202	CCC1(C)CCC(N)CC1	141,26	C9H19N
Z1692721911	CN1N=CC=C1NCC1=C(Br)C=CS1	272,16	C9H10BrN3S
Z138328496	CNCCN1CCOCC1	144,22	C7H16N2O
Z228589394	NCC1=CC2=C(C(OCO2)C(Cl)=C1	199,63	C9H10ClNO2
Z1259339759	CC(OC1CCCC1)C(O)=O	158,20	C8H14O3
Z1333717723	CC1(CN)CCCCC1O	143,23	C8H17NO
Z1333043418	OC(=O)COC1CCOC1	146,14	C6H10O4
Z2218585849	CN(C)CCN1N=CC=C1N	154,22	C7H14N4
Z1347206051	CNS(=O)(=O)C1=CC(OC)=C(Cl)C=C1	235,68	C8H10ClNO3S
Z1346385378	CCN1N=C(N)C=C1C1CC1	151,21	C8H13N3
Z1342879026	COC(C)C1=NC(C)=C(S1)C(O)=O	201,24	C8H11NO3S
Z905065930	OC(=O)C1CC2CCC(C1)N2C1CC1	195,26	C11H17NO2
Z1336457495	CCOC1=C(N=CC=C1)C(O)=O	167,16	C8H9NO3
Z1333761729	OC1CCC2=C(C1)C=NN2	138,17	C7H10N2O
Z905065908	O=C1CC2CCC(CN1)N2	140,19	C7H12N2O
Z100449516	CC1=C(C=CO1)C(=O)NCC1=CC=CO1	205,21	C11H11NO3
Z1333043381	CC1=CC2=C(OC(N)=N2)C(C)=C1	162,19	C9H10N2O
Z1333043379	NC1=NN(CC2=CC=C(Cl)C=C2)C=N1	208,65	C9H9ClN4
Z1333043373	CNC(C)(C(O)=O)C1=CC=C(F)C=C1	197,21	C10H12FNO2
Z1815155448	CC1=NN2C(CN)=NN=C2C=C1	163,18	C7H9N5
Z85891019	OC(=O)C1CCCN1C(=O)C1=CC=CS1	225,26	C10H11NO3S
Z1814381679	CNC1=C(C=CC(F)=C1)C(O)=O	169,16	C8H8FNO2
Z1693055082	CC1CN(CCS1(=O)=O)C1=NC=CC=C1	226,29	C10H14N2O2S
Z1787355378	OCC1=C(Cl)C=C(C=C1)C#N	167,59	C8H6ClNO
Z444349690	OC(=O)CC1=NN(N=C1)C1=CC=CC=C1	203,20	C10H9N3O2
Z440824948	OC(=O)CC1=CC(=O)NN1	142,11	C5H6N2O3
Z432066922	CC1=NC(=O)NC(=C1)C(O)=O	154,13	C6H6N2O3
Z431973752	COCC1=NNC(N)=C1C1=CC=CC=C1	203,25	C11H13N3O
Z31112127	N#CC1=C(C(NCC2=CC=CS2)N=CC=C1	215,27	C11H9N3S
Z425484984	CN1C=C(C=CC1=O)C(O)=O	153,14	C7H7NO3
Z425449752	OC(=O)CC1=CS(C(=N1)N1CCNC1=O	227,24	C8H9N3O3S
Z425389558	CC1=C(C=CC(=N1)C(F)(F)F)C(O)=O	205,14	C8H6F3NO2
Z415636674	NC1CCN(CC1)C1=NC=CC=N1	178,24	C9H14N4
Z839575642	CC1=NOC(Cl)=C1CCC(O)=O	189,60	C7H8ClNO3
Z857666964	NC1=CC2=C(OC(=N2)C(F)(F)F)C=C1	202,14	C8H5F3N2O
Z839575850	CC1CCC(CC1)(NC(C)=O)C(O)=O	199,25	C10H17NO3
Z839028500	OC(=O)CN1C=CC(=O)C2=C1C=CC=C2	203,20	C11H9NO3
Z992716964	NC1=NN=C(CCC2=CC=CC=C2)O1	189,22	C10H11N3O
Z645562380	N#CC1=CN=C(C(NCC2=NC=CS2)C=C1	216,26	C10H8N4S
Z33545911	CCC1=C(C)SC(=C1)C(N)=O	169,24	C8H11NOS
Z225892438	CC1CC1C(=O)NCC1=NC(C)=CS1	210,30	C10H14N2OS
Z32366804	CC1=NC(CC(=O)NC2CC2)=CS1	196,27	C9H12N2OS
Z437351256	CC1=CC=C(CNC(=O)C2=CC=CO2)S1	221,27	C11H11NO2S
Z432725268	BrC1=C(SC=C1)C(=O)N1CCOCC1	276,15	C9H10BrNO2S
Z384362790	O=C(NCC1CCOC1)C1=NC=CN=C1	207,23	C10H13N3O2
Z1832147138	ClC1=CN=C(C(NCC2=CSN=N2)C=C1	226,68	C8H7ClN4S
Z169851686	CC1=CC(C)=C(N1)C1=CC=NC=C1	172,23	C11H12N2
Z2106600022	CN1C=CC(=N1)N1CC(C1=O)C(O)=O	209,21	C9H11N3O3
Z2510258114	CC(O)(CN1C=CC=CC1=O)C(O)=O	197,19	C9H11NO4
Z240127660	CC1=NN=C(O)C(N1)=CC1=CC=CC=C1	201,23	C11H11N3O
Z57842305	CC1=NC2=C(C(N)=NS2)C(C)=C1	179,24	C8H9N3S
Z223656256	CC(N1C=CC=C1)C(O)=O	139,15	C7H9NO2
Z135439900	CCN(CC)C(=O)C1=CC(C)=NO1	182,22	C9H14N2O2
Z1259086957	OCCN1CCC2=C(C1)C=CC=C2	177,25	C11H15NO
Z1267773500	CN1N=C(C)C(C2CCCN2)=C1C	179,27	C10H17N3
Z1465369619	CC1=C(C=CC(F)=C1)C(=O)N1CCCC1	207,25	C12H14FNO
Z228589876	CC(C)C(N)C1=NN=C2C=CC=CN12	190,25	C10H14N4
Z1415893926	CN1N=C(C)C(OCO(O)=O)=C1C	184,20	C8H12N2O3
Z228584062	COC1=C(CN2CCNCC2)C=CC=C1	206,29	C12H18N2O

Z1263820389	OCCN1C(=O)NCC2=C1C=CC=C2	192,22	C10H12N2O2
Z228569070	CC(CN)N1CCN(C)CC1	157,26	C8H19N3
Z2213893395	NC1=NC(C2CC2)=C(Br)C=C1	213,08	C8H9BrN2
Z26823525	CCC1=NN=C(NC(=O)C2CCCO2)S1	227,28	C9H13N3O2S
Z285925540	CC1=C(F)C=C(C=C1)C(=O)NCCN	196,23	C10H13FN2O
Z86430604	O=C(NC1CCS(=O)(=O)C1)C1CCCC1	231,31	C10H17NO3S
Z234898151	CC(=O)NC1(CCCC1)C(O)=O	171,20	C8H13NO3
Z234898083	O=C1NCCOC2=C1C=CC=C2	163,18	C9H9NO2
Z118257746	NC1=CC(=CC=C1)C(=O)NC1CC1	176,22	C10H12N2O
Z234897391	NCC1=CC=C(CN2CCCC2=O)C=C1	204,27	C12H16N2O
Z32412988	CC1=NC(CC(=O)NC2CCCC2)=CS1	224,32	C11H16N2OS
Z104753984	CC1=CC(CI)=C(NCC(N)=O)C=C1	198,65	C9H11ClN2O
Z26743843	COC1=C(CI)C=C(C(NC(=O)C2CC2)C=C1	225,67	C11H12ClNO2
Z220616780	C1CNCC(C1)C1=NC2=C(N1)C=CC=C2	201,27	C12H15N3
Z220383530	CN1NC(=O)C2=C(N=CC=N2)C1=O	178,15	C7H6N4O2
Z1750885079	CN1C=NN=C1NC(=O)C1CCCCO1	210,24	C9H14N4O2
Z111634624	CC1=NN2C(NC(C)=C(C)C2=O)=N1	178,20	C8H10N4O
Z1860991525	COC1=C(N)C=C(CI)C(CI)=C1	192,04	C7H7Cl2NO
Z1889710301	CN1CCC2=C(C1)C(=O)NC(C)=N2	179,22	C9H13N3O
Z1222278672	CN(C)C(C)(C(O)=O)C1=CC=C(F)C=C1	211,24	C11H14FNO2
Z1222278659	CC(C)C1=C(Br)C(=NN1)C(O)=O	233,07	C7H9BrN2O2
Z1166180442	CC1CN(C)CCN1C(=O)C1=CSN=N1	226,30	C9H14N4OS
Z433657690	CN(C)C(=O)CNC(=O)C1=C(Br)C=CS1	291,16	C9H11BrN2O2S
Z1022803746	CNC(=O)C(C)(C)C1=CC(Br)=CC=C1	256,14	C11H14BrNO
Z1836339155	C1CC(C1)C1=NC(=CS1)C1=NC=CC=C1	216,30	C12H12N2S
Z300114476	CC1CC(C)CN(C1)S(=O)(=O)N(C)C	220,33	C9H20N2O2S
Z1171979208	CNC(=O)C1(CCC1)C(O)=O	157,17	C7H11NO3
Z1205221212	CN(C)C(=O)C(C)(C)NC1CCCC=C1	210,32	C12H22N2O
Z1262237488	CC1=CC(=CC=C1)C(C)(C)CN	163,26	C11H17N
Z1269702257	CC(CN)OC1=CC=C(Br)C=C1	230,11	C9H12BrNO
Z1220645147	CC(C)N1C=CC(CN2C=C(CI)C=N2)=N1	224,69	C10H13ClN4
Z1103238697	CC(C)CN1CCCC1C1=CN(C)N=C1	207,32	C12H21N3
Z1262237327	OC(=O)C1=C(OC2CCC2)C=CC=C1	192,21	C11H12O3
Z2217052364	FC1=CN=C(C=C1)C1CCCCN1	180,23	C10H13FN2
Z2509351114	OC(=O)C1=CC2=C(COCC2)C=C1	178,19	C10H10O3
Z1955122823	COC1=C(N=CC=C1)C#N	134,14	C7H6N2O
Z2179017020	CC1=NC(NC2CC2)=CC(=C1)C#N	173,22	C10H11N3
Z2507919897	C1CC(CCO1)C1=NC=CN1	152,20	C8H12N2O
Z2507870689	CC1=NC(N)=C(C(N)=O)C(C)=C1	165,20	C8H11N3O
Z2492774535	CC(C)CCC1=NN=C(N)S1	171,26	C7H13N3S
Z2492774459	CC(CC(O)=O)N1CCC2=C1C=CC=C2	205,26	C12H15NO2
Z2379767265	CC(C)CC1=CSC(=N1)C1=NN=CN1	208,28	C9H12N4S
Z2379767447	NC1=C(N=NS1)C1=NC(=CS1)C1CC1	224,30	C8H8N4S2
Z2472860002	NC(C(O)=O)C1=C(F)C=C(F)C=C1	187,15	C8H7F2NO2
Z2088385280	N#CC1=NC=CC(=C1)N1CCCC1	187,25	C11H13N3
Z1269799982	CC1=CC=C(O1)C(=O)NCC1=CC=CN1	204,23	C11H12N2O2
Z1238477757	CN(C)C(=O)N1CCNCC1	157,22	C7H15N3O
Z71177490	CNC1=C(C=CC=N1)C(O)=O	152,15	C7H8N2O2
Z2471262531	OCC1=NN2C=CC=NC2=N1	150,14	C6H6N4O
Z2510258098	CC1NC2=C(NC1=O)C=CC=C2C(O)=O	206,20	C10H10N2O3
Z2510258288	OC(=O)C1=NC=CC(=C1)C1CC1	163,18	C9H9NO2
Z2510258172	CC(C)C1=NC(C)=C(O1)C(O)=O	169,18	C8H11NO3
Z2509351168	COC1=CC=C(C=C1)C1=NC(N)=NC=C1	201,23	C11H11N3O
Z2509351196	CC(C(N)C(O)=O)C1=CC=CC=C1	179,22	C10H13NO2
Z1982493931	OC(=O)CC1CC(C1)C1=CC=CC=C1	190,24	C12H14O2
Z353247326	CC(CO)NC(=O)C1=C(CI)C=C(F)C=C1	231,65	C10H11ClFNO2
Z1966493094	CC(C)(C1CCOCC1)C(O)=O	172,22	C9H16O3
Z1966492233	CC(N)(C(O)=O)C1=C(F)C=CC(Br)=C1	262,08	C9H9BrFNO2
Z1966487993	CCC1NC(=O)CCN(C)C1=O	170,21	C8H14N2O2
Z1948935031	COC1=CC=C(C=C1)C1=C(N)N=CC=N1	201,23	C11H11N3O
Z1947444015	CCC(C)C1=NC=C(N)C=N1	151,21	C8H13N3
Z839706072	CN(C1CC1)C(=O)CN1C=C(Br)C=N1	258,12	C9H12BrN3O
Z29418354	CC(C)C(=O)NC1=CC(CI)=C(C=C1)C#N	222,67	C11H11ClN2O
Z1272426173	CN1CCC(NC2=NC(C)=NS2)C1=O	212,27	C8H12N4OS
Z1983080486	OC1CCC(CC1)N1CCCC1=O	183,25	C10H17NO2
Z360008080	BrC1=CN(CC(=O)N2CCC2)C(=O)C=C1	271,11	C10H11BrN2O2
Z1664380857	COC1=NC(N)=C(N)C=C1	139,16	C6H9N3O

Z1632890379	NC(CC(O)=O)C1=CC(Cl)=CC(Cl)=C1	234,08	C9H9Cl2NO2
Z915781066	CCC(C)(C)NC(=O)C1=CN=C(C)S1	212,31	C10H16N2OS
Z235344291	CC1=C(SC2=C1C(C)=NC(C)=N2)C(O)=O	222,26	C10H10N2O2S
Z403317908	COCC(=O)NC1CCCCNC1=O	200,24	C9H16N2O3
Z56948440	CC(C)(N)C1=NC2=C(N1)C=CC=C2	189,26	C11H15N3
Z56822248	OC(=O)CNC(=O)C1=C(F)C=CC=C1	197,17	C9H8FNO3
Z57967260	O=C(NC1=NN=CS1)C12CCC(CC1)C2	223,29	C10H13N3OS
Z56782009	COC1=C(N)C=C(Cl)C=C1	157,60	C7H8ClNO
Z56764669	OC1CS(=O)(=O)CC1N1CCCCC1	219,30	C9H17NO3S
Z56763571	CN(C)C(=O)NC1CCS(=O)(=O)C1	206,26	C7H14N2O3S
Z1230023781	CC(=O)NC1=C2N=CNC2=CC=C1	175,19	C9H9N3O
Z2692095039	OC(=O)C1=CC=C(O1)C(F)F	162,09	C6H4F2O3
Z2692095137		152,20	C7H12N4
Z409512682	CC1CCCN(C1)C(=O)NC1=NN=CS1	226,30	C9H14N4OS
Z744843848	CC1=NN(C(=O)C1)C1=CC(N)=CC=C1	189,22	C10H11N3O
Z228589684	COC1=C(N)C(C(O)=O)=C(C)C=C1	181,19	C9H11NO3
Z1741957061	OC(=O)C1=C(C=C(F)C=C1)C(F)(F)F	208,11	C8H4F4O2
Z1749294408	ClC1=C(CN2N=CS2=O)N=NS1	234,68	C5H3ClN4OS2
Z1839480414		170,21	C9H14O3
Z1348371854	N#CC1=NC=C(C=C1)N1CCCOCC1	203,25	C11H13N3O
Z1348403112	CCC1=NSC(NC2CCN(C)C2=O)=N1	226,30	C9H14N4OS
Z1744194310	COC1=CC(OC)=C(Br)C=C1NC(C)=O	274,11	C10H12BrNO3
Z1699554930	CN1N=C(C)N=C1NCC1=CC=CS1	208,28	C9H12N4S
Z1331708554	O=C(NCC1=CCN=N1)C1CCCCC1	208,27	C10H16N4O
Z1824511110	CC1=C(OC(CC2CC2)=N1)C(O)=O	181,19	C9H11NO3
Z1627023416	CC1=NN(CCC(N)=O)C=C1Br	232,08	C7H10BrN3O
Z1258992483	CCC1=NNC(=O)C(C#N)=C1CC	177,21	C9H11N3O
Z31602731	CC1=C(SC=C1)C(=O)N1CCNC(=O)C1	224,28	C10H12N2O2S
Z822382694	CS(=O)(=O)CC(O)C1=CC=CC=C1	200,25	C9H12O3S
Z1255523318	OCCNC(=O)C1=NC=C(Br)C=C1	245,08	C8H9BrN2O2
Z1123870588	CNC(=O)COC1=C(F)C=CC(F)=C1	201,17	C9H9F2NO2
Z1250132721	CC(N)(CO)C1CCCCC1	157,26	C9H19NO
Z1250132677	NC1=C(C(OC(F)F)C=CC(=C1)C#N	184,15	C8H6F2N2O
Z1250132631	NCC1=CC(=CC=C1)N1CC=CC1	174,25	C11H14N2
Z1250132344	CN1N=NC2=C1C=CC(CO)=C2	163,18	C8H9N3O
Z1250132320	CC1=NC2=C(N1)C=C(Br)C=N2	212,05	C7H6BrN3
Z1196037098	OCC1CCCN(C1)C1CCCC=C1	209,33	C13H23NO
Z816005728	CCNC(=O)N(C)CC1=CSC(Br)=C1	277,18	C9H13BrN2OS
Z1259339957	CC(C)C1=C(C=NC(C)=N1)C(O)=O	180,21	C9H12N2O2
Z275170094	CCN1C=C(C=N1)C(O)=O	140,14	C6H8N2O2
Z275170014	CN1C=C(C(O)=O)C(C)=N1	140,14	C6H8N2O2
Z1259335802	CC1=C(C)C(=O)N=C(N1)C1=NC=CC=C1	201,23	C11H11N3O
Z1259273393		198,17	C10H8F2O2
Z85886697	OC(=O)CNC(=O)C1=C(Cl)C=CC=C1F	231,61	C9H7ClFNO3
Z1259273098	NC(C(O)=O)C1=C(F)C=CC=C1	169,16	C8H8FNO2
Z2689031620	OCC1=NN=C(S1)C1CC1	156,20	C6H8N2OS
Z1259339726	CC(O)(CN)C1=CC=CO1	141,17	C7H11NO2
Z1984948429	CC1(COC1)C(=O)NC1=CC(F)=CN=C1	210,21	C10H11FN2O2
Z1578034630	CN1C=C(C=N1)C(C)(O)CN	155,20	C7H13N3O
Z106307058	CC(C)N1CCN(CC1)C(=O)C(C)C	198,31	C11H22N2O
Z2527680084	CC1=CC(C(O)=O)=C(C)N1C1CCOC1	209,25	C11H15NO3
Z1994237215	FC(F)(F)C1=CC(CN2CCCC2)=NN1	219,21	C9H12F3N3
Z383325512	CC(=O)NCC1=CCN=C1	139,16	C6H9N3O
Z1171979275	CN1C=CC2=C1C=CC=C2C(O)=O	175,19	C10H9NO2
Z1171978796	CS(=O)(=O)C1=C(SC=C1)C(O)=O	206,23	C6H6O4S2
Z57335261	OC(=O)CN1CC2=C(C1)C=CC=C2	177,20	C10H11NO2
Z1171978814	OC(=O)CC1=CO(C=N1)C1=CC=CS1	209,22	C9H7NO3S
Z1171978854	CC(C)CC1=NC(=CS1)C(O)=O	185,24	C8H11NO2S
Z32016484	CNC(=O)C1=CC=C(Cl)S1	175,63	C6H6ClNOS
Z438096750	CC(=O)N1CCCC(CNS(C)(=O)=O)C1	234,31	C9H18N2O3S
Z1162910729	OC(C1CCNCC1)C1=CC=C(Cl)C=C1	225,72	C12H16ClNO
Z296759562	CC1=NOC(=N1)C1=CC=C(C=C1)C(N)=O	203,20	C10H9N3O2
Z203520994	ClC1=C(C=C(NC(=O)C2CC2)C=C1)C#N	220,66	C11H9ClN2O
Z19739280	CN(C)C(=O)COC1=CC=C(C=C1)C#N	204,23	C11H12N2O2
Z1160900191	NCCN1C(=O)CC2=C1C=CC=C2	176,22	C10H12N2O
Z1770193433	CC1=CC(=CS1)C1=C(N)C=CC=N1	190,26	C10H10N2S
Z1768428824	OC(=O)C1=CC(=NC=C1)C1CC1	163,18	C9H9NO2

Z1768160437	CC(=O)NC1(CCCCC1)C(O)=O	199,25	C10H17NO3
Z1259335792	OC(=O)C1=NC(=NC=C1)C1CC1	164,16	C8H8N2O2
Z1762997314	CC1=C(C1)C=CC(=C1)C(N)C(O)=O	199,63	C9H10CINO2
Z1762772460	CN(CC(O)=O)C1=CC=NC=C1	166,18	C8H10N2O2
Z1079512010	CC1=NOC(CN2N=C(C)C=CC2=O)=C1	205,22	C10H11N3O2
Z2467208649	CC(C)NC1=NC2=C(N1)C=CC=C2	175,24	C10H13N3
Z1603606316	OC(=O)C1(CC1)NC(=O)C1=CC=C(C1)S1	245,68	C9H8CINO3S
Z1715153919	CN1C(CCC1=O)C(O)=O	143,14	C6H9NO3
Z2211246663	COCCN1N=NC2=C1CCNC2	182,23	C8H14N4O
Z1263714198	C(N1CCNCC1)C1=NOC=C1	167,21	C8H13N3O
Z45537374	O=S(=O)(NC1CCCC1)C1=CC=CS1	231,33	C9H13NO2S2
Z2065616520	CCNC1CCN(CC1)C1=CC=NC=C1	205,31	C12H19N3
Z2073741691	C[C@H]1CN(C[C@H](C)O1)C(=O)COC(F)F	223,22	C9H15F2NO3
Z1583292089	CC1=NN=C(CNC2=CC(F)=CC=C2)S1	223,27	C10H10FN3S
Z2146515384	COC(C)(C)C1=NC(C)=C(S1)C(O)=O	215,27	C9H13NO3S
Z85923165	OCC1=CNC2=C1C=CC=C2	147,18	C9H9NO
Z2111525966	Cl.C1.NC1CCCN(CC(F)(F)F)C1	255,11	C7H15Cl2F3N2
Z2111526094	CN(C)C1=C(N=CC=C1)C#N	147,18	C8H9N3
Z2096659384	OC(=O)CCC1=C2C=CC=CC2=CN=C1	201,23	C12H11NO2
Z1273141584	NC(=O)C1=CC=C(OC2CCC2)C=C1	191,23	C11H13NO2
Z1218259484	CC1=C2CCN(CC(O)=O)CC2=CC=C1	205,26	C12H15NO2
Z2160887284	C1CCC2NCCNC2C1	140,23	C8H16N2
Z2160887173	NC(=O)C1CC1C(O)=O	143,14	C6H9NO3
Z2160887463	COC1=CNC(C)=NC1=O	140,14	C6H8N2O2
Z1438447167	CCN1CCC2=C(C1)C=CC=C2N	176,26	C11H16N2
Z1348417096	CN(CC1CCOC1)C1=C(C1)C=NC=C1	226,70	C11H15CIN2O
Z1694645445	NC1CCOC(C1)C1CC1	141,21	C8H15NO
Z265638758	NCC1=C(OC(F)F)C=CC(C1)=C1	207,60	C8H8ClF2NO
Z1230130478	CC(C)NC1=C(C=CC=N1)C(=O)N(C)C	207,28	C11H17N3O
Z212232234	CCC1=NN=C(CN2CCCC(C)C2)O1	209,29	C11H19N3O
Z1497321453	CC1=NC(C1=O)N2CCCC2=C(C)S1	210,30	C10H14N2OS
Z1359502847	C1CN(C2CCCC12)C1=NC=CN=C1	203,29	C12H17N3
Z1130244753	OC[C@H]1CCCN1CC1=C(C1)SN=N1	233,71	C8H12CIN3OS
Z1723418946	CC1=C(C=CC(N)=C1)C1CC1	147,22	C10H13N
Z1266823327	CC1=C(CCN)C(C)=NO1	140,19	C7H12N2O
Z1238477877	CC1=CC=C(O1)C1CCCN1	151,21	C9H13NO
Z234895145	NCC1CCCC2=C1C=CC=C2	161,25	C11H15N
Z2065543066	CC(C)OC1=CC2=C(NC=C2CN)C=C1	204,27	C12H16N2O
Z1276496842	CC(N)C1=CC(=CC=C1)C#N	146,19	C9H10N2
Z1142870697	CCC(CN)N1CCC2=C(C1)C=CC=C2	204,32	C13H20N2
Z422516090	CC1=C(SC=N1)C(=O)NCC1CCC1	210,30	C10H14N2OS
Z45527702	CNS(=O)(=O)C1=CC=C(C1)S1	211,68	C5H6CINO2S2
Z57229604	CC(C)(OC1=CC=C(Br)C=C1)C(O)=O	259,10	C10H11BrO3
Z373771058	CN1C=C(NC(=O)C2=CSC(Br)=C2)C=N1	286,15	C9H8BrN3OS
Z927756816	CC1=CN=C(NC(=O)CCN)C=C1	179,22	C9H13N3O
Z375692646	CN(CC1=NOC(C)=C1)C(=O)C1CCC1	208,26	C11H16N2O2
Z90507763	CC1CCC(CC1)NCC1=CN=CC=C1	204,32	C13H20N2
Z220996120	CC(NC(=O)C1CC1)C1=CN=CC=C1	190,25	C11H14N2O
Z31720228	CC1=NC(CC(=O)N2CCOCC2)=CS1	226,29	C10H14N2O2S
Z208155164	NC1CCC2=C1C=CC=C2	133,19	C9H11N
Z458888310	CC1=C(N=C(O1)C1=CC=CS1)C(N)=O	208,24	C9H8N2O2S
Z1891776347	OCC1CCCCN1C1=NC=NC=C1	193,25	C10H15N3O
Z1273141646	COCC1=CC(=NO1)C(N)=O	156,14	C6H8N2O3
Z2327039876	CC1=CC2=CNC(=O)C=C2C=C1	159,19	C10H9NO
Z2309759195	CN1N=CC=C1C1=NN=C(N)C=C1	175,20	C8H9N5
Z2309759186	NC1=CC(=CC=C1)C1CCC(=O)N1	176,22	C10H12N2O
Z2306625664	OC1=NC2=C(CCCC2)N=C1	150,18	C8H10N2O
Z2301438417	CN1N=C(C)C2=C1C(O)=NN=C2	164,17	C7H8N4O
Z2293607285	OCC1(CCOCC1)C(O)=O	160,17	C7H12O4
Z2284393895	CN1C(CC(O)=O)CCC1=O	157,17	C7H11NO3
Z1267881643	CC1NC2=C(NC1=O)C=CC=N2	163,18	C8H9N3O
Z1267773729	CC(C)S(=O)(=O)CC1=CC(N)=CC=C1	213,30	C10H15NO2S
Z1266933803	OC(=O)CN1CCOC2=C1C=C(C1)C=C2	227,64	C10H10CINO3
Z1258519607	CC1=CN=C(O1)C1=CC(N)=CC=C1	174,20	C10H10N2O
Z1266854838	CC(C)C1=NN(C)C(N)=N1	140,19	C6H12N4
Z1266854833	CC(C)(C1=NN=C(N)O1)C1=CC=CC=C1	203,25	C11H13N3O
Z1266854824	COC1=C(N)C(=CC(F)=C1)C(O)=O	185,15	C8H8FNO3

Z1263820422	CN1C=C(C=N1)C1=NN=C2CNCCN12	204,24	C9H12N6
Z1263820367	OCC(=O)N1CCOCC1	145,16	C6H11NO3
Z111583018	COC1=CC=C(C=C1)C1=NC(CN)=NO1	205,22	C10H11N3O2
Z1263716020	CN(C)C1=CC(=CC=C1)C1=NN=C(N)O1	204,23	C10H12N4O
Z1263602457	CCC1=CC=C(C=C1)C1=NOC(N)=C1	188,23	C11H12N2O
Z1263602430	CC(C)C1NCCNC1=O	142,20	C7H14N2O
Z2233919746	CC1=NSC(NCC2=C(C)N=CO2)=N1	210,26	C8H10N4O5
Z2417927388	CC1=CC(=O)N(CCC2(O)CCC2)C=C1	207,27	C12H17NO2
Z2234185684	O=C1CCCC(N1)C1=CC=CC=C1	175,23	C11H13NO
Z1413780550	CC(C)C(N)C1=C(F)C=C(F)C=C1	185,22	C10H13F2N
Z1569715342	COCCCN1(N)CCCC1	143,23	C8H17NO
Z275189668	NC1=C(F)C=CC(=C1)C(F)(F)F	179,12	C7H5F4N
Z1263529765	NCC1=CC2=C(C(OCCCO2)C=C1	179,22	C10H13NO2
Z275728064	CCC1=NOC(=N1)C(C)N1CCOCC1	211,27	C10H17N3O2
Z90517862	CC1=CC=C(CNC2CC2)O1	151,21	C9H13NO
Z1354376234	OC1CN(C1)C1=C(F)C=C(Cl)C=N1	202,61	C8H8ClFN2O
Z1250120913		196,67	C11H13ClO
Z1575143883	CC1=NOC(=N1)C(N)CO	143,15	C5H9N3O2
Z744843378	CC1=C(N=NN1C1=CC=CC=C1)C(O)=O	203,20	C10H9N3O2
Z744754626	COC1=C(C=CC(C)=N1)C#N	148,17	C8H8N2O
Z2179640362	CC1=C(N=CC=N1)N1CCC=C(F)C1	193,23	C10H12FN3
Z1373447292	CN(CC1=NC=CS1)C1=C(F)C=CC=N1	223,27	C10H10FN3S
Z2272040458	FC1=CCN(C1)C(=O)C1=NSC=C1	212,24	C9H9FN2O5
Z1798482785	CC1CCN(C1CO)C1=C(F)C=CC=N1	210,25	C11H15FN2O
Z1270783121	CN(C)S(=O)(=O)C1=C(C)C(F)=CC=C1	217,26	C9H12FNO2S
Z1583292057	CC1=NN=C(CNC2=CC=C(F)C=C2)S1	223,27	C10H10FN3S
Z172492308	NCC1=C(OC(F)(F)F)C=CC=C1	191,15	C8H8F3NO
Z2272532508	NC1=CC(CC2CC2)=NN1	137,19	C7H11N3
Z2235831703	CN1C=C(N)C(=N1)C(=O)NC1CCCC1	208,27	C10H16N4O
Z2235831719	CN1C=C(N)C(=N1)C(=O)NC1CCCC1	194,24	C9H14N4O
Z31424008	O=C(CC1=CC=CS1)N1CCCCC1	209,31	C11H15NO5
Z1255451841	NC1CCC2=C(CC1)C=CC=C2	161,25	C11H15N
Z1849012580	COC1(CCCC1)C(O)=O	144,17	C7H12O3
Z2235681153	COC1COCCC1CC(O)=O	174,20	C8H14O4
Z2309761167	COCC1CCC(N)CC1	143,23	C8H17NO
Z2442270563	C(C1CCNCC1)C1=NC(=NO1)C1CC1	207,28	C11H17N3O
Z2240988424	COCC1(CN)CCCC1	143,23	C8H17NO
Z2293643743	COCC1(CCCC1)C(O)=O	158,20	C8H14O3
Z85935506	OCC1=CC2=C(OCCO2)C(Cl)=C1	200,62	C9H9ClO3
Z57054208	CC1=CC=C(CN2N=CC=C2N)O1	177,21	C9H11N3O
Z85923459	CC(=O)N1CCC[C@H]1C(O)=O	157,17	C7H11NO3
Z85920643	CC1=NC2=C(O1)C=CC(N)=C2	148,17	C8H8N2O
Z27749489	CC(=O)NCC1=CC=CC=C1	149,19	C9H11NO
Z57900336	COC1=CC(OC)=C(OC)C=C1C#N	193,20	C10H11NO3
Z57980675	CC1=C(CN2N=CC=C2N)SC=C1	193,27	C9H11N3S
Z57049319	CCNC1=NN=C(S1)C1=CC=NC=C1	206,27	C9H10N4S
Z57047005	CC(C)(OC1=CC=C(F)C=C1)C(O)=O	198,19	C10H11FO3
Z57041992	CC1=NN(N=C1C(O)=O)C1=CC=CC=C1	203,20	C10H9N3O2
Z57002442	Cl.CN(C)S(=O)(=O)C1=C(Cl)C=CC(N)=C1	271,16	C8H12Cl2N2O2S
Z55692894	CC1=NC2=C(N1)C=CC=C2	132,17	C8H8N2
Z823291756	CC1CN(CCO1)C1=NC=C(CN)C=C1	207,28	C11H17N3O
Z45527656	CNS(=O)(=O)C1=CC=CS1	177,24	C5H7NO2S2
Z815264188	OC(=O)C1=CC2=C(NC(=O)C2)C=C1	177,16	C9H7NO3
Z815264300	CC1=C(F)C=C(C=C1)C1=NN=C(N)O1	193,18	C9H8FN3O
Z815264098	CC1=C(C=CC=C1N)C(=O)NCCO	194,23	C10H14N2O2
Z815264032	COC1=CC(N)=C(NC(C)=O)C=C1	180,21	C9H12N2O2
Z396120220	CN1C=C(NC(=O)CC2=CC=CS2)C=N1	221,28	C10H11N3O5
Z332767782	CNC(=O)CN(C)C(=O)C1=CSC(Br)=C1	291,16	C9H11BrN2O2S
Z351739896	CN(C)S(=O)(=O)N1CCN(CC1)C(C)=O	235,30	C8H17N3O3S
Z25081029	NC(=O)COC1=C(Br)C=C(F)C=C1	248,05	C8H7BrFNO2
Z79434398	ClC1=CC=C(O1)C(=O)N1CCOCC1	215,63	C9H10ClNO3
Z752989054	CC1=NN2C=C(C=NC2=C1)C#N	158,16	C8H6N4
Z752371208	N#CC1=CN=C(C=C1)N1CCNCC1	188,23	C10H12N4
Z19727416	CC(OC1=CC=C(Cl)C=C1)C(N)=O	199,63	C9H10ClNO2
Z228465246	FC1=CC(CN2C=NC(=N2)C#N)=CC=C1	202,19	C10H7FN4
Z57451303	CC(=O)NC1C2CC3CC(C2)CC1C3	193,29	C12H19NO
Z31490284	CC1=CC=C(S1)C(=O)NCC1CCCO1	225,31	C11H15NO2S

Z394693564	CS(=O)(=O)NC1CCCNC1	178,25	C6H14N2O2S
Z285782398	CN(C)C1=NC=CC(=C1)C(O)=O	166,18	C8H10N2O2
Z381429064	CC1=C(C=CC=C1N)C(N)=O	150,18	C8H10N2O
Z228463944	FC1=CC=C(CN2C=NC(=N2)C#N)C=C1	202,19	C10H7FN4
Z344080996	C1C1=CC=C(CNC(=O)C2=CC=CO2)S1	241,69	C10H8ClNO2S
Z219098968	CN(CCO)C1=NC=C(C=C1)C#N	177,21	C9H11N3O
Z367678734	CN(C)C1=NC=CC(=C1)C#N	147,18	C8H9N3
Z367451180	OC(=O)CN1C=CC=NC1=O	154,13	C6H6N2O3
Z367450968	CC1=CC=C(O1)C1=NC(CC(O)=O)=CS1	223,25	C10H9NO3S
Z63851050	C1C1=CC=C(O1)C(=O)NCC1=CC=CS1	241,69	C10H8ClNO2S
Z2469998600	O=C1CCC2=C(N1)N=CC=C2	148,17	C8H8N2O
Z2469606500	COC1=CC2=C(C=C1)C(=O)NCCO2	193,20	C10H11NO3
Z2466617840	CN1C(C)=CC(N)=C(N)C1=O	153,19	C7H11N3O
Z2442102818	OC(=O)C1CCOC2=C1C=C(Br)C=C2	257,08	C10H9BrO3
Z2007151852	CC(O)CS(=O)(=O)C1=C(C)C=C(C)C=C1	228,31	C11H16O3S
Z2412196571	CN1N=NC2=C1C=CC(N)=C2	148,17	C7H8N4
Z1266823370	CC(N)CN1C=C(C)C=N1	139,20	C7H13N3
Z1263529811	CCN1CCC(CCN)CC1	156,27	C9H20N2
Z1436181107	CC(N)CC1=CC(Br)=C(F)C=C1	232,10	C9H11BrFN
Z1269750463	CC1COC2=C(N1)C=CC=C2	149,19	C9H11NO
Z1269702290	CCC1=CC=C(O1)C1CCCN1	165,24	C10H15NO
Z235336609	COC1=CC(Br)=C(OC)C=C1C(O)=O	261,07	C9H9BrO4
Z223688272	CN(C(C)=O)C1=C(C=CC=C1)C(O)=O	193,20	C10H11NO3
Z234855718	OC(=O)C1=CC2=C(OC1)C=CC(Br)=C2	255,07	C10H7BrO3
Z45509018	FC1=CC=C(C=C1)S(=O)(=O)N1CCCC1	229,27	C10H12FNO2S
Z33546508	NC(=O)CC1=CC=CC=C1	135,17	C8H9NO
Z169856680	CC1=CC=C(S1)S(=O)(=O)N1CCNCC1	246,34	C9H14N2O2S2
Z53111117	OC(=O)CCN1C=CN=C1	140,14	C6H8N2O2
Z1250080950	CC1=C(C)C(=CC=C1)C(N)CC(O)=O	193,25	C11H15NO2
Z335931386	OCCN1C=NC2=C(SC=C2)C1=O	196,22	C8H8N2O2S
Z1250080895	CCC1=NN=C(CO)N1C	141,17	C6H11N3O
Z1238477814	CC(C)C(O)C1=NC=CN1C	154,21	C8H14N2O
Z319545618	CC1=NC=CN1CC1=CC(=CC=C1)C#N	197,24	C12H11N3
Z274553584	CC(CC(O)=O)N1N=C(C)C=C1C	182,22	C9H14N2O2
Z31602953	BrC1=CC=C(S1)C(=O)N1CCNC(=O)C1	289,15	C9H9BrN2O2S
Z228589680	CC1=C(N)C(C(O)=O)=C(F)C=C1	169,16	C8H8FNO2
Z1222423407	CC1=NNC(=N1)C1=CC=C(C=C1)C#N	184,20	C10H8N4
Z1222331426	CC(N)(C(O)=O)C1=C(F)C=CC(F)=C1	201,17	C9H9F2NO2
Z1222331421	CC(N)(C(O)=O)C1=CC(Br)=CC=C1	244,09	C9H10BrNO2
Z31407850	CC(=O)NCC1=CC=CO1	139,15	C7H9NO2
Z1209494589	COCC(C)N1CCN(CC1)C(C)=O	200,28	C10H20N2O2
Z1258955447	CCOC1=C(C)C=C(CO)C=C1C	180,25	C11H16O2
Z1250132782	NC1(CCCCC1)C1=CC=CS1	181,30	C10H15NS
Z1269702473	CC(N1CCC(N)CC1)C1=CC=CC=C1	204,32	C13H20N2
Z1139408804	CC(C)=CCNC1CCC2=NC=NN2C1	206,29	C11H18N4
Z1259087075	CC1=CC2=C(CC(C)(C)CC2N)O1	179,26	C11H17NO
Z1139247397	CNC1CCCN(C1)C1=NN=C(C)C=C1	206,29	C11H18N4
Z2235814827	OCC1(CCC(=O)NC1)C1=CC=CC=C1	205,26	C12H15NO2
Z1255445535	COC1=C(C)N=CC(=C1)C#N	148,17	C8H8N2O
Z361819214	C1C1=CC=C(CNC2=C(C=NN2)C#N)S1	238,69	C9H7ClN4S
Z1509046220	OC(=O)CC1=CC2=C(C=CC=C2)C(=O)N1	203,20	C11H9NO3
Z2236664380		154,21	C8H14N2O
Z2235810124	CC(C)C1=C(SC=N1)C(O)=O	171,21	C7H9NO2S
Z1795826584	COCC1CNCC(C)O1	145,20	C7H15NO2
Z1262254434	CC1=NOC(N)=C1C1=CCCCC1	178,24	C10H14N2O
Z2255110188	COC1=C2C=CC=C(N)C2=CC=N1	174,20	C10H10N2O
Z1262237471	CC(C)OCC1=C(C)C(N)=CC=C1	179,26	C11H17NO
Z85895577	CN(CC(O)=O)C(=O)C1=CC=C(Br)S1	278,12	C8H8BrNO3S
Z1245580492	NCC1=C(C=C(F)C=C1)C(F)(F)F	193,15	C8H7F4N
Z1992316315	CN1CCN(CCN)CC1(C)C	171,29	C9H21N3
Z1962356423	CCC1=C(ON=C1N)C(F)(F)F	180,13	C6H7F3N2O
Z1956875765	CC(C)C1=NN(C)C=C1N	139,20	C7H13N3
Z1318110042	CC#CCN(C)C1CCS(=O)(=O)CC1	215,31	C10H17NO2S
Z168883358	CC(=O)N1CCCNCC1	142,20	C7H14N2O
Z1895554336	CNCC1CCC2=NC=CN2C1	165,24	C9H15N3
Z217102746	NC(C1CC1)C1=CC=CS1	153,24	C8H11NS
Z1649893385	CC1=NOC(=C1C(O)=O)C1=CC=CC=C1	203,20	C11H9NO3

Z1696861512	OC1=NN=C2CCNCC2=C1	151,17	C7H9N3O
Z1696822743	OC(C1CCOCC1)C(O)=O	160,17	C7H12O4
Z1917790067	OCC1=NC(=CS1)C1=NC=CC=C1	192,24	C9H8N2O5
Z1998612790	C1CNC(CN1)C1=CC=NC=C1	163,22	C9H13N3
Z32279730	COCC(=O)N1CCCC(C1)C(N)=O	200,24	C9H16N2O3
Z1741969215	OC(=O)[C@H]1CCCC(=O)N1	143,14	C6H9NO3
Z2017679577	O=C1CC=NN1CC1=CC=CC=C1	174,20	C10H10N2O
Z2010051583	COC(C)C1=NSC(N)=N1	159,21	C5H9N3O5
Z2009850714	NC1=C(C=C2CCCC2=C1)C(O)=O	191,23	C11H13NO2
Z2009851541	OC(=O)C1=C2NCCC2=CC=C1	163,18	C9H9NO2
Z1642061111	CCC1=NO(C(=N1)C1=CC(CI)=C(N)C=C1	223,66	C10H10CIN3O
Z1625822300	CC(C)CC1CC(C(C(=O)N1)C(O)=O	199,25	C10H17NO3
Z1601554962	CC1CC(CCO1)C(O)=O	144,17	C7H12O3
Z1601555025	NC(C(O)=O)C1=CC=C(CI)C=C1	185,61	C8H8CINO2
Z227975776	CN(C)C1=NC(C)=C(S1)C(O)=O	186,23	C7H10N2O2S
Z319024806	CC1=C(C)C(C#N)=C(NCC2CC2)N=N1	202,26	C11H14N4
Z1575304440	O=C1CC2=C(N1)C=CC=N2	134,14	C7H6N2O
Z1575143797	CCS(=O)(=O)C1=C(CI)C=CC(N)=C1	219,68	C8H10CINO2S
Z1642389924	COC1=C(C=CC=C1N)C(N)=O	166,18	C8H10N2O2
Z1642389727	CCC1=CC(=CC(=O)N1)C(O)=O	167,16	C8H9NO3
Z1699556624	CN1C=C(CNC2=NC(C)=NN2C)C=N1	206,25	C9H14N6
Z228586822	O=C(CCN1=CC=CS1)N1CCNCC1	210,30	C10H14N2O5
Z241190530	O=C(CCN1C=NC=N1)N1CCOCC1	210,24	C9H14N4O2
Z1270246351	OC(=O)C1CCCCC1	142,20	C8H14O2
Z1269702273	NCCN1C=C(C=N1)C#N	136,16	C6H8N4
Z27797391	COC1=C(NC(=O)C(C)C)C=CC=C1	193,25	C11H15NO2
Z1357827195	CC1CCC2=C(C=CC=C2F)C1N	179,24	C11H14FN
Z1160899527	CC1(N)CCC2=C1C=CC=C2	147,22	C10H13N
Z1979756072	CC1CN(CC2=C(C)N(C)N=C2C)C1	193,29	C11H19N3
Z1262252948	NC1=CC=NN1CC1CCOC1	167,21	C8H13N3O
Z927756398	CC1=NC(NC(=O)C(C)C(N)=CC=C1	193,25	C10H15N3O
Z228589692	CC1=C(C(O)=O)C(N)=C(F)C=C1	169,16	C8H8FNO2
Z1675167140	CN1N=NC2=C1C=C(C=C2)C(O)=O	177,16	C8H7N3O2
Z2235810235	CC1=C(CO)N=CC=C1N	138,17	C7H10N2O
Z2235790653	OC(=O)CC1=CNC(=O)C=C1	153,14	C7H7NO3
Z2235790638	CC1=C(F)C=C(CC(O)=O)C(F)=C1	186,16	C9H8F2O2
Z2235681414	OC(=O)C1=C2CCCN2N=C1	152,15	C7H8N2O2
Z2235681291	CCC1=NC(=O)C(C)=C(N)N1	153,19	C7H11N3O
Z2230911536	O=C1CC2=C(CN1)C=CC=C2	147,18	C9H9NO
Z2230911380	CC1=CC2=C(C=NN2C=C1)C(O)=O	176,18	C9H8N2O2
Z2218555757	CCN1N=NC(C)=C1C(O)=O	155,16	C6H9N3O2
Z2218555806	NCCC1=CN2N=CC(CI)=C2N=C1	196,64	C8H9CIN4
Z1781322218	BrC1=CC=C(CNC(=O)C2=NNC=C2)O1	270,09	C9H8BrN3O2
Z2574360289	CNC1=C(F)C=C(C=C1)C(O)=O	169,16	C8H8FNO2
Z2568751830	NC(=O)C1CNCCN1C1CC1	169,23	C8H15N3O
Z2568751751	OC(=O)C1=C2CCCCN2C=C1	165,19	C9H11NO2
Z2523459941	CC1=CC=CN2C(N)=CN=C12	147,18	C8H9N3
Z2466639957	COC1=C(C=CC=C1)C1=NC(N)=NC=C1	201,23	C11H11N3O
Z2517219392	CC1(C)CNC(=O)CC(C)(C)C1	169,27	C10H19NO
Z2515399703	O=C1NCC(N1)C1=CC=CC=C1	162,19	C9H10N2O
Z2515207584	FC(F)C1=NC=C(C=C1)C#N	154,12	C7H4F2N2
Z2512942913	OCC1=CC2=C(O1)C=CN=C2	149,15	C8H7NO2
Z2512942927		143,19	C7H13NO2
Z2512942883	CC1=NC(NC2CC2)=CC(=C1)C(O)=O	192,22	C10H12N2O2
Z1245537934	CC(C)C1=CC(=NO1)C(O)=O	155,15	C7H9NO3
Z1924086866	NC(=O)C1=C(C(C(O)=O)C=CC=C1	179,18	C9H9NO3
Z57111831	CC1=C(C=NN1C1=CC=CC=C1)C(O)=O	202,21	C11H10N2O2
Z137579644	C(NC1=CC=CC=C1)C1=CSC=N1	190,26	C10H10N2S
Z90666965	CC1=NNC(=O)C(C#N)=C1C	149,15	C7H7N3O
Z94599150	COC1=C(F)C=C(C=C1)C(C)N	169,20	C9H12FNO
Z94601171	NC(CC(O)=O)C1=CC=CC=C1	165,19	C9H11NO2
Z90123329	CC(N)C1=CC2=C(C(CCC2)C=C1	175,28	C12H17N
Z31408631	CC1=CC=C(O1)C(O)=NCC1=CC=CO1	205,21	C11H11NO3
Z56887675	CC1=CC(=CC(C)=C1)C(=O)NCC(O)=O	207,23	C11H13NO3
Z56945500	C[C@H](NC(=O)C1=C(C)C=CC=C1)C(O)=O	207,23	C11H13NO3
Z56871698	OC(=O)CC1=NNC(=O)C2=C1C=CC=C2	204,19	C10H8N2O3
Z56912098	NC(=O)N1CCCCC1	142,20	C7H14N2O

Z56911968	CN1N=C(C=CC1=O)C(O)=O	154,13	C6H6N2O3
Z56907638	CCC(CC)C1=NN=C(N)S1	171,26	C7H13N3S
Z56899123	NC(CC(O)=O)C1=CC(Br)=CC=C1	244,09	C9H10BrNO2
Z56899025	CN1C(=O)CC2=C1C=CC=C2	147,18	C9H9NO
Z56895352	CC1=CC(=O)NC(=N1)N1CCOCC1	195,22	C9H13N3O2
Z56893095	CC(=O)NC1=C(Br)C=CC(OC(F)F)=C1	280,07	C9H8BrF2NO2
Z56887666	OC(=O)CNC(=O)C1CCCCC1	185,22	C9H15NO3
Z56886577	COC1=CC2=C(OC(C(O)=O)=C2C)C=C1	206,20	C11H10O4
Z56858180	CC(=O)NC1=CC(OC(F)F)=C(C)C=C1	215,20	C10H11F2NO2
Z56827662	OC(=O)CNC(=O)C1=CC=C(Br)C=C1	258,07	C9H8BrNO3
Z56824302	NC(CC(O)=O)C1=CC(F)=CC=C1	183,18	C9H10FNO2
Z56798541	C1CCN=C(CC1)NC1=NN=CS1	196,27	C8H12N4S
Z56757309	OC1C2CC3CC(C2)CC1C3	152,24	C10H16O
Z86417440	O=C(NC1=NN=CS1)C1CCC=CC1	209,27	C9H11N3OS
Z281802060	CNC1=NC(OC)=CC=N1	139,16	C6H9N3O
Z1431904023	CS(=O)(=O)C1=CC2=C(OCCN2)C=C1	213,25	C9H11NO3S
Z1428158219	FC(F)(F)C1CCCC(=O)N1	167,13	C6H8F3NO
Z1416282409	NC1=C(N=CN=C1)N1CCCCC1	164,21	C8H12N4
Z1407673104	CCC1=NNC(=O)C(C(O)=O)=C1CC	196,21	C9H12N2O3
Z1272495640	OCCCCCN(C1)C1=NC=C(Br)C=N1	272,15	C10H14BrN3O
Z228589694	CC1=C(N)C(C(O)=O)=C(CI)C=C1	185,61	C8H8ClNO2
Z1407007540	CC1=C(C)C(=O)NNC1=O	140,14	C6H8N2O2
Z1407007537	COC1=C(OC)C=C(C(O)=O)C(C)=C1	196,20	C10H12O4
Z1275480355	CC1=NSC(NC(=O)C2=CN=CC=C2)=N1	220,25	C9H8N4OS
Z1365534348	CCC1=NOC(=N1)C1=C(N)C=CC(CI)=C1	223,66	C10H10ClN3O
Z1362754540	C1CNC2=C(N1)C=CN=C2	135,17	C7H9N3
Z1362754516	COC1=COC(CO)=CC1=O	156,14	C7H8O4
Z1359881911	CCC1(C)CCNC(=O)CC1	155,24	C9H17NO
Z1217910533	NCC1CC2=C(O1)C=CC=C2	149,19	C9H11NO
Z1192379004	NCC1=C(C=CC=C1)N1CCNCC1	191,28	C11H17N3
Z1259197166	CC(O)(CN)CN1CCOCC1	174,24	C8H18N2O2
Z1259339799	CC1CCCC(C1)OCC(O)=O	172,22	C9H16O3
Z56957556	CNCC1=C(OC)C=CC(Br)=C1	230,11	C9H12BrNO
Z1252398313	OC1(CNC2=NC=CC=C2)CCOCC1	208,26	C11H16N2O2
Z600584282	CC1=C(CN)C(F)=CC=C1	139,17	C8H10FN
Z1267773566	CC(C)C(N)C1=NC(C)=NO1	155,20	C7H13N3O
Z1267773595	CCC1=NC(=CS1)C(C)N	156,25	C7H12N2S
Z2168515496	COC1=CC2=C(C=CN2)C(F)=C1	165,17	C9H8FNO
Z1891775757	CC(=O)N1CCNCC1(C)C	156,23	C8H16N2O
Z1431002647	CCOC1=C(N)C=CC(Br)=C1	216,08	C8H10BrNO
Z1381271437	CC(O)COC1CCOC1	146,19	C7H14O3
Z2050725052	CC(C)OC1=C(C=CC=N1)C#N	162,19	C9H10N2O
Z1878656559	CC1CC(C)(C)CC1NCC1=NNC=C1	207,32	C12H21N3
Z56347482	CC(N)C1=CC(=CC=C1)C(F)(F)F	189,18	C9H10F3N
Z1878440717	FC1=C(NCC2=NC=CS2)C(CI)=CC=C1	242,70	C10H8ClFN2S
Z431807512	CC(C)N(C)S(=O)(=O)N1CCNC(=O)C1	235,30	C8H17N3O3S
Z643741552	CC1=CN2N=C(NCC3CC3)SC2=N1	208,28	C9H12N4S
Z391963058	CNC(=O)C1=CC(=NO1)C1=CC=CC=C1	202,21	C11H10N2O2
Z422500504	CNC(=O)C1=C(C)OC(=N1)C1=CC=CS1	222,26	C10H10N2O2S
Z33547160	NC(=O)CC1CCCCC1	141,21	C8H15NO
Z594293916	CCC(C)N(C)C(=O)NC1=NN=CS1	214,29	C8H14N4OS
Z1272684690		191,23	C11H13NO2
Z274554318	CC(CN1N=C(C)C(Br)=C1C)C(O)=O	261,12	C9H13BrN2O2
Z1271843038	CCC1CCNC(=O)CC1	141,21	C8H15NO
Z2680629402	CCC1=NOC(=N1)C1(O)CCNC1	183,21	C8H13N3O2
Z1309300216	CC1=CC2=C(NC=C2CCC(O)=O)C=C1	203,24	C12H13NO2
Z29885101	CC(=O)NCC1COC2=C(O1)C=CC=C2	207,23	C11H13NO3
Z274553704	CN(C)S(=O)(=O)N1N=C(C)C(CI)=C1C	237,70	C7H12ClN3O2S
Z1717425227	FC1=CCCN(CC2=NNC=C2)C1	181,21	C9H12FN3
Z2001746360	CC1(C)CNC(=O)CN1C(=O)CCC=C	210,28	C11H18N2O2
Z1993937260	CC(O)CS(=O)(=O)C1=C(CI)C=CC=C1	234,69	C9H11ClO3S
Z57719465	CCN(CC)C(=O)C1=C(C)N=C(C)S1	212,31	C10H16N2OS
Z228576766	CC(C)C(CN)N1CCCC(C)CC1	184,33	C11H24N2
Z927400026	CC(C)C(N)C(=O)N1CCOCC1	186,26	C9H18N2O2
Z1259339823	CN1C=C(C=N1)C1CCCN1	151,21	C8H13N3
Z1262396047	CC1=CC(=NO1)C1CCCN1	152,20	C8H12N2O
Z2182115556	CC(C)C1=NC(C)=C(CO)O1	155,20	C8H13NO2

Z2001745807	COCC(=O)N1CC(=O)NCC1(C)C	200,24	C9H16N2O3
Z1891772416	CC1=NOC(C2CC2)=C1C(O)=O	167,16	C8H9NO3
Z2065464277	CCN(C1CCCC1)C1=NC(N)=NC=C1	206,29	C11H18N4
Z1286244967	CC1=NC(=CS1)C(=O)NCC(C)(C)O	214,28	C9H14N2O2S
Z68591039	COC1=CC2=C(OC(C(N)=O)=C2C)C=C1	205,21	C11H11NO3
Z980250586	CN1N=CC=C1NC(=O)C1=CN=CC=C1	202,22	C10H10N4O
Z1796663008	CC1=CSC(=O)N1CC1=NC=C(Cl)C=C1	240,71	C10H9ClN2OS
Z2037273251	CC(C)C1=CC(C(O)=O)=C(C)O1	168,19	C9H12O3
Z1874299552	CC(C)=CCNC1=C(Cl)C(N)=NC=N1	212,68	C9H13ClN4
Z1899186978	CC(=CC1=CC(Cl)=CS1)C1=NC=CN=C1	236,72	C11H9ClN2S
Z2033454399	CCOC1(CCCC1)C(O)=O	158,20	C8H14O3
Z1270502322	CC(O)(CN)C1=CC=CS1	157,23	C7H11NOS
Z1270446342	NCCC(O)C1=CC=CC=C1	151,21	C9H13NO
Z1270399997	N[C@@H](CC(O)=O)C1=C(F)C=CC=C1F	201,17	C9H9F2NO2
Z1270392238	OC(=O)C1=NC=CC(NC2CC2)=C1	178,19	C9H10N2O2
Z1270387220	CC1CC2=C(O1)C(=CC=C2)C(O)=O	178,19	C10H10O3
Z1270358387	COC1=C(SC(C)=C1)C(O)=O	172,20	C7H8O3S
Z1269638567	CS(=O)(=O)C1=C(N)SC=C1	177,24	C5H7NO2S2
Z1269638426	CC(C)C(C(O)=O)C1=CC=CC=C1	178,23	C11H14O2
Z1268152385	CNC1=CC=C(OC2=NC=CC=C2)C=C1	200,24	C12H12N2O
Z1268152298	OC(=O)C1=CN(CC2=CC=CS2)N=N1	209,22	C8H7N3O2S
Z32733538	COCC(=O)NC1=CC(=CC=C1)C#N	190,20	C10H10N2O2
Z1262250857	NC1=NN(CC2=NC=CC=C2)C=N1	175,20	C8H9N5
Z1262246182	CC1=CC(=C(C)C=C1)C1=NC(N)=NN=C1	200,25	C11H12N4
Z2658865738	CCC1CCCC(N)(CC1)C(O)=O	185,27	C10H19NO2
Z2630949151	OCC#CC1=C(F)C(F)=CC=C1	168,14	C9H6F2O
Z2588063768	CN1C=C(C(O)=O)C(=N1)C1=CC=CO1	192,17	C9H8N2O3
Z1741980286	CC1=CC(F)=C(C(O)=O)C(F)=C1	172,13	C8H6F2O2
Z2582143609	OC(CC1=CC=CC=C1)C(O)=O	166,18	C9H10O3
Z2574910555	NC(C(O)=O)C1=C(Cl)C(Cl)=CC=C1	220,05	C8H7Cl2NO2
Z2106599118	CCC1=NOC(=C1)C(O)=O	141,13	C6H7NO3
Z2106594207	CCC(C)N1C=C(Cl)C(=N1)C(O)=O	202,64	C8H11ClN2O2
Z2510259566	CC(C)OC1=C(C=CC=N1)C(O)=O	181,19	C9H11NO3
Z275169746	CCN1C=CC(=N1)C(O)=O	140,14	C6H8N2O2
Z223658280	CCC(N1C=CC=N1)C(O)=O	154,17	C7H10N2O2
Z2510259351		198,17	C10H8F2O2
Z2510259339	CC1=NOC=C1CC(O)=O	141,13	C6H7NO3
Z2106601614	CC1=CC2=CN(CC(O)=O)N=C2N=C1	191,19	C9H9N3O2
Z2412196484	CC1=C(C2CCC(=O)N2)C(C)=NN1	179,22	C9H13N3O
Z2412196603	CCC1=C(C)C(=O)N=CN1	138,17	C7H10N2O
Z1154745738	OC(=O)CN1C=NC=CC1=O	154,13	C6H6N2O3
Z2379802671	CNC1=NC=CC(OC)=C1	138,17	C7H10N2O
Z2379087815	CC1=C2OC=C(C(O)=O)C2=CC=C1	176,17	C10H8O3
Z2372279075	CS(=O)(=O)C1=CC=C(S1)C(O)=O	206,23	C6H6O4S2
Z2350907421	CCN1CCC(=O)NC2(CCCC2)C1=O	210,28	C11H18N2O2
Z1263529630	CS(=O)(=O)C1=C(F)C=C(N)C=C1F	207,19	C7H7F2NO2S
Z1263529612	CC(N)C1=CC(=CC=C1)S(=O)(=O)N(C)C	228,31	C10H16N2O2S
Z1263529583	CC(C)CC1=NN=C(N)O1	141,17	C6H11N3O
Z1213677549	CC1=CC=C(C=C1)C1=NN=C(N)O1	175,19	C9H9N3O
Z86893741	CC(C)C(=O)NC1=NON=C1C	169,18	C7H11N3O2
Z57780905	CC1=C(C#N)C(=O)N(CC=C)C(O)=C1	190,20	C10H10N2O2
Z1262691671	CC1=C(C=CC(=C1)N1C=NC=N1)C(O)=O	203,20	C10H9N3O2
Z1262398517	NC1(CCCCC1)C(O)=O	157,21	C8H15NO2
Z1262398415	CNC1=NNC(=C1)C1=CC=CC=C1	173,22	C10H11N3
Z1422127285	OC1CN(C1)C1=NC(=CS1)C(F)(F)F	224,20	C7H7F3N2OS
Z2679906885	COC1=NC=C(Br)C(CO)=C1	218,05	C7H8BrNO2
Z1896595977	CNC1=C(F)C(C)=NC(C)=N1	155,18	C7H10FN3
Z2169650265	NC(=O)CC1=C(F)C(Cl)=CC=C1	187,60	C8H7ClFNO
Z138702688	CN(CCO)C1=CC=CC=C1	151,21	C9H13NO
Z1440873590	CC1OCCN(C1C)C(=O)C1=CCCC1	209,29	C12H19NO2
Z1699555218	CN1N=C(C)N=C1NCC1=NC(C)=CS1	223,30	C9H13N5S
Z1169060901	CNC1(CO)CCOCC1	145,20	C7H15NO2
Z1834223506	OC(=O)C1(CC=C)CCC1	140,18	C8H12O2
Z1694636438	CCC1=C(C=C(C)N=N1)C(O)=O	166,18	C8H10N2O2
Z1824497862	CN(C)C1=NC(CN)=CC(C)=N1	166,23	C8H14N4
Z1824497679	CC(N1C=C(C)C(N)=N1)C1=CC=CC=C1	201,27	C12H15N3
Z1823262959	CCNCC1=CC2=C(NC=C2)C=C1	174,25	C11H14N2

Z1703432371	CC(O)C1CCCN(CC2=CSN=N2)C1	227,33	C10H17N3OS
Z1607356994	CNC1=CC(CO)=CC=C1	137,18	C8H11NO
Z1318356911	CNC1=C(OC)N=CC=C1	138,17	C7H10N2O
Z1276751986	C1CC2(CN1)CCOCC2	141,21	C8H15NO
Z1787185107	CNC1=C(OC)C=CC(OC)=C1	167,21	C9H13NO2
Z1787184927	CC1CC(N)CCN1CC1=CC=CC=C1	204,32	C13H20N2
Z1542123042	CC#CCNC(=O)N1CCC2(CCC2)C1	206,29	C12H18N2O
Z2168282741	O=C1CC(CC2=CC=CC=C2)CCN1	189,26	C12H15NO
Z1982493939	CN1C=C2C(CCCC2=N1)C(O)=O	180,21	C9H12N2O2
Z1948024945	FC(F)C1=NN(C(=O)C1)C1=CC=NC=C1	211,17	C9H7F2N3O
Z1889997416	NC(=O)N1CCC2=C1C=C(N)C=C2	177,21	C9H11N3O
Z1868430497	OC(=O)C1=CNC=C1C1CC1	151,17	C8H9NO2
Z1863617849	CN1C=C(C(O)=O)C2=C(C(=CC=C2)C1=O	203,20	C11H9NO3
Z1836338798	OC(=O)CC1=CC2=NNC=C2C=C1	176,18	C9H8N2O2
Z1429858214	COC1=CC=C(C=C1)N1C=CC=N1	174,20	C10H10N2O
Z1741785991	OC(=O)CC1=C2CCCCC2=NN1	180,21	C9H12N2O2
Z2087739430	NCC1CCC2=C(C=NN2C1)C(N)=O	194,24	C9H14N4O
Z1198298267	CC1=CSC(=O)N1CC1=CC=C(F)C=C1	223,27	C11H10FNOS
Z1930291176	CC1(C)CN(CC2=CC=CS2)CC1O	211,32	C11H17NOS
Z1602637364	C(NC1CCCOCC1)C1=CC=CS1	211,32	C11H17NOS
Z1440427866	OC1CN(C1)C(=O)C1=C(Br)C=CC=C1F	274,09	C10H9BrFNO2
Z2405262317	CC1CCC(CN)CC1	156,27	C9H20N2
Z1330142692	CC(=O)N1CCNC(C)C(C)C1	156,23	C8H16N2O
Z2092145118	N[C@H]1CC[C@H](CC1)NCC1=CN=CC=C1	205,31	C12H19N3
Z1891776421	CC(C)OC1=NC=CC(CN)=C1	166,22	C9H14N2O
Z1262396049	CN(C)C1=C2CNCCC2=NC=N1	178,24	C9H14N4
Z763366278	CC(C)N1CCC(CN)C1	142,25	C8H18N2
Z1551463557	CC1=NC(=NC(CO)=C1)N1CCCCC1	207,28	C11H17N3O
Z1536943084	CC(C)N1N=CC(C(N)=O)=C1N	168,20	C7H12N4O
Z1526503457	CCC1=C(C=C(C=C1)S(C)=O)=O)C(O)=O	228,26	C10H12O4S
Z1520646252	CN1C(=O)OC2=C1C=CC=C2C(O)=O	193,16	C9H7NO4
Z1511502430	CC(CC(O)=O)C1=C(C)ON=C1C	183,21	C9H13NO3
Z1511494443	CN1C=CN=C1C1=NN=C(N)S1	181,22	C6H7N5S
Z1511494808	NC(C(O)=O)C1=C(F)C=CC=C1F	187,15	C8H7F2NO2
Z1495385307	CNC1=CC(NC)=C(Cl)C=C1	170,64	C8H11ClN2
Z1495385214	CC1CNC(=O)CC(C)C1	141,21	C8H15NO
Z56921150	CN1C(=O)CC2=C1C=CC(Br)=C2	226,07	C9H8BrNO
Z952016246	CN1C(=O)N(C)C2=C1C=CC(Br)=C2	241,09	C9H9BrN2O
Z54160747	CNC1=C(Cl)C=C(Cl)C=N1	177,03	C6H6Cl2N2
Z1463349723	CC1=C(C=CC=C1N)S(C)(=O)=O	185,24	C8H11NO2S
Z1454736877	OCC1=CN2C=CN=C2C=C1	148,17	C8H8N2O
Z1272672419	CC1CC(N)C(=O)N1C1=CN(C)N=C1	194,24	C9H14N4O
Z1263811758	CCOC1=C(F)C=C(CN)C=C1	169,20	C9H12FNO
Z1333043417	CC1=NC(=CC=N1)N1CCC(N)CC1	192,27	C10H16N4
Z1431919938	CCC1=NC2=C(S1)C(CCC2)NC	196,31	C10H16N2S
Z105930004	CC(C)N1CCNC(=O)C1	142,20	C7H14N2O
Z1263529744	COC1=C2NCCCC2=C(C)C=C1	177,25	C11H15NO
Z1266823311	COCCN1CCC(N)C1	144,22	C7H16N2O
Z1661371730	COC1CCN(CC1)C1=NC=C(C)S1	212,31	C10H16N2OS
Z228569944	CCN1CCN(CC1)C(C)CN	171,29	C9H21N3
Z287485530	NC(=O)CC1=CSC(=N1)C1=CC=CO1	208,24	C9H8N2O2S
Z1945695969	CC(C)N1N=C(C=C1N)C1=CC=CO1	191,23	C10H13N3O
Z1699554297	CN1N=C(C)N=C1NCC1=CC=C(Br)S1	287,18	C9H11BrN4S
Z1260735442	COC1=C(C=C(Br)C=C1)C(=O)N(C)C	258,12	C10H12BrNO2
Z57815696	CN1C(=O)N(C)C2=C1C=CC=C2	162,19	C9H10N2O
Z1925930040	OC(=O)C1CCCC(=O)N1	157,17	C7H11NO3
Z1729209079	BrC1=CC=C(C(N2C=CN=N2)S1	244,11	C7H6BrN3S
Z1741976870	COC1=C(C=CC(C)=C1)C#N	147,18	C9H9NO
Z1895742026	CC(C)NC1=NC(C)=NO1	141,17	C6H11N3O
Z1889997503	CC1=C(N)C=C(C=C1)N1CCNC1=O	191,23	C10H13N3O
Z1889917114	COC1=CC2=NNC(N)=C2C=C1	163,18	C8H9N3O
Z373773714	CN1C=C(NC(=O)C2=C(C)C=CO2)C=N1	205,22	C10H11N3O2
Z600428546	CNC1=NC=C(C=C1)C(O)=O	152,15	C7H8N2O2
Z600428566	NC1=CC(=CC=C1)C1=NC(=NO1)C1CC1	201,23	C11H11N3O
Z373773750	CN1C=C(NC(=O)C2=CC(Br)=CN2)C=N1	269,10	C9H9BrN4O
Z381114838	CN(C(=O)C1=CC=C(Br)O1)C1=NC=CS1	287,13	C9H7BrN2O2S
Z372501532	CC1=CC(C(=O)NC2=CCN=C2)=C(C)S1	221,28	C10H11N3OS

Z594413662	CC1=C(C=CO1)C(=O)NCC(O)=O	183,16	C8H9NO4
Z594038310	NC1=CN(CC(=O)NC2CC2)N=C1	180,21	C8H12N4O
Z594038204	CNC(=O)CN1C=C(N)C=N1	154,17	C6H10N4O
Z373775848	CN1C=C(NC(=O)C2=C(C)C=CS2)C=N1	221,28	C10H11N3OS
Z317500324	NC(=O)C1=CC(=CC=C1)C(=O)NC1CC1	204,23	C11H12N2O2
Z2186882445	O=S1(=O)NCCC1C1=CC=CC=C1	197,25	C9H11NO2S
Z371827086	CNS(=O)(=O)C1=C(C)C=C(OC)C=C1C	229,29	C10H15NO3S
Z458894644	CCOC1=NC=C(C=C1)C(N)=O	166,18	C8H10N2O2
Z540727674	CCOC1=NC=C(C=C1)C(O)=O	167,16	C8H9NO3
Z212122838	CC1=CSC(CNC(=O)C2CCC2)=N1	210,30	C10H14N2OS
Z372501060	CC1=CC(C(=O)NC2=CN=C2)=C(C)O1	205,22	C10H11N3O2
Z29672808	CC1=NN=C(NC(=O)C2=CC=NC=C2)S1	220,25	C9H8N4OS
Z45528338	CCNS(=O)(=O)C1=CC=C(C)C=C1	199,27	C9H13NO2S
Z1259155930	FC(F)(F)C1=CC(=CC=C1)C1=NC=CN1	212,18	C10H7F3N2
Z1235963286	OC(=O)CCC1CCNCC1	157,21	C8H15NO2
Z385158968	O=C(NC1CCCCC1)C1=CSN=N1	225,31	C10H15N3OS
Z190780124	CC(NC(=O)C1=C(C)N=CC=C1)C1CC1	206,25	C11H14N2O2
Z231744492	CC(N1CCC2=C(C1)C=CS2)C(N)=O	210,30	C10H14N2OS
Z1570998378	CC1CC(CCO1)NC1=C(F)C=CC=N1	210,25	C11H15FN2O
Z2067099522	C1C1=C(CN2CCCS2(=O)=O)SC=C1	251,74	C8H10ClNO2S2
Z90502205	CC(C)NCC1=CC=CO1	139,20	C8H13NO
Z1517452179	N#CC1=CN(CC2=CC=CC=C2)C=C1	182,23	C12H10N2
Z1262237386	NCC1CCN(C1)C1=CC(F)=C(F)C=C1	212,24	C11H14F2N2
Z2233922897	CC1C(CCN1C1=NC(C)=NS1)N(C)C	226,34	C10H18N4S
Z2199618152	CC(C)C1=NN(C)C=C1C#N	149,20	C8H11N3
Z31479147	FC1=CC(=CC(F)=C1)C(=O)N1CCCC1	211,21	C11H11F2NO
Z1741973699	COC1=CC(OC)=CN=C1	139,15	C7H9NO2
Z31504642	COC(C=O)NC1=CC=CC=C1	165,19	C9H11NO2
Z1782259387	CNC(C1=NC=CN1)C1=CC=CC=C1	187,25	C11H13N3
Z1954801633	CC1(C)C(C(O)=O)C1(C)C	142,20	C8H14O2
Z2211231747	OC(=O)CC1CCCS(=O)(=O)C1	192,23	C7H12O4S
Z2205958381	CC(C)N1N=NC(C(O)=O)=C1C	169,18	C7H11N3O2
Z90664455	CC(=O)N1CCC(N)CC1	142,20	C7H14N2O
Z2186881894	OC(=O)CCC1=NC=CC=N1	152,15	C7H8N2O2
Z2186882520	OC(=O)C1C(C(O)=O)C1=C	142,11	C6H6O4
Z2034457351	BrC1=C(NC2CCCN2=O)N=CC=C1	270,13	C10H12BrN3O
Z332370018	CNC(=O)C1=NC2=C(C=CC=C2)C(=O)N1	203,20	C10H9N3O2
Z332722126	CN1C=CC(NC(=O)C2=CSC(Br)=C2)=N1	286,15	C9H8BrN3OS
Z30242049	CCC(=O)NC1=CC=C(C=C1)C(N)=O	192,22	C10H12N2O2
Z228588548	CCS(=O)(=O)N1CCCC(C1)C(O)=O	221,27	C8H15NO4S
Z32414450	OC1=NC=C(C=C1)C(=O)NC1CCCC1	206,25	C11H14N2O2
Z27782626	O=C(CC1=CC=CS1)NC1=CC=CC=C1	217,29	C12H11NOS
Z316170458	OC(=O)CN1N=CC2=C(C=CC=C2)C1=O	204,19	C10H8N2O3
Z228463938	C1C1=C(CN2C=NC(=N2)C#N)C=CC=C1	218,64	C10H7ClN4
Z45527569	CN(C)S(=O)(=O)C1=C(C)C=CC(C)=C1	213,30	C10H15NO2S
Z271099570	[Na+].[CC1=NC2=C(C(N)=C(S2)C([O-])=O)C(C)=C1	244,24	C10H9N2NaO2S
Z119916498	CNC1=C(C(=O)NC2CC2)C(C)=NS1	211,28	C9H13N3OS
Z31725198	OCCNC(=O)C1=CC=NC=C1	166,18	C8H10N2O2
Z234895219	COC1=C(OC)C(CN)=CC=C1	167,21	C9H13NO2
Z1653341213	CC1CC1C(=O)N(C)C1=C(Br)C=CC=N1	269,14	C11H13BrN2O
Z1632776942	CC(O)C1CCCN(CC2=CN=CS2)C1	226,34	C11H18N2OS
Z1863667371	CC1(O)CN(C1)C(=O)NC1=NC=CC=C1	207,23	C10H13N3O2
Z1342206622	CS(=O)(=O)CC1=C(CN)C=CC=C1	199,27	C9H13NO2S
Z1295559787	NCC1(CCO)CCCC1	143,23	C8H17NO
Z1250132418	CC1=CC=C(O1)C1CCCCN1	179,26	C11H17NO
Z1318186459	CC(C)OC1=CC(CO)=CC=C1	166,22	C10H14O2
Z1250132469	NCC1(C1)C1=C(F)C=CC=C1	165,21	C10H12FN
Z402037718	CN(C)CC1=CSC(=N1)C1=CC=C(C)O1	222,31	C11H14N2OS
Z1891777161	CCN1C=C(C=N1)C1CNCCO1	181,24	C9H15N3O
Z1350606429		173,21	C8H15NO3
Z57611438	CNS(=O)(=O)C1=C(OC)C=CC(C)=C1	215,27	C9H13NO3S
Z1342208354	NC1=NN(CC2=CC=C(C=C2)C#N)C=N1	199,22	C10H9N5
Z1336457504	CN(C)CC1=CC(N)=C(C)C=C1	164,25	C10H16N2
Z1359429544	COC1=C(C=C(Br)C=C1)C(N)CO	246,10	C9H12BrN2O2
Z1357774256	CC(C)OC1=C(N=CC=C1)C(O)=O	181,19	C9H11NO3
Z1357774207	CN1CC(=O)NC2=C1N=CC=C2	163,18	C8H9N3O
Z1354602504	O=C1CCN(CCN1)C1CC1	154,21	C8H14N2O

Z1354602501	NCC1CC(=O)NC2=C1C=CC=C2	176,22	C10H12N2O
Z1354432960	COCCN1N=C(C)C(N)=C1C	169,23	C8H15N3O
Z1815155531	O=C1NCCCC11CCNC1=O	182,22	C9H14N2O2
Z1238956385	CN1C(C)=NN=C1CN1C=C(Cl)C=N1	211,65	C8H10ClN5
Z30847226	CCC(=O)NC1=CC(F)=C(F)C=C1	185,17	C9H9F2NO
Z203976296	NC(=O)C1=CC=C(CN2C=CN=C2)C=C1	201,23	C11H11N3O
Z57301586	CC1=CN2C(S1)=NC=C(C(O)=O)C2=O	210,21	C8H6N2O3S
Z55928828	CC1=C(C)C=C2N=CNC2=C1	146,19	C9H10N2
Z381471538	O=C(NCC1=CC=CS1)C1COCCO1	227,28	C10H13NO3S
Z363109604	CC1=C(C=CC(=N1)C(=O)NCC=C)C#N	201,23	C11H11N3O
Z432066748	CCOC1=CC(=CC=C1)C1=NNC(N)=C1	203,25	C11H13N3O
Z111781372	CN1C=CC=C1C1=NNC(=C1)C(O)=O	191,19	C9H9N3O2
Z18430620	CC(OC1=CC(Cl)=C(F)C=C1)C(N)=O	217,62	C9H9ClFNO2
Z251977366	CC(C)C(C)NC(=O)C1=NNC(=O)C=C1	209,25	C10H15N3O2
Z425484916	CNS(=O)(=O)C1=CC(N)=C(C)C=C1	200,26	C8H12N2O2S
Z228585974	OCC1=C(Br)C=C2OCCOC2=C1	245,07	C9H9BrO3
Z425389776	OCC1=NC(=CS1)C1=CC=CC=C1	191,25	C10H9NOS
Z234895273	NCC1=CN=C(C=C1)N1C=NC=N1	175,20	C8H9N5
Z415727992	CS(=O)(=O)C1=NC=C(N)C=C1	172,20	C6H8N2O2S
Z398556892	CC1=CC=C(O1)C1=NC(C)=C(S1)C(O)=O	223,25	C10H9NO3S
Z398557008	CC(C)S(=O)(=O)C1=C(C=CC=C1)C(O)=O	228,26	C10H12O4S
Z434667014	CCOC1=C(NC(=O)N(C)C)C=CC=N1	209,25	C10H15N3O2
Z857666908	CC(=O)NC1=C(N)C=C(C=C1)C(F)(F)F	218,18	C9H9F3N2O
Z240299288	CN1C=CC(NC(=O)C2=CC(Cl)=CN2)=N1	224,65	C9H9ClN4O
Z491457098	CC1=CSC(CNC(=O)N2CCCC2)=N1	211,28	C9H13N3OS
Z283726940	CC1=NSC2=C1C=C(C=N2)C(O)=O	194,21	C8H6N2O2S
Z1868430544	OC(=O)C1=CC2=C(CCC2)N1	151,17	C8H9NO2
Z1868409671	CN1N=NC(C(O)=O)=C1C	141,13	C5H7N3O2
Z1500735155	O=C(NC1CCOC1)C1CCCOC1	199,25	C10H17NO3
Z104341886	CC1=NOC2=C1C=CC=C2	133,15	C8H7NO
Z2522870727	CN1C=C(C(O)=O)C(=N1)C1CCOCC1	210,23	C10H14N2O3
Z1891772659	CN1C=C(C(O)=O)C(=N1)C1CCOC1	196,21	C9H12N2O3
Z381429030	CC(C)NC(=O)N1CCCC(C1)C(O)=O	214,27	C10H18N2O3
Z1597853149	CC(C)NC1CCCCC1O	157,26	C9H19NO
Z2235810242	COC1=C(Cl)C=CC(CC(O)=O)=C1	200,62	C9H9ClO3
Z2234186138	FC1=CC2=C(NC(=N2)C2CCNC2)C=C1	205,24	C11H12FN3
Z2213893306	OC(=O)C12CC(C1)(C2)C1=CC=CC=C1	188,23	C12H12O2
Z1250132459	C1CC(CCO1)N1CCCNCC1	184,28	C10H20N2O
Z2230864881	CC1=CC(C)=C(C=C1)C1(CN)CC1	175,28	C12H17N
Z221429978	NCCC1=CC=C(C=C1)N1C=CC=N1	187,25	C11H13N3
Z1269702310	CC1=NC(=CC=C1)N1CCC(N)CC1	191,28	C11H17N3
Z228588590	NCCN1CCC2=C(C1)C=CC=C2	176,26	C11H16N2
Z1245537816	NCC1=CC(=NC=C1)N1C=CC=N1	174,21	C9H10N4
Z1270210786	NC1=NC(=NC=C1)N1CCCC1	164,21	C8H12N4
Z1430814775	C1CC2=C(CN1)C=NN2C1=CC=CC=C1	199,26	C12H13N3
Z1170135337	NC1=CC(=CC=C1)C1=NOC(=N1)C1CC1	201,23	C11H11N3O
Z803153260	CC1=CNC(=O)N1C1=CC(N)=CC=C1	189,22	C10H11N3O
Z1276745159	OC(=O)C1CC11CCCC2=C1C=CC=C2	202,25	C13H14O2
Z1266933833	CCC1=C2NC=C(CCN)C2=CC=C1	188,27	C12H16N2
Z1263820464	CN1CC(=O)NC2=C(C=CC=C2)C1=O	190,20	C10H10N2O2
Z1946684538	CN1N=CC(C(O)=O)=C1C#N	151,13	C6H5N3O2
Z1820077950	OC(=O)C1CCCC2=CN=C1C2	166,18	C8H10N2O2
Z2255682695	CC(C)OCC1CNCCO1	159,23	C8H17NO2
Z2106601922	CC(C)N1C=C(C)C(N)=N1	139,20	C7H13N3
Z26489203	CCC(=O)NC1=C(C=CC=C1)C#N	174,20	C10H10N2O
Z32367961	O=C(NC1CC1)C1CCCC1	153,23	C9H15NO
Z56871585	CC1=NN=C(NC2CCCC2)S1	183,27	C8H13N3S
Z221430028	NC1CCN(CC(N)=O)CC1	157,22	C7H15N3O
Z221429086	OC(=O)C1=CC=C(NC(=O)C2CC2)S1	211,24	C9H9NO3S
Z105004294	CC1=C(NCC(N)=O)C=C(Cl)C=C1	198,65	C9H11ClN2O
Z27073204	CC1=CC=CC(C)=C1NC(=O)C1CCC1	203,29	C13H17NO
Z29414613	CC(C)C(C)NC(=O)C1=C(Br)C=CC=C1	270,17	C12H16BrNO
Z1867069683	CC1=C(SC2=C1C=CC(C)=N2)C(O)=O	207,25	C10H9NO2S
Z1863617803		141,17	C7H11NO2
Z1692557993	CC1=NOC(NCC2=C(Br)C=CS2)=N1	274,14	C8H8BrN3OS
Z1743521947	CN1C=NN=C1NCC1=C(Br)C=CS1	273,15	C8H9BrN4S
Z1738063683	OCC1=CC=C(CN2N=CSC2=O)C=C1	222,26	C10H10N2O2S

Z839988838	CC1=C(CNC2CCCC2)C(C)=NN1	207,32	C12H21N3
Z1889902453	CNC1=CC=C(C=C1)S(=O)(=O)N(C)C	214,28	C9H14N2O2S
Z1699519010	CN1N=CN=C1NCC1=C(Br)C=CS1	273,15	C8H9BrN4S
Z1699557134	CN1N=C(C)N=C1NCC1=CSC=N1	209,27	C8H11N5S
Z1127203805	O[C@H]1CCN(C1)C(=O)NCC1CCCC1	212,29	C11H20N2O2
Z1222278664	NC(C(O)=O)C1=CC=C(C=C1)C(F)(F)F	219,16	C9H8F3NO2
Z1119739690	OC(CN1C=CN=C1)C1=CC=C(Br)C=C1	267,13	C11H11BrN2O
Z975839228	CN(CC1=CC=CO1)C1=C(N)N=CC=N1	204,23	C10H12N4O
Z1140027744	BrC1=CC=C(S1)C(=O)NC1CCCOC1	290,18	C10H12BrNO2S
Z153345584	CCN1N=C(OC1=O)C1=CC=C(F)C=C1	208,19	C10H9FN2O2
Z221429968	NC1=CN=C(C=C1)N1CCCC1	163,22	C9H13N3
Z404208434	CNC(=O)C1=CC=C(CN2C=CC=N2)O1	205,22	C10H11N3O2
Z2273962468		213,30	C9H15N3OS
Z2273411596	CCN(C1COC1)C1=NC(C)=NS1	199,27	C8H13N3OS
Z1575308473	CN1C=C(C=N1)C(O)CN	141,17	C6H11N3O
Z1245580450	CC1CC(C)CN(CCN)C1	156,27	C9H20N2
Z1245633176	COCC1=CC(CN)=CC=C1	151,21	C9H13NO
Z1245580523	COC1=CC=C(CC2CCCN2)C=C1	191,27	C12H17NO
Z1139253378	CNCC1CCCN1C1=NN=CC=C1	192,27	C10H16N4
Z1575143886	NCC(N)C1=CC=CC=C1	136,20	C8H12N2
Z90122385	OCCC1=NC2=C(S1)C=CC=C2	179,24	C9H9NOS
Z134783700	CC(C)N1CCN(CC1)S(C)(=O)=O	206,30	C8H18N2O2S
Z228465586	N#CC1=NN(CC2CCCO2)C=N1	178,20	C8H10N4O
Z1172115923	CC(=O)NCC1=CC=C(S1)C(O)=O	199,22	C8H9NO3S
Z1171979209	CCN1C=C(C1)C=C1C(O)=O	173,60	C7H8CINO2
Z85923420	CC(C)CN1N=CC=C1N	139,20	C7H13N3
Z1259339803	CNCC1=C(OC)C(Br)=CC=C1	230,11	C9H12BrNO
Z996001650	CCN(C)C(=O)CC1=CC(Br)=CC=C1	256,14	C11H14BrNO
Z2509346437	NC1=NC=C(CC2CCCN2)C=C1	191,28	C11H17N3
Z1255497795	CC1=NNC2=C1C=C(C=C2)C(O)=O	176,18	C9H8N2O2
Z2507870736	C1CC1C1=C2NCCCN2N=C1	163,22	C9H13N3
Z2507870657	CC1=C(Br)C=C2N=CC=NC2=N1	224,06	C8H6BrN3
Z2572825303	CCNS(=O)(=O)C1=C(C)C=C(C)C(C)=C1	227,32	C11H17NO2S
Z1267881617	OC(=O)C1=C(C1)C=C2NC(=O)CC2=C1	211,60	C9H6CINO3
Z1741967647	CC1=C(F)C(Br)=CC=C1N	204,04	C7H7BrFN
Z57475114	CC1=NC(=CS1)C1=CC=C(C=C1)C(O)=O	219,26	C11H9NO2S
Z57101151	CC1=NC2=C(C=NN2)C(N)=N1	149,16	C6H7N5
Z1981870422	CC1=CC(N)=CC(C)=C1Cl	155,63	C8H10ClN
Z1954856453	CC1C(=O)NC2=C1C=CC=C2	147,18	C9H9NO
Z1945984155	CC(C)C(N)(C(O)=O)C1=CC=CC=C1	193,25	C11H15NO2
Z1992316394	CC1=C(C=C(C=C1)C(O)=O)C#N	161,16	C9H7NO2
Z1398461990	OC1CCC2=C(C1)NN=C2	138,17	C7H10N2O
Z276130164	CC1=C(Br)C=C(N)C(N)=N1	202,06	C6H8BrN3
Z992946910	O=C1NN=C2CCCC2=C1	136,15	C7H8N2O
Z84563384	CCC1=C(C)C=C(S1)C(N)=O	169,24	C8H11NOS
Z135394292	CC(C)NC(=O)C1=CC(C)=NO1	168,20	C8H12N2O2
Z17829253	NC(=O)COC1=C(Br)C=CC=C1	230,06	C8H8BrNO2
Z2692093593	NC1=C(C=CC=C1)C1CCC(=O)N1	176,22	C10H12N2O
Z2677920990	NC(=O)C1CCN(CC2=CC(Br)=CN2)C1	272,15	C10H14BrN3O
Z1259155959	CC1=C(CCO)C(=O)NN1	142,16	C6H10N2O2
Z1741969107	COC1=C(C=CC=C1Br)C(O)=O	231,05	C8H7BrO3
Z1694794850	CN1C=NN=C1NC(=O)C1=C(C)OC=C1	206,21	C9H10N4O2
Z1728624024	CC(=CC1=CN=CS1)C1=NC=CN=C1	203,26	C10H9N3S
Z1728193453	CC1=CC(C)=C(O1)C(=O)N1CC(CO)C1	209,25	C11H15NO3
Z1743520862	CN1C=NN=C1NCC1=CC=C(S1)C#N	219,27	C9H9N5S
Z909942618	NC(=O)CN1CC2CC3CC(C2)CC1C3	208,31	C12H20N2O
Z1834265833	CC1CNC2=C(C=CC=C2)S1=O	181,25	C9H11NOS
Z1694793088	CN1C=NN=C1NC(=O)C1CCC=CC1	206,25	C10H14N4O
Z1824482611	COC1=C(C(O)=O)C(=O)NC=C1	169,14	C7H7NO4
Z1259041047	COC1=C(C=CC=C1)C(C)(C)C(O)=O	194,23	C11H14O3
Z1258943241	CC1(CCC1(O)=O)C1=C(F)C=CC=C1F	212,20	C11H10F2O2
Z1258620048	CC1=NOC2=C1C=C(N)C=N2	149,15	C7H7N3O
Z445914158	CCC(C)NC(=O)N1CCCC1	156,23	C8H16N2O
Z1255523297	NC1=CC(CCC2=CC=CC=C2)=NN1	187,25	C11H13N3
Z1250888348	CCOC1=C(N)C(C(O)=O)=C(F)C=C1	199,18	C9H10FNO3
Z927535612	NC1=C(C=C(C1)C=C1)C(=O)NCC1CC1	224,69	C11H13ClN2O
Z1250132669	CCN1C=C(C(O)=O)C(N1)C(C)C	182,22	C9H14N2O2

Z1250100774	NCC1=CC(=CC=C1)C1=CC=C(S1)C#N	214,29	C12H10N2S
Z1823256834	CCNC1=CC2=C(NC(=O)N2)C=C1	177,21	C9H11N3O
Z1262237449	CN(C)C1=CN=C(N)C=C1	137,19	C7H11N3
Z1262237268	CC1=C(C(N)=NN1)C1=CC(CI)=CC=C1	207,66	C10H10ClN3
Z1262237225	OC1(CCOCC1)C1=CC=CC=C1	178,23	C11H14O2
Z1259273388	CN(C)C(=O)CN1C=NC(N)=N1	169,19	C6H11N5O
Z1259273094	NC(C(O)=O)C1=CC(=CC=C1)C(F)(F)F	219,16	C9H8F3NO2
Z1259162157	OC(=O)CCN1CCCC1=O	157,17	C7H11NO3
Z162878494	CCN1C(CNC)=NC2=C1C=CC=C2	189,26	C11H15N3
Z1262327517	CC1=NC(NCC2CCNC2)=CC=C1	191,28	C11H17N3
Z1176190687	BrC1=CN(CCN2CCCC2)N=C1	244,14	C9H14BrN3
Z905065786	CCC1=NC(CCN)=CS1	156,25	C7H12N2S
Z1262237439	CC(C)N(C)C(=O)C1CCNC1	184,28	C10H20N2O
Z137907758	CN1C=C(CNC2=C(F)C=CC2)C=N1	205,24	C11H12FN3
Z1673972503	CS(=O)(=O)NCC1=CN=CS1	192,25	C5H8N2O2S2
Z2687203707	OCC(O)C1=C(CI)C(CI)=CC=C1	207,05	C8H8Cl2O2
Z2687203820		151,21	C9H13NO
Z165143678	CC(=O)NC1=C(OC(F)(F)F)C=CC=C1	219,16	C9H8F3NO2
Z2218204415	CC#CCN(C)C1=NC=C(F)C=N1	179,20	C9H10FN3
Z1262515715	CC1=NSC(CC(O)=O)=C1	157,19	C6H7NO2S
Z1171979266	CC1(CCOCC1)C(O)=O	144,17	C7H12O3
Z1171979201	CN(C)C(=O)C1=NC(C)=C(C=C1)C(O)=O	208,22	C10H12N2O3
Z432792294	CN1CCN(CC1)C(=O)C1=C(Br)C=CS1	289,19	C10H13BrN2OS
Z2177030758	FC(F)C1=NC2=C(C=C(F)C=C2)C(=O)N1	214,15	C9H5F3N2O
Z1171978900	CC1=CC(C(O)=O)=C(C)N1CC1CC1	193,25	C11H15NO2
Z1171978887	CC(NC(=O)C1CCC1)C(O)=O	171,20	C8H13NO3
Z373102456	OC(=O)C1CCCN(C1)C1=NC=CS1	212,27	C9H12N2O2S
Z1171978885	OC(=O)CC1=CC2=C(O1)C=CC=C2	176,17	C10H8O3
Z1171978844	CN1C(=O)NC2=C1C=CC(=C2)C(O)=O	192,17	C9H8N2O3
Z1171978786	CN1C=CC=C(C(O)=O)C1=O	153,14	C7H7NO3
Z751623148	CC(N1CCNC(=O)C1)C1=NN=C(C)O1	210,24	C9H14N4O2
Z955198822	OCCN1C(=O)ON=C1C1=CC=CC=C1	206,20	C10H10N2O3
Z355202286	CCC1CN(CCO1)S(=O)(=O)N(C)C	222,30	C8H18N2O3S
Z220816104	CC(=O)N1CCCC(C1)C(N)=O	170,21	C8H14N2O2
Z32399802	CC(=O)N1CCC(CC1)C(N)=O	170,21	C8H14N2O2
Z370745496	CNC(=O)C1=NC=C(C=C1)C(O)=O	180,16	C8H8N2O3
Z1768428780	CN1C=C(C(O)=O)C(=N1)C1=CC=CS1	208,24	C9H8N2O2S
Z1762997351	CC(N)(C(O)=O)C1=C(F)C=CC=C1	183,18	C9H10FN2O2
Z458897272	CC1=C(C=CC=C1)C1=NNC(=C1)C(N)=O	201,23	C11H11N3O
Z1737940706	COC1=C(C=CN=C1)C#N	134,14	C7H6N2O
Z1723849112	CC1CC(C(C1)C(O)=O)C(O)=O	172,18	C8H12O4
Z1723549277	COC1=CC(=NN1C)C(O)=O	156,14	C6H8N2O3
Z1723549311	COC1=C(F)C=C(C=C1)C(N)C(O)=O	199,18	C9H10FN3O3
Z1602246704	NC(=O)C1=C(C=C(Br)C=C1)C(F)(F)F	268,03	C8H5BrF3NO
Z1618338338	CC1=CC(Br)=C(C)C=C1OCC(N)=O	258,12	C10H12BrNO2
Z90539275	CC1CCC(CC1)NCC1=CSC(C)=N1	224,37	C12H20N2S
Z90713719	CCC1=C(SN=N1)C(=O)N1CCOCC1	227,28	C9H13N3O2S
Z2754910894	Cl.CC(C)1OCCCC1CN	179,69	C8H18ClNO
Z1416282851	CN1CCOC2CNCC12	142,20	C7H14N2O
Z1259339139	NC1=CN=C(NC2CCCC2)C=C1	177,25	C10H15N3
Z927323122	CC(C)C(=O)N1CCCNCC1	170,26	C9H18N2O
Z285973104	CNCC1=NC2=C(C=CC=C2)C(C)=N1	187,25	C11H13N3
Z1359761587	CC(C)N1N=C2CCNCC2=CC1=O	193,25	C10H15N3O
Z1263771201	C1CC(CN1)C1=NC=CC=C1	148,21	C9H12N2
Z2689031550	CN1C=C(C(O)=O)C(=N1)C1=CC=C(C)O1	206,20	C10H10N2O3
Z2146515842	FC(F)C1=C(C#N)C(F)=CC=C1	171,12	C8H4F3N
Z2146515164	CC(C)C1=C(N=CS1)C(O)=O	171,21	C7H9NO2S
Z2146515720	CC1(C)CNCC(C)(C)N1	142,25	C8H18N2
Z2146515522	OC(=O)C1=C(C=CC=C1)C1CCC1	165,19	C9H11NO2
Z2144245215	CC1(C)CC(O)CC(C)(C)N1	157,26	C9H19NO
Z2143570482	CN1C=C(C=N1)C1NCCNC1=O	180,21	C8H12N4O
Z2130644351	OC(=O)CC1CCCC(=O)N1	157,17	C7H11NO3
Z2122400671	CC1=C(N)C=C(C=C1)C1CNCCN1	191,28	C11H17N3
Z2120060941	FC(F)C1=CC(=O)C2=C(N1)C=CC(CI)=C2	229,61	C10H6ClF2NO
Z2111526120	OC(=O)C1=C(N=CO1)C1CC1	153,14	C7H7NO3
Z2096088066	OCC1=CN=NN1C1=CC=CC=C1	175,19	C9H9N3O
Z2096088430	CC1=C(C=CC(O)=N1)C#N	134,14	C7H6N2O

Z1803709444	NC(=O)CN1CCC=CC2=C1C=CC=C2	202,26	C12H14N2O
Z2070537331	CC1=NOC(CC(O)=O)=C1	141,13	C6H7NO3
Z2168282733	CC1=C(C)C2=C(NC=N2)C=C1	146,19	C9H10N2
Z2160887345	CCC1=C(C=CN1C)C(O)=O	153,18	C8H11NO2
Z2160887321	COCC1=CC(=O)C2=C(N1)C=CC(F)=C2	207,20	C11H10FNO2
Z1741981838	OC(=O)C1=C(N=NS1)C1CC1	170,19	C6H6N2O2S
Z1258578224	NC(CCO)C1=CC=CS1	157,23	C7H11NOS
Z1501469697	CN1C(C)=CC=C(N)C1=O	138,17	C7H10N2O
Z1337810783	CN(CC1CCCCO1)C1=CN(C)N=C1	209,29	C11H19N3O
Z1428018534	OC1CC(C1)C1=CC=CC=C1	148,21	C10H12O
Z1139545993	CC1=CN(N=C1)C1CN(CC(C)(C)O)C1	209,29	C11H19N3O
Z1741794236	CN(C)C1=NOC(CO)=N1	143,15	C5H9N3O2
Z104346692	CN(C)CC(N)C1=CC=CC=C1	164,25	C10H16N2
Z1172115976	OC(=O)CN1CCCS1(=O)=O	179,19	C5H9NO4S
Z1404661584	CC(N)C1=CC(=CC=C1)N1CCCC1	190,29	C12H18N2
Z227830216	NC1=CN=C(C=C1)N1CCCC1	177,25	C10H15N3
Z910841110	CC(=O)NC1=C(C=C(C)C=C1Br)C(O)=O	272,10	C10H10BrNO3
Z234897285	CN1C(=O)OC2=C1C=C(C)C=C2	163,18	C9H9NO2
Z30272045	CNC(=O)C1=CC=C(CS(C)(=O)=O)C=C1	227,28	C10H13NO3S
Z234895869	NCC(O)C1CCCCC1	143,23	C8H17NO
Z19648288	NC(=O)CN1C=NC2=C1C=CC=C2	175,19	C9H9N3O
Z969560530	NC(=O)CC1CCCCN1	142,20	C7H14N2O
Z33545772	CS(=O)(=O)C1=CC=C(C=C1)C(N)=O	199,22	C8H9NO3S
Z370277954	CCC1=CC=C(O1)C(=O)N(C)C	167,21	C9H13NO2
Z370278114	COCC1=C(C=CC=C1)C(=O)N(C)C	193,25	C11H15NO2
Z102767808	CNCC1=C(C)ON=C1C	140,19	C7H12N2O
Z52314092	CC(=O)NCCC1=C(C)C=CC=C1	177,25	C11H15NO
Z140637446	COCC(=O)NC1=C(F)C=C(C)C=C1	197,21	C10H12FNO2
Z203974470	COC1=C(CN2C=CN=C2)C=C(C)C=C1	202,26	C12H14N2O
Z138108940	CNCC1=CC(=CC=C1)C#N	146,19	C9H10N2
Z2327226104	CC1=C(C=CC=C1)N1C=C(N=N1)C(O)=O	203,20	C10H9N3O2
Z2327224819	NC(=O)C1(CCCCC1)C1=CC=NC=C1	204,27	C12H16N2O
Z2327224800	CN1N=C(C=C1N)C1=CN=NC=C1	175,20	C8H9N5
Z1526503475	N#CC1=CC(OC2CCC2)=NC=C1	174,20	C10H10N2O
Z2301499792	COC1=CN=C(C=C1)N1CCNCC1	193,25	C10H15N3O
Z2301438391	NC1=C(C#N)C(OC(F)(F)F)=CC=C1	202,14	C8H5F3N2O
Z2301438477	CCN1C=CC=C(N)C1=O	138,17	C7H10N2O
Z2284386121	CC(N)(C(O)=O)C1=CC(Cl)=CC(Cl)=C1	234,08	C9H9Cl2NO2
Z1896597864	CNC1=C(N=CC=N1)C#N	134,14	C6H6N4
Z1267875535	CC(C)C1=NN(C)C2=C1C=C(S2)C(O)=O	224,28	C10H12N2O2S
Z1266933952	OC(=O)CC1CCOCC1	144,17	C7H12O3
Z1020680242	NCC(O)C1=C(Cl)C=C(Cl)C=C1	206,07	C8H9Cl2NO
Z1266854919	CCNC(=O)CN1C=CC(N)=N1	168,20	C7H12N4O
Z1266854886	CCC(O)C1CCCCN1	143,23	C8H17NO
Z927746932	CC(C)(N)C(=O)NC1=CC=CC=C1	178,24	C10H14N2O
Z277110394	NC1=NN=C(CC2CCCC2)S1	183,27	C8H13N3S
Z1263602433	COC1=C(C=CC=C1)C1=NN=C(N)O1	191,19	C9H9N3O2
Z52214433	CC1=C(CC(N)=O)C=CC=C1	149,19	C9H11NO
Z1259161694	OC(=O)C1CC(C1)C1=CC(F)=CC=C1	194,21	C11H11FO2
Z992422476	NC1CCC2=NC=CN2C1	137,19	C7H11N3
Z275728452	CC(N1CCC(C)CC1)C1=NC(C)=NO1	209,29	C11H19N3O
Z2177153697	C1CC1C1=NOC(=N1)C1CCNC1	179,22	C9H13N3O
Z2234631226	OCC1=CC(Br)=C(OC(F)F)C=C1	253,04	C8H7BrF2O2
Z123977486	C(NC1CC1)C1=NC2=C(O1)C=CC=C2	188,23	C11H12N2O
Z172492200	COC1=CC=C(C=C1)C(N)C1CC1	177,25	C11H15NO
Z198249910	CC(C)NC(=O)C1=CC2=C(NN=N2)C=C1	204,23	C10H12N4O
Z2379560414	CC1CN(C1C)C1=NC(C)=NS1	183,27	C8H13N3S
Z1259339810	COC1=CC(=CC=C1)C(O)C(O)=O	182,18	C9H10O4
Z1259087019	OC(=O)C1CC(C1)C1=CC=CC=C1	176,22	C11H12O2
Z2037257441	NCCN1C=CC2=C1C=CC(Cl)=C2	194,66	C10H11ClN2
Z744843458	NC1(CC2=C(C1)C=CC=C2)C(O)=O	177,20	C10H11NO2
Z2026432004	CS(=O)C1=NN=CN1CC1(C)CCC1	213,30	C9H15N3OS
Z1988459579	CN1N=C(C=C1C)C(O)C1=CN=CN=C1	204,23	C10H12N4O
Z2273074160	OC(C1CCC1)C(=O)N1CCC=C(F)C1	213,25	C11H16FNO2
Z1885626052	CC1=CC(=NS1)C(=O)N1CCC=C(F)C1	226,27	C10H11FN2OS
Z1389189457	FC1=C(F)C=C(CC(=O)N2CCCC2)C=C1	211,21	C11H11F2NO
Z738792498	COCC(=O)N(C)C1=CC=C(F)C=C1	197,21	C10H12FNO2

Z1644841773	CC1(COC1)C(=O)N1CCC=C(F)C1	199,23	C10H14FNO2
Z2362618963	CN1N=C(C)C=C1CN1CCC=C(F)C1	209,27	C11H16FN3
Z2074076908	FC(F)OCC(=O)N1CCCC2(CC2)C1	219,23	C10H15F2NO2
Z2277255954	CC1(CC1)S(=O)(=O)N1CCC=C(F)C1	219,27	C9H14FNO2S
Z1573313752	CC1=C(NCC2=CSN=N2)C=CC(F)=C1	223,27	C10H10FN3S
Z1613883823	CC1=CC=C(O1)C(=O)N1CCC=C(F)C1	209,22	C11H12FNO2
Z1231644380	CN(C)C(=O)C1(CC1)C1=C(F)C=CC=C1	207,25	C12H14FNO
Z1395924173	NC(=O)CN1CCOC2=C1C=C(F)C=C2	210,21	C10H11FN2O2
Z1337784682	OCCN1CCOC2=C1C=CC(F)=C2	197,21	C10H12FNO2
Z32664952	CC1CCN(CC1)C(=O)CC1=CC=CS1	223,33	C12H17NOS
Z2234631196	NCC1CCCCN1CCO	158,25	C8H18N2O
Z2235330340	CCN1N=C(C)C(CO)=N1	141,17	C6H11N3O
Z1250132377	CC(C)N1C=C(Br)C=C1C(O)=O	232,08	C8H10BrNO2
Z2379087997	OCCC1CCC2=C(N1)C=CC=C2	177,25	C11H15NO
Z2234185629	OC(=O)C1=C2CCCCC2=NO1	167,16	C8H9NO3
Z2236619777	C1CCC2(CC1)COCN2	155,24	C9H17NO
Z2240988379	COCC1(CCOC1)C(O)=O	160,17	C7H12O4
Z2106594617	CC(C)(N)CN1CCOCC1	158,25	C8H18N2O
Z29693719	O=C(NCC1=CC=CS1)C1=CN=CC=C1	218,27	C11H10N2OS
Z56884346	CC1=C(C)C=C(C=C1)C(=O)NCC(O)=O	207,23	C11H13NO3
Z57040448	OC(=O)CN1NC(=O)C=CC1=O	170,12	C6H6N2O4
Z89283367	CC1=CC2=NC(=CN2C=C1)C(O)=O	176,18	C9H8N2O2
Z85923408	CC1=NN2C=NN=C2NC1=O	151,13	C5H5N5O
Z85921050	OC(=O)[C@@H]1CCCN1C(=O)C1=CC=CO1	209,20	C10H11NO4
Z29672921	CC1=NN=C(NC(=O)C2CCCC2)S1	211,28	C9H13N3OS
Z57069978	OC(=O)CN1N=NC2=C1C=CC=C2	177,16	C8H7N3O2
Z57050098	COC1=CC(C(O)=O)=C(OC)C=C1	182,18	C9H10O4
Z56791867	CCN(CC)C1=CC(C)=NC2=NC=NN12	205,27	C10H15N5
Z53116464	NC(=O)CCN1C=NC2=C1C=CC=C2	189,22	C10H11N3O
Z219094774	N#CC1=CN=C(NCC2=CC=CO2)C=C1	199,21	C11H9N3O
Z815264310	NC1=CC(=CC=C1)N1CCS(=O)(=O)CC1	226,29	C10H14N2O2S
Z18769001	CC(OC1=C(C=CC=C1)C#N)C(N)=O	190,20	C10H10N2O2
Z810541796	NC(CC(O)=O)C1=CC(Cl)=CC=C1	199,63	C9H10ClNO2
Z812517122	CC1=CC(C)=C(C=C1)C1=NN=C(N)O1	189,22	C10H11N3O
Z412132834	CC(C)C1=NN=C(NC(=O)N(C)C)S1	214,29	C8H14N4OS
Z803145534	CCC(=O)NC1=C(N)C=C(OC)C=C1	194,23	C10H14N2O2
Z384359552	ClC1=CC=C(O1)C(=O)NCC1CCOC1	229,66	C10H12ClNO3
Z281113396	CCC1N(CCC2=C1C=CS2)C(=O)NC	224,32	C11H16N2OS
Z19743974	NC(=O)COC1=C(Cl)C=C(Cl)C=C1	220,05	C8H7Cl2NO2
Z802665960	CC1=CC(N)=C(C=C1)S(C)(=O)=O	185,24	C8H11NO2S
Z31791484	CC1=CC=C(S1)C(=O)NC1=CN=CC=C1	218,27	C11H10N2OS
Z235361249	OC(=O)C1CCCC2=C1C=CC=C2	176,22	C11H12O2
Z27381628	CC(=O)NC1=CC(Cl)=C(OC(F)F)C=C1	235,61	C9H8ClF2NO2
Z57472350	CN1CC(CC1=O)C(O)=O	143,14	C6H9NO3
Z361993816	NCCN1=NC=C(C=C1)C#N	162,20	C8H10N4
Z360010094	OC(=O)CN1C=C(Br)C=CC1=O	232,03	C7H6BrNO3
Z955369596	COC1=C(CNC(C)=O)C=C(Br)C=C1	258,12	C10H12BrNO2
Z394693584	CC1CN(CC(C)O1)S(=O)(=O)CCN	222,30	C8H18N2O3S
Z45498050	O=S(=O)(N1CCCCC1)C1=CC=CS1	231,33	C9H13NO2S2
Z235353833	CC1=NC2=C(O1)C=C(N)C=C2	148,17	C8H8N2O
Z235344767	COC1=NC=CC(=C1)C#N	134,14	C7H6N2O
Z235344617	CN1N=C(C)C2=C1N=C(C)C=C2C(O)=O	205,22	C10H11N3O2
Z27167104	CC(=O)NC1=NN=C(S1)C1CC1	183,23	C7H9N3OS
Z381061488	NCC1(CCOC1)C(N)=O	158,20	C7H14N2O2
Z33546338	CN1N=C(C(N)=O)C2=C(C=CC=C2)C1=O	203,20	C10H9N3O2
Z30271799	CNC(=O)C1=C(C)C=CC(=C1)S(C)(=O)=O	227,28	C10H13NO3S
Z219104216	CCNC1=NC=C(C=C1)C#N	147,18	C8H9N3
Z367452400	O=S(=O)(N1CCNCC1)C1=CN=CC=C1	227,28	C9H13N3O2S
Z367678526	CC(C)C1=NC2=C(O1)C=CC(N)=C2	176,22	C10H12N2O
Z367452324	CC1=CC2=C(N1)C=CC(N)=C2	146,19	C9H10N2
Z228586424	CC(N)C1=CC2=C(OC(=O)N2)C=C1	192,22	C10H12N2O2
Z85895273	CN(CC(O)=O)C(=O)C1=CC=CS1	199,22	C8H9NO3S
Z230661148	CC(C)NC(=O)N1CCC2=C(C1)C=CS2	224,32	C11H16N2OS
Z285675390	CC1=C(C)C(C#N)=C(N=N1)N1CCCC1	202,26	C11H14N4
Z2469606466	CN1N=NC2=C1CCC(N)C2	152,20	C7H12N4
Z2467523230	OCC1=C2CCCCN2N=C1	152,20	C8H12N2O
Z2466617838	OC(=O)C1=C2OCCOC2=CC=C1	194,19	C10H10O4

Z2442047935	<chem>O[C@H]1C[C@H](C1)C1=C(F)C=CC=C1</chem>	166,20	C10H11FO
Z2440429242	<chem>FC(F)(F)OC1=CNC(=O)C=C1</chem>	179,10	C6H4F3NO2
Z2418194328	<chem>NC1=CN(CCO)C(=O)C=C1</chem>	154,17	C7H10N2O2
Z2418194268	<chem>OC(=O)C1(CC1)NC1=CC=CC=C1</chem>	177,20	C10H11NO2
Z1891775689	<chem>CNC1=NNC(=C1)C1=C(OC)C=CC=C1</chem>	203,25	C11H13N3O
Z2418194188	<chem>O=S1(=O)CC2=C(C1)C=CC=C2</chem>	168,21	C8H8O2S
Z2418194280	<chem>OC1CCC2=C(NC1=O)C=CC=C2</chem>	177,20	C10H11NO2
Z1421484484	<chem>CCC(=O)N1CCC(N)C1</chem>	142,20	C7H14N2O
Z1263529721	<chem>CC(NC1CC1)C1=CN=CC=C1</chem>	162,24	C10H14N2
Z1507563282	<chem>CC(C)(CN)C1CCCC1</chem>	141,26	C9H19N
Z1427941552	<chem>CN1N=CC(CCN)=C1C</chem>	139,20	C7H13N3
Z1415893948	<chem>CCOC1=C(N)C=CC(Cl)=C1</chem>	171,62	C8H10ClNO
Z1350579458	<chem>CC(C)(N)C1=CC(F)=C(F)C=C1</chem>	171,19	C9H11F2N
Z1342206625	<chem>CN1CCC(N)(CCO)CC1</chem>	158,25	C8H18N2O
Z1262395898	<chem>OC1CCCC1CC1=CC=CC=C1</chem>	176,26	C12H16O
Z235336569	<chem>Cl.CC(=O)NC1=CC=C(CN)C=C1</chem>	200,67	C9H13ClN2O
Z53827650	<chem>CS(=O)(=O)N1CCCC1C(O)=O</chem>	207,24	C7H13NO4S
Z212045062	<chem>O=S(=O)(NC1CCNCC1)C1=CC=CS1</chem>	246,34	C9H14N2O2S2
Z210803598	<chem>CC1=C(C=C(F)C=C1)C(O)=O</chem>	154,14	C8H7FO2
Z55148803	<chem>CC1=NN(C(C)=C1)C1=NC(O)=CC(C)=N1</chem>	204,23	C10H12N4O
Z235362709	<chem>CN1N=C(C)C(C)=C(C(O)=O)C1=O</chem>	182,18	C8H10N2O3
Z826553418	<chem>NC(=O)CN1C(=O)ON=C1C1=CC=CS1</chem>	225,22	C8H7N3O3S
Z906021418	<chem>CC(C)C1=NC(C(N)=O)=C(Cl)C=N1</chem>	199,64	C8H10ClN3O
Z1250080926	<chem>CCNC1=NN=C2CCNCC2=C1</chem>	178,24	C9H14N4
Z1139740116	<chem>CN1C=NC2=C1CCN(CC=C(C)C)C2</chem>	205,31	C12H19N3
Z1222331433	<chem>OCC1=CC=C(OC2=CN=CC=C2)C=C1</chem>	201,23	C12H11NO2
Z1222331423	<chem>CC1=CSC(=N1)N1CCC(CC1)C(O)=O</chem>	226,29	C10H14N2O2S
Z1335657489	<chem>OCC1CCCN1CC1CCCN1</chem>	184,28	C10H20N2O
Z1269702243	<chem>CC(N)C1=C(Cl)C(Cl)=CC=C1</chem>	190,07	C8H9Cl2N
Z1354432957	<chem>COC1=CC(F)=C(C(C)O)C(F)=C1</chem>	188,17	C9H10F2O2
Z1160899480	<chem>CC1=CN=C(NCC2CCNC2)C=C1</chem>	191,28	C11H17N3
Z1259339808	<chem>CNC1=NNC(=C1)C1=C(C)C=CC=C1</chem>	187,25	C11H13N3
Z1276745040	<chem>CCC1=NSC(=N1)N1CCCNCC1</chem>	212,32	C9H16N4S
Z1602958158	<chem>C[C@@H](O)CN1CCOCC1</chem>	145,20	C7H15NO2
Z1741972644	<chem>OC(=O)C1=NN2CCCCC2=C1</chem>	166,18	C8H10N2O2
Z2158786398	<chem>CC1=NN=C(S1)C(=O)N1CCCCN1</chem>	212,27	C8H12N4O5
Z1741778448	<chem>CN1N=CC=C1C1CC(N)CCO1</chem>	181,24	C9H15N3O
Z1592032458	<chem>CN1CCC2=C1C=C(N)C=C2</chem>	148,21	C9H12N2
Z1272672333	<chem>CC(CN)C1=CC(F)=C(F)C=C1</chem>	171,19	C9H11F2N
Z2255112965	<chem>CNCC1=NC=C(C=C1)C(O)=O</chem>	166,18	C8H10N2O2
Z2255110176	<chem>CC(C)N1CC2=C(NC1=O)C=CC=C2</chem>	190,25	C11H14N2O
Z1741967101	<chem>ClC1=C(C=CC=C1)C1CNCCN1</chem>	196,68	C10H13ClN2
Z1238949196	<chem>FC(F)N1C=CN=C1CN1C=C(Br)C=N1</chem>	277,07	C8H7BrF2N4
Z1250089954	<chem>CC1=NN=C(O1)C1=CC=C(N)C=C1</chem>	175,19	C9H9N3O
Z113296902	<chem>CC1=CC(COC2=C(Br)C=CC=C2)=NO1</chem>	268,11	C11H10BrNO2
Z1245646830	<chem>OC1C(=O)NC2=C1C=C(F)C=C2</chem>	167,14	C8H6FNO2
Z1245635827	<chem>CCOC1=NC=C(C=C1)C#N</chem>	148,17	C8H8N2O
Z104584152	<chem>CN(C)C(=O)CNC1=CC=CC=C1</chem>	178,24	C10H14N2O
Z104590676	<chem>CC1=C(NCC(N)=O)C=CC=C1</chem>	164,21	C9H12N2O
Z228585534	<chem>CC1CCCN(C1)C(=O)CO</chem>	157,21	C8H15NO2
Z1983132682	<chem>CN1C=C(C=N1)C(O)C1=CC=CC=C1</chem>	188,23	C11H12N2O
Z1925961378	<chem>NC1=NNC(=C1)C1CCOC1</chem>	167,21	C8H13N3O
Z1172449162	<chem>CCN1N=C(CC)C(CC)=C(C#N)C1=O</chem>	205,26	C11H15N3O
Z1966400979	<chem>OC(=O)COC1CCCC2=C1C=CC=C2</chem>	206,24	C12H14O3
Z1741977827	<chem>NC1=C2CCOC2=CC=C1</chem>	135,17	C8H9NO
Z1945984179	<chem>OC(=O)CC1CCOC1</chem>	144,17	C7H12O3
Z31723394	<chem>CCN(CC)C(=O)C1=C(C)C=CC=C1</chem>	191,27	C12H17NO
Z1267773582	<chem>CC(N)CCN1CCCC1=O</chem>	156,23	C8H16N2O
Z104378298	<chem>NC(CN1CCOCC1)C1=CC=CC=C1</chem>	206,29	C12H18N2O
Z1655104004	<chem>CNC1=CN=C(C=C1)N1CCOCC1</chem>	193,25	C10H15N3O
Z1649677768	<chem>NC1=CC(=NO1)C1CCCO1</chem>	154,17	C7H10N2O2
Z1708089972	<chem>CC1=CC(=O)C(CO)=NN1</chem>	140,14	C6H8N2O2
Z1708089985	<chem>NC1=C(OC(F)(F)F)C=CC(=C1)C(O)=O</chem>	221,14	C8H6F3NO3
Z1708089983	<chem>CC1=CC(=CC(C)=C1)C(N)C(O)=O</chem>	179,22	C10H13NO2
Z31182213	<chem>NC(=O)C1CCCN(C1)C1=NC=CN=C1</chem>	206,25	C10H14N4O
Z1696861484	<chem>CC(N)CN1C=NC2=C(C=NN2C)C1=O</chem>	207,24	C9H13N5O
Z1696844471	<chem>OC(=O)CN1N=C(CC1=O)C(F)(F)F</chem>	210,11	C6H5F3N2O3

Z53116498	CC1=NC2=C(C=CC=C2)N1CCC(N)=O	203,25	C11H13N3O
Z1427430205	OC(=O)C1=COC(CN2C=C(Br)C=N2)=C1	271,07	C9H7BrN2O3
Z1696091826	CC(C)C1=C(C(O)=O)C(C)=NN1	168,20	C8H12N2O2
Z1515654336	CN1C=C(C(N)=O)C(=N1)C(F)F	175,14	C6H7F2N3O
Z2004547654	CC1=C2C=CC=C2C(N)N=N1	159,19	C9H9N3
Z1998636718	O=C1C=CNC(=N1)N1CCCC1	179,22	C9H13N3O
Z1993522733	CN(C)C(=O)NC1=CC(N)=C(C)C=C1	193,25	C10H15N3O
Z1993522712	OCC(O)C1=CC(F)=C(Cl)C=C1	190,60	C8H8ClFO2
Z423238660	OCCNC(=O)C1=CC(Br)=CC(F)=C1	262,08	C9H9BrFNO2
Z1992316428	CC1=NSC2=C1C(=O)NC=N2	167,19	C6H5N3O5
Z2028214430	CC1=NC=C2C=CC(=CN12)C(O)=O	176,18	C9H8N2O2
Z54615640	CC1(CCS(=O)(=O)C1)NC(=O)C1CC1	217,28	C9H15NO3S
Z2027049450	CC1(C)CNC2=NC(O)=CC(=O)N2C1	195,22	C9H13N3O2
Z1631503821	CCC(=O)NC1=NC=CC(=C1)C(F)(F)F	218,18	C9H9F3N2O
Z2017843061	CS(=O)(=O)C1=CC(N)=NC=C1	172,20	C6H8N2O2S
Z1791180142	CC(C(=O)NC1=CN=NS1)C1=CC=CS1	239,31	C9H9N3O5S2
Z2010009899		190,24	C12H14O2
Z1837073420	CCOC1=C(C=CC(C)=N1)C(O)=O	181,19	C9H11NO3
Z1737000014	CC1=NC(=CO1)C(=O)NCC=C	166,18	C8H10N2O2
Z1416537705	CNC(=O)CC1=NOC(C=C2CCC2)=N1	207,23	C10H13N3O2
Z1642061119	OC(=O)C1=C(C=NC=C1)N1CCCC1	192,22	C10H12N2O2
Z1642061357	CCC1=NN=C(O1)C1=CC(N)=CC=C1	189,22	C10H11N3O
Z445856640	CC(C)NC(=O)N(C)C1CCS(=O)(=O)C1	234,31	C9H18N2O3S
Z1419630209	CC1=NN(CC2CCOC2)C(N)=C1C#N	206,25	C10H14N4O
Z1349163663	CN(C1CCC1)C1=NN=C(C=C1)C(N)=O	206,25	C10H14N4O
Z1575312101	CC1=C(OC=C1)C1=NN=C(N)S1	181,21	C7H7N3O5
Z56767838	CNC1=NC2=C(N1)C=CC=C2	147,18	C8H9N3
Z1082510666	CC1N(CCN1=O)C(=O)C1=CC=CO1	208,22	C10H12N2O3
Z1569709044	COC1CNC(C1)C(O)=O	145,16	C6H11NO3
Z829561790	CCC(=O)NC1CCCN(C1)S(C)(=O)=O	234,31	C9H18N2O3S
Z741559898	NC(=O)CN1C=C(Br)C=N1	204,03	C5H6BrN3O
Z1642389859	CC1=CN2CCNCC2=N1	137,19	C7H11N3
Z1738061746	CCN1C=CN=C1CN1N=CSC1=O	210,26	C8H10N4O5
Z1632777925	CC(O)C1CCCN(CC2=CC=CO2)C1	209,29	C12H19NO2
Z1667561760	CN1N=C(C)N=C1NC(=O)C1CCCO1	210,24	C9H14N4O2
Z1609052448	COC1=NC(C)=C(NC2CCOC2)C=C1	208,26	C11H16N2O2
Z1241573127	CC1=CSC(CCN2CCCC2=O)=N1	210,30	C10H14N2O5
Z280806554	CCC(=O)N(C)C(C)C1CC1	155,24	C9H17NO
Z1235963386	COC1=C(CN)C=CC=N1	138,17	C7H10N2O
Z48858593	CC1=CSC(=N1)N1CCOCC1	184,26	C8H12N2O5
Z1269702383	NCC1=C(F)C(Cl)=CC=C1	159,59	C7H7ClFN
Z265437038	CCC1=NOC(CN2CCCC2)=N1	195,27	C10H17N3O
Z729603874	OC(=O)C1CN(C(=O)C1)C1=CN=CC=C1	206,20	C10H10N2O3
Z1683068139	O=C1NN=C2CNCCN12	140,15	C5H8N4O
Z1373975464	CNC(=O)C1=CC2=C(O1)C(Cl)=CC=C2	209,63	C10H8ClNO2
Z2235681444	COC1=NN=C(C=C1)C#N	135,13	C6H5N3O
Z2235681457	CC1=C(C=C(N1)C#N)C(O)=O	150,14	C7H6N2O2
Z2033637875	CN(CC(N)=O)C1=C(C#N)C(C)=NS1	210,26	C8H10N4O5
Z1741972405	OC(=O)C1=CN=C(N=C1)C1CC1	164,16	C8H8N2O2
Z2034495247	CN(C)C1CN(C1)C1=C(C#N)C(C)=NS1	222,31	C10H14N4S
Z1741976372	OC(=O)C1=NN2CCCC2=C1	152,15	C7H8N2O2
Z2235387992	NC(=O)[C@@H]1CCC[C@@H]1NC1CCCC1	196,29	C11H20N2O
Z2218554991	CCN1N=NC=C1C(O)=O	141,13	C5H7N3O2
Z2217033067		157,17	C7H11NO3
Z1419497132	OCCN1C=NC=CC1=O	140,14	C6H8N2O2
Z2522503195	OCC1=CN=C(N=C1)C1=CC=CC=C1	186,21	C11H10N2O
Z1255428434	C1CC(CCN1)C1=CSC=N1	168,26	C8H12N2S
Z2519037609	COC1=C(C=CC=C1)C1=NOC(N)=C1	190,20	C10H10N2O2
Z2519002105	CN1N=CC(C2CC2)=C1C(O)=O	166,18	C8H10N2O2
Z2515207596	CC(C)(CO)N1C=CC=N1	140,19	C7H12N2O
Z2513337808	CN1C=CC(C(O)=O)=C1C1=CC=CC=C1	201,23	C12H11NO2
Z2512942993	OC(=O)C1=C2OCCOC2=CC(Br)=C1	259,06	C9H7BrO4
Z2512942973	COC1=C(C=CC=C1)C(O)=O)C#N	177,16	C9H7NO3
Z1172115949	CC1=NN(CCO)C=C1C(O)=O	170,17	C7H10N2O3
Z94598730	COC1=C(F)C=C(C(C(O)=O)C=C1	184,17	C9H9FO3
Z172492234	CC1=C(C=C(CO)O1)C(O)=O	156,14	C7H8O4
Z188924454	OC(=O)CC1=CC2=C(C(CCO2)C(Cl)=C1	228,63	C10H9ClO4

Z45681495	CS(=O)(=O)N1CCCC1C(O)=O	193,22	C6H11NO4S
Z57127432	CC1(C)C(CCC1(C)C(O)=O)C(O)=O	200,23	C10H16O4
Z90664474	COC1=CC(C2CCCN2)=C(OC)C=C1	207,27	C12H17NO2
Z30841040	BrC1=C(C=CC=C1)C(=O)NC1CC1	240,10	C10H10BrNO
Z57101199	CCN(CC)C1=C2C=NN(C)C2=NC=N1	205,27	C10H15N5
Z45527646	CNS(=O)(=O)C1=CC=C(Cl)C=C1	205,66	C7H8ClNO2S
Z56931797	OC(=O)C1CN(CC2=CC=CO2)C(=O)C1	209,20	C10H11NO4
Z56928941	CC1=C(CNC2=CC=CC=C2)C(C)=NO1	202,26	C12H14N2O
Z56921108	CC1=CC(=O)N2N=C(N)SC2=N1	182,20	C6H6N4OS
Z29672791	CC(=O)NC1=NN=C(C)S1	157,19	C5H7N3OS
Z55692907	CCC1=NC2=C(N1)C=CC=C2	146,19	C9H10N2
Z56889385	NC(=O)N1CCCC1C(O)=O	158,16	C6H10N2O3
Z56865289	NC(=O)CN1CCCC1=O	142,16	C6H10N2O2
Z56853704	CNC(=O)C12CC3CC(CC(C3)C1)C2	193,29	C12H19NO
Z56854346	NC(CC(O)=O)C1=C(Cl)C=CC=C1	199,63	C9H10ClNO2
Z234969377	N#CC1=CC(=NC=C1)N1CCOCC1	189,22	C10H11N3O
Z234969369	CC1=C(C=NN1CCO)C(O)=O	170,17	C7H10N2O3
Z56757306	NC(=O)C12C3CC(CC(C3)C1)C2	179,26	C11H17NO
Z1416282382	OC(=O)CC1=CNCC2=C1C=CC=N2	176,18	C9H8N2O2
Z285690798	CC1=NC(C)=NC(=C1)N1CCNC(=O)C1	206,25	C10H14N4O
Z1166191036	CC(C)N1C=C(NC2=NC=CC=N2)C=N1	203,25	C10H13N5
Z1312590836	NC(=O)C1(O)CC2=C(C1)C=CC=C2	177,20	C10H11NO2
Z1365534371	COC1=C(C=C(Br)C=C1)C(N)C(O)=O	260,09	C9H10BrNO3
Z166605294	OCC1=CC2=C(O1)C=CC=C2	148,16	C9H8O2
Z54524377	CC(=C)COC1=CC(=CC=C1)C#N	173,22	C11H11NO
Z1263714204	CC(N)CCC1=CC=C(C)O1	153,23	C9H15NO
Z927412236	CC(N)C(=O)N1CCCCC1C	170,26	C9H18N2O
Z905065808	NCCC1=CC(F)=CC(F)=C1	157,16	C8H9F2N
Z314452408	CCN(C1CC1)C(=O)C1=C(C)C=CO1	193,25	C11H15NO2
Z1162911836	NC1CCCN(C1)C1CCCCC1	182,31	C11H22N2
Z1272684551	NCCC1=NC(=CS1)C(F)(F)F	196,19	C6H7F3N2S
Z204695454	FC1=C(CN2CCCC2)C=CC(=C1)C#N	204,25	C12H13FN2
Z26286176	CC1=NN=C(COC2=C(Br)C=CC=C2)O1	269,10	C10H9BrN2O2
Z1267773609	CCN1CCCCC1CN	142,25	C8H18N2
Z197277614	CC1CCN(CCO)CC1	143,23	C8H17NO
Z1768918374	CN(C1CCC(O)CC1)C(=O)C1CCC1	211,31	C12H21NO2
Z2168515525	OC(=O)C1CCN(C1)C1=C(Cl)C=CC=C1	225,67	C11H12ClNO2
Z1318153868	OCCN1CCC2=C1C=CC=C2	163,22	C10H13NO
Z1583117108	CC1(C)CCCC1NCC1(O)CCOC1	213,32	C12H23NO2
Z2094144722	NCC1CCC2=NC=CN2C1	151,21	C8H13N3
Z1263529726	COC1=C(C=CC=C1)C1CCCN1	177,25	C11H15NO
Z2092396921	CCOC1CC(C1)C(O)=O	144,17	C7H12O3
Z1267882023	CC(C)(CN)C1=CC=CS1	155,26	C8H13NS
Z1891775046	COCC1=C(F)C=CC(CN)=C1	169,20	C9H12FNO
Z2044949055	OCC1=CC2=C(OC=C2)C=C1	148,16	C9H8O2
Z1945710531	COC(C)C1=NC(=CS1)C1=C(C)ON=C1	224,28	C10H12N2O2S
Z1741970163	CC1=C(CCN)N=CC=C1	136,20	C8H12N2
Z285675006	CC1=NC(N)=NC(=C1)N1CCCCC1	206,29	C11H18N4
Z82283343	O=C(NCC1=CC=CO1)C1CCOCC1	209,25	C11H15NO3
Z105653968	CN(C)C(=O)C1CCN(CC(C)=C)CC1	210,32	C12H22N2O
Z434911400	CN(CC(N)=O)C(=O)C1=CSC(Br)=C1	277,14	C8H9BrN2O2S
Z404922778	CC(N1C=CC=N1)C(=O)N(C)C	167,21	C8H13N3O
Z534296060	CCN1C=NN=C1CNC(=O)N1CCC1	209,25	C9H15N5O
Z729024430	CCN(CC)C(=O)C1=NC(C)=NC=C1	193,25	C10H15N3O
Z119516856	CC(NC(=O)C1=C(C)C=CO1)C1CC1	193,25	C11H15NO2
Z395781192	CC(=O)N1CCCCC1NS(C)(=O)=O	234,31	C9H18N2O3S
Z756724188	CC1=CSC(CNC(=O)C2=NSN=C2)=N1	240,30	C8H8N4OS2
Z409512732	O=C(NC1=NN=CS1)N1CCCCC1	226,30	C9H14N4OS
Z131516158	CC(NC(C)=O)C1=NN=C2C=CC=CN12	204,23	C10H12N4O
Z915925122	OC[C@H]1CCCN1C1=NC=C(C=C1)C#N	203,25	C11H13N3O
Z274554552	CC(CN1N=C(C)C(Cl)=C1C)C(O)=O	216,67	C9H13ClN2O2
Z1318356910	CC1=C2C(CCC(O)=O)=CNC2=CC=C1	203,24	C12H13NO2
Z1318268690	CC(N)(C(O)=O)C1=C(Cl)C=CC=C1	199,63	C9H10ClNO2
Z1318147454	COC1=C(Br)C=CC(N)=C1	202,05	C7H8BrNO
Z1313483213	NC1=C(C=CC=C1)C1=NC(=NO1)C1CC1	201,23	C11H11N3O
Z208334664	CN(C)C(=O)NC1=CC(Cl)=CC(Cl)=C1	233,09	C9H10Cl2N2O
Z1213687273	CN1C(=O)COC2=C1C=C(N)C=C2	178,19	C9H10N2O2

Z274553506	CC(CC(O)=O)N1N=C(C)C(C)=C1C	196,25	C10H16N2O2
Z1208912529	CNC(=O)CN1CCCC(CC1)C(C)C	212,34	C12H24N2O
Z818727262	C(NC1CC1)C1CCOC1	141,21	C8H15NO
Z1609161188	CCN1C=C(NC2CCCC2C)C=N1	193,29	C11H19N3
Z1263529780	COC1=C(CN)C(C)=CC(C)=N1	166,22	C9H14N2O
Z1162448860	CN(C)C1=NC=CC(CN)=C1	151,21	C8H13N3
Z1190318575	CC(C)OC1=CC(CN)=CC=C1	165,24	C10H15NO
Z223353618	CN1N=C(C)C=C1NC(=O)C1CCCO1	209,25	C10H15N3O2
Z265541128	CCC1=NOC(CN2CCCC(O)C2)=N1	211,27	C10H17N3O2
Z389867078	NCC1=CC(=CC=C1)C(=O)N1CCCC1	204,27	C12H16N2O
Z2574918328	CN1N=CC=C1CC1CCNCC1	179,27	C10H17N3
Z1416282827	CNC1CCN(CC1)C1=NN=CC=C1	192,27	C10H16N4
Z2065788426	CC1=C(N)C=C(C(O)=O)C(Br)=C1	230,06	C8H8BrNO2
Z2065788347	COC1=C(CO)C(C)=CC(C)=N1	167,21	C9H13NO2
Z2050687995	CCC1=C(C=CN1)C(O)=O	139,15	C7H9NO2
Z2050688026	C1C1=C2CNC(=O)C2=CC=C1	167,59	C8H6ClNO
Z2045034941	NC1=CN=C(CC2CC2)N=C1	149,20	C8H11N3
Z2037273275	CC(CN1C=CC2=C1C=CC=C2)C(O)=O	203,24	C12H13NO2
Z1827603335	O=C(NC1=CN=NS1)C1CCCCC1	225,31	C10H15N3O5
Z2034364269	CNC1=NC=C(OC)C=C1	138,17	C7H10N2O
Z1270446309	CC(C)N1C(=O)CNCC1(C)C	170,26	C9H18N2O
Z1218252078	OCC1CCCN1CC(O)=O	159,19	C7H13NO3
Z1270384361	COC1=C(C=CC(Br)=C1)C(O)=O	231,05	C8H7BrO3
Z274535144	CC(C)(OC1=CC(Cl)=CC=C1)C(O)=O	214,65	C10H11ClO3
Z1270326281	CCOC1=C(Cl)C=C(C=N1)C(O)=O	201,61	C8H8ClNO3
Z31725404	OCCNC(=O)C1=CC(Br)=CN=C1	245,08	C8H9BrN2O2
Z57229047	CC(NC(=O)C1=CC=C(Cl)C=C1)C(O)=O	227,64	C10H10ClNO3
Z57229045	CC(NC(=O)C1=CC=C(Br)C=C1)C(O)=O	272,10	C10H10BrNO3
Z1269702266	CS(=O)CC1=CC(N)=C(Cl)C=C1	203,68	C8H10ClNOS
Z1268703711	CC1=NN=C(O1)C1=CC(N)=CC=C1	175,19	C9H9N3O
Z1267881751	CC1=C(N)C=CC(=C1)S(C)=O	185,24	C8H11NO2S
Z1267881746	NC1(CO)CC2=C(C1)C=CC=C2	163,22	C10H13NO
Z1262250750	C1CC(CN1)NC1=CC=CC=C1	162,24	C10H14N2
Z1262246117	CC1=NC2=C(S1)C(O)CCC2	169,24	C8H11NOS
Z1262246115	CC(O)CS(=O)(=O)C1=CC=C(C)C=C1	214,28	C10H14O3S
Z2658865272	COC1=C(OC)N=CC(N)=C1	154,17	C7H10N2O2
Z2597964385	NC(CO)C1=CC=CC=C1	137,18	C8H11NO
Z2588063658	OC(=O)C1CN(C1)C1CCOC1	171,20	C8H13NO3
Z2446040567	CC(C)C1=NC=CN1CC(O)=O	168,20	C8H12N2O2
Z2583036300	O=C1NCCCN1C1=CC=C(C=C1)C#N	201,23	C11H11N3O
Z270979606	CC(C)(C(N)=O)C1=CC=CC=C1	163,22	C10H13NO
Z2106594221	CC(C)N1N=CC(Cl)=C1C(O)=O	188,61	C7H9ClN2O2
Z1431005396	CC(C)C(N1C=C(C)C=N1)C(O)=O	182,22	C9H14N2O2
Z2106598636	CCC(N1N=CC=C1C)C(O)=O	168,20	C8H12N2O2
Z2510944731	CC1=C(C=CC(Cl)=C1)C1(CC1)C(O)=O	210,66	C11H11ClO2
Z1741958104	COC1=C(F)C=CC(=C1)C(O)=O	170,14	C8H7FO3
Z2106594216	CCC(C)N1N=CC=C1C(O)=O	168,20	C8H12N2O2
Z2510259379	CC(C)N1C=C(N=N1)C(O)=O	155,16	C6H9N3O2
Z2235389495		166,18	C8H10N2O2
Z221603924	CC(=O)NC1=C(C=CC=C1C)C(O)=O	193,20	C10H11NO3
Z2510259343	CC1=NN=C2C=CC=C(C(N12)C(O)=O	177,16	C8H7N3O2
Z431537238	CC(CC(O)=O)N1C=CC=N1	154,17	C7H10N2O2
Z2510259511	OC(=O)CC1CS(=O)(=O)C1	164,18	C5H8O4S
Z2510259303	OC(=O)C1=CN(CC2CC2)N=N1	167,17	C7H9N3O2
Z1741960937	CC1=C(C=CC=C1Cl)C(O)=O	170,59	C8H7ClO2
Z2510258250	COC1=C(C=CC(CO)=C1)C(O)=O	182,18	C9H10O4
Z2510258302	COC1=C(C=CC(=C1)C(F)(F)F)C(O)=O	220,15	C9H7F3O3
Z1741978912	NC1CCCC(C1)C(O)=O	143,19	C7H13NO2
Z2379802567	FC(F)(F)C1=CC(=O)NN1	152,08	C4H3F3N2O
Z2379087723	OCC1=C2CCCN2N=C1	138,17	C7H10N2O
Z1741980032	CC1=C2C=CNC(=O)C2=CC=C1	159,19	C10H9NO
Z2372279593	OC(C1CCCC1)C1=NC=CN1	180,25	C10H16N2O
Z2372279480	CC1=CC(C(O)=O)=C(C=C1)C1CC1	176,22	C11H12O2
Z235344899	N#CC1=CC(=NC=C1)N1CCNCC1	188,23	C10H12N4
Z2327883779	CN(C(C)=O)C1=NC=C(N)C=C1	165,20	C8H11N3O
Z2327531729	CC(C)CC1=CNC(=C1)C(O)=O	167,21	C9H13NO2
Z1213674920	CCOC1=CC=C(C=C1)C1=NON=C1N	205,22	C10H11N3O2

Z1151517069	CC1=CC(=CC(C)=C1OC(F)F)C(N)=O	215,20	C10H11F2NO2
Z1262398505	NCC(O)C1=CC=CC=C1	137,18	C8H11NO
Z2680629340	OC(=O)C1CCC2=C(C(C1)C=CC=C2	190,24	C12H14O2
Z2680629316	CC(=O)N1CC(C1)OCC(O)=O	173,17	C7H11NO4
Z2679906771	FC(F)(F)OC1=CC(=O)NC=C1	179,10	C6H4F3NO2
Z2678251571	CC1=C(N)C(=O)N2C=CC=CC2=N1	175,19	C9H9N3O
Z2678251327	CC1=NN(C2CCOCC2)C(=C1)C(O)=O	210,23	C10H14N2O3
Z2283225344	CCC1(CC1)NC(=O)C1=CC(F)=CN1	196,23	C10H13FN2O
Z1262327411	CNC(=O)CN1C=CC2=C1C=C(N)C=C2	203,25	C11H13N3O
Z198194364	CC1CCCN(C1)C(N)=O	142,20	C7H14N2O
Z1889909829	CC1COCCCN1C(O)=O	144,17	C7H12O3
Z1889709964	CC1=CC=C(O1)C1=NNC(N)=C1	163,18	C8H9N3O
Z1699554788	CN1N=C(C)N=C1NCC1=C(Br)C=CS1	287,18	C9H11BrN4S
Z1705151001	CN(C)CC(=O)N1CCCC1C(C)(C)O	214,31	C11H22N2O2
Z1681936395	CN(CC1=NNC=C1)C1=CC(C)=CC=C1	201,27	C12H15N3
Z1787627869	CN(CC1CCOC1)C1=C(Cl)C=NC=N1	227,69	C10H14ClN3O
Z1407659698	CC1CN(CC1N)C1CC1	140,23	C8H16N2
Z1416200832	COC1=NC(C)=C(N)C=C1	138,17	C7H10N2O
Z1259161721	OCCOC1=CN=CC=C1	139,15	C7H9NO2
Z2156626388	O[C@H]1C[C@H](C1)C1=CC=CC=C1	148,21	C10H12O
Z221429096	NCC1=CN=C(C=C1)N1C=CC=N1	174,21	C9H10N4
Z2327226367	COC1=CC2=C(C(OC[C@H]2O)C=C1	180,20	C10H12O3
Z2177030625	CC(C)C1(CNC(=O)C1)C(O)=O	171,20	C8H13NO3
Z2027049523	CC1=C(N=NN1)C1=CC=C(Cl)C=C1	193,63	C9H8ClN3
Z1945702023	NC1=CN2C(C=C1)=NN=C2C(F)F	184,15	C7H6F2N4
Z1495385242	C1CC1N1C=NC2=C1C=CN=C2	159,19	C9H9N3
Z1717424191	CN1C=C(CN2CCC=C(F)C2)C(C)=N1	209,27	C11H16FN3
Z1220672383	NC(=O)C1CCCN1CC1=CC(Br)=CS1	289,19	C10H13BrN2OS
Z1624945762	CC(=CC1=CSC(Br)=C1)C1=NC=CN=C1	281,17	C11H9BrN2S
Z2012924471	NC(=O)C1=CC(OC(F)F)F)=C(Br)C=C1	284,03	C8H5BrF3NO2
Z1455023936	OC(=O)CNC(=O)C1=CC(Br)=CS1	264,09	C7H6BrNO3S
Z2293643386	CC(=O)N1CCCC(O)(C1)C(O)=O	187,20	C8H13NO4
Z55997155	CC(C)NCC(=O)N1CCCCC1	198,31	C11H22N2O
Z2680304681	CS(=O)(=O)NCC1=NNC=C1	175,21	C5H9N3O2S
Z1558209795	CS(=O)(=O)C1=CC(=CS1)C(O)=O	206,23	C6H6O4S2
Z1520645392	OC(=O)C1=CSC(=N1)C1CCC1	199,22	C8H9NO3S
Z1516115797	CN1C=C(C(N)=O)C(N)=N1	140,15	C5H8N4O
Z1414093197	COC1=C(C)C=CC(=C1)C#N	147,18	C9H9NO
Z1511483984	COC1=C(OC)C=C(C(O)=O)C(Cl)=C1	216,62	C9H9ClO4
Z1507502325	OC(=O)C(C1CC1)C1CC1	140,18	C8H12O2
Z196118774	OCCNC1=C2SC=CC2=NC=N1	195,24	C8H9N3OS
Z2442033986	NCC1=C(C=C=CC1F)N1CCCC1	194,25	C11H15FN2
Z2442033938	NC1CCN(CC1)C1=C(F)C=CC=C1	194,25	C11H15FN2
Z285718998	CC1=C(C)C(C#N)=C(N=N1)N1CCCC1	188,23	C10H12N4
Z30904272	CC1=C(NC(=O)C2CCC2)C=C(F)C=C1	207,25	C12H14FNO
Z32016173	CNC(=O)CNC(=O)C1=CC(Br)=CC=C1	271,11	C10H11BrN2O2
Z30271975	CNC(=O)C1=CC2=C(S1)C=CC=C2F	209,24	C10H8FNOS
Z241832786	CN1CCN(CC1)C(=O)C1CCCN1	197,28	C10H19N3O
Z1258578137	CC(C(O)=O)C1=CC=C(C)O1	154,17	C8H10O3
Z1245633158	COC1=CC(CCN)=CC=C1	151,21	C9H13NO
Z1245633104	NCC1=CN(CC2=CC=CC=C2)N=C1	187,25	C11H13N3
Z1235963376	CC(N)CC1=CC=C(C)S1	155,26	C8H13NS
Z33546668	COC1=C(OC)C(=CC=C1)C(N)=O	181,19	C9H11NO3
Z1945700452	COCCCN1=NSC(N)=N1	159,21	C5H9N3OS
Z1729206778	COC1=C(F)C=C(CN2C=CN=N2)C=C1	207,21	C10H10FN3O
Z1272517105	CC1=NSC(NC2CCCC2(C)CO)=N1	227,33	C10H17N3OS
Z1925930638	CC1=C2NC(=O)NC2=NC=C1	149,15	C7H7N3O
Z1925930237	OC(=O)C1=NN(C=C1)C1CCCC1	194,23	C10H14N2O2
Z1741978268	OC(=O)CC1=CC(F)=C(Cl)C=C1	188,58	C8H6ClFO2
Z1729210493	BrC1=CC(CN2C=CN=N2)=CS1	244,11	C7H6BrN3S
Z54572643	OCC1CCCCN1C1=NC=CN=C1	193,25	C10H15N3O
Z1699556994	CN1N=C(C)N=C1NCC1=C(C)C=CS1	222,31	C10H14N4S
Z1343696013	CNC(=O)C1=C(OC)C=C(Cl)C(Cl)=C1	234,08	C9H9Cl2NO2
Z1895583063	CN(C)C1=NC=NC(N)=C1	138,17	C6H10N4
Z1889917335	CC1=C(Br)C(C(O)=O)=C(F)C=C1	233,04	C8H6BrFO2
Z85886894	CC1=CC(C(=O)NCC(O)=O)=C(C)O1	197,19	C9H11NO4
Z85890614	CC(NC(=O)C1=CC=C(Br)S1)C(O)=O	278,12	C8H8BrNO3S

Z600428548	OC(=O)C1CCCN1C1CCNCC1	198,27	C10H18N2O2
Z237880160	CNC(=O)C1=C(OC)C(Br)=CC(OC)=C1	274,11	C10H12BrNO3
Z373774388	CN1C=C(NC(=O)C2=C(C)OC=C2)C=N1	205,22	C10H11N3O2
Z135384154	CC1=NOC(=C1)C(=O)NCC1=CC=CO1	206,20	C10H10N2O3
Z86949260	CC1=CC=C(O1)C(=O)NC1=NOC(C)=C1	206,20	C10H10N2O3
Z225339168	CC1=CC(NC(=O)C2=CC=C(CI)O2)=NO1	226,62	C9H7ClN2O3
Z1255523423	NC1=NC2=C(C=CC=C2)N1C1CCCC1	201,27	C12H15N3
Z1222283871	C1CNCC(C1)N1C=NC2=C1C=CC=C2	201,27	C12H15N3
Z2350941316	CN1N=C(CC(O)=O)C2=C1C=CC=C2	190,20	C10H10N2O2
Z415252234	CC(N1C=CN=C1)C(=O)NC1=NN=CS1	223,25	C8H9N5O5
Z422396686	CC1CCCN1C(=O)C1=C(C)N=CS1	224,32	C11H16N2O5
Z68248055	CN(C)(=O)C1=C(C(OC(F)F)C=CC=C1	215,20	C10H11F2NO2
Z1318161309	CC1CN(CCO)CCO1	145,20	C7H15NO2
Z280757432	CC(C)N(C)C(=O)C1=C(C)N(C)C(C)=C1	208,31	C12H20N2O
Z1511499407	OCCN1CCC(CC1)C1=NC=CC=C1	206,29	C12H18N2O
Z802671662	NCCNC1=NC=CN=C1	138,17	C6H10N4
Z2582143817	FC(F)(F)C1=NC(=CO1)C#N	162,07	C5HF3N2O
Z1324255779	CS(=O)(=O)NCC1=NOC=C1	176,19	C5H8N2O3S
Z68639747	CCN1C(NC(C)=O)=NC2=C1C=CC=C2	203,25	C11H13N3O
Z2186895169	CC1=C(Cl)C=CC(CCN)=C1	169,65	C9H12ClN
Z2011901248	BrC1=C(CNC(=O)C2CC=CC2)C=CS1	286,19	C11H12BrNOS
Z2216303045	CCN1N=C(C)C(=N1)C(O)=O	155,16	C6H9N3O2
Z2216303131	CN1C=NC=C1C(O)C1=CN=C(C)C=C1	203,25	C11H13N3O
Z2213893339	CN1C=CC(C(O)=O)=C1C1CCC1	179,22	C10H13NO2
Z2213893326	COC1=C(Cl)C=CC(C(O)=O)=C1N	201,61	C8H8ClNO3
Z2205958928	CC1CC(O)C2=NC=CN12	138,17	C7H10N2O
Z2197092525	CC1=C2C(O)CCOC2=CC=C1	164,20	C10H12O2
Z2197092181	C[C@H]1NCC[C@H]1N(C)CCO	158,25	C8H18N2O
Z2186882337	CN1N=CC=C1[C@@H]1NC(=O)CC[C@H]1N	194,24	C9H14N4O
Z2177030724	CN1C=C(N)C(=N1)C1CC1	137,19	C7H11N3
Z2168564218	CNC1=NOC2=C1C=C(Cl)C=C2	182,61	C8H7ClN2O
Z2168541790	CC1=C(C=CC=C1N)N1C=NNC1=O	190,21	C9H10N4O
Z2168390419	COC1=C(N=C(C)C=C1)C(O)=O	167,16	C8H9NO3
Z2168282687	CN(C)C1=NC=CC(N)=C1	137,19	C7H11N3
Z89404895	CC1=C(C=CO1)C(=O)NCC1=CC=CS1	221,27	C11H11NO2S
Z235362323	CCC1=NC(C)=C(C#N)C(=O)N1	163,18	C8H9N3O
Z68162877	OCCNC(=O)C1=CC2=C(CCCC2)S1	225,31	C11H15NO2S
Z32024416	CCNC(=O)C1=CC(=CC=C1)C(F)(F)F	217,19	C10H10F3NO
Z271004940	NC(CC(O)=O)C1=CC=CS1	171,21	C7H9NO2S
Z237578888	C1CCN(C1)C1=C2C=NNC2=NC=N1	189,22	C9H11N5
Z33545777	CS(=O)(=O)CC1=CC=C(C=C1)C(N)=O	213,25	C9H11NO3S
Z234897455	OC(=O)C1=CC(F)=C(C=C1)N1CCCC1	209,22	C11H12FNO2
Z432788010	BrC1=C(SC=C1)C(=O)NCC1=CC=CO1	286,14	C10H8BrNO2S
Z267487136	CC1=NOC(CN2C=C(Br)C=CC2=O)=N1	270,09	C9H8BrN3O2
Z1700082131	CC1=NN(CC2=NC=C(Cl)C=C2)C(C)=C1	221,69	C11H12ClN3
Z231745152	CN(C)C(=O)CN1CCC2=C(C1)C=CS2	224,32	C11H16N2O5
Z32384710	CC(C)CNC(=O)C1=NN(C)C(=O)C=C1	209,25	C10H15N3O2
Z1262396038	COC1=C(N)C=CC(F)=C1	141,15	C7H8FNO
Z1664359523	COC1=C(N)C=C(F)C=C1	141,15	C7H8FNO
Z1218186922	CC1=CC=C(O1)C1CCCN1S(C)(=O)=O	229,29	C10H15NO3S
Z1267882033	CCN1C=C(CNC)C=N1	139,20	C7H13N3
Z1335657447	COC1=CC(=CC=C1)C(O)C1CC1	178,23	C11H14O2
Z1276496841	CC1CCNC(C1)C1=CC=C(C)O1	179,26	C11H17NO
Z415735030	CC1=CC(Br)=CC(C)=C1CN	214,11	C9H12BrN
Z1262395953	CC1=C(C=CC=C1)C1(CN)CC1	161,25	C11H15N
Z1259339816	OC(=O)CC1=CCCCC1	140,18	C8H12O2
Z1324054923	CC(N)C(C)C1=CC=CC=C1	149,24	C10H15N
Z275170058	CCN1N=C(C)C(CN)=C1C	153,23	C8H15N3
Z1262237455	CC1=CN=C(S1)C(N)C1CC1	168,26	C8H12N2S
Z103706784	CNC(=O)CN(C)C1CCS(=O)(=O)C1	220,29	C8H16N2O3S
Z1263828503	CC1CN(CC2=CN=C(C)S2)CCC1N	225,35	C11H19N3S
Z1295619820	CC1CNC(CO1)C1=CC=CC=C1	177,25	C11H15NO
Z57269988	CNS(=O)(=O)C1=CC(C)=C(OC)C=C1	215,27	C9H13NO3S
Z1347206062	CNS(=O)(=O)C1=C(OC)C=C(C)C(Cl)=C1	249,71	C9H12ClNO3S
Z45528324	CCNS(=O)(=O)C1=CC=C(Cl)C=C1	219,68	C8H10ClNO2S
Z1347206044	CNS(=O)(=O)C1=C(C)C=C(C)C(C)=C1	213,30	C10H15NO2S
Z1347206038	CNS(=O)(=O)C1=C(C)C=C(C)C(OC)=C1	229,29	C10H15NO3S

Z1286244717	CC(C)(O)CNC(=O)C1=NC=C(Cl)C=C1	228,68	C10H13ClN2O2
Z1342208419	CC(O)C1=NC2=C(C=CC(Cl)=C2)N1C	210,66	C10H11ClN2O
Z1342208411	C1COC2=C(N1)C=CC=N2	136,15	C7H8N2O
Z1333717633	CC(C)N1CCC(N)C1=O	142,20	C7H14N2O
Z31767568	CC1CC(C)CN(C1)C(=O)C1CCC1	195,31	C12H21NO
Z133629916	CS(=O)(=O)NC1CCC(O)CC1	193,26	C7H15NO3S
Z1357774184	CNC1=CC2=C(C=C1)N=C(C)S2	178,25	C9H10N2S
Z1815157369	COC1=C(C(O)=O)C(N)=C(F)C=C1	185,15	C8H8FNO3
Z1815157352	CC1=NC(=CS1)C1=CNC=C1C(O)=O	208,24	C9H8N2O2S
Z992717294	COC1=CC(Br)=C(C=C1)C(O)=O	231,05	C8H7BrO3
Z1815157424	CCOC1=C(N=C(C)C=C1)C(O)=O	181,19	C9H11NO3
Z1815156880	CS(=O)(=O)C1=C(C(O)=O)C(Cl)=CC=C1	234,65	C8H7ClO4S
Z1741980868	COC1=C(OC)C(C(O)=O)=C(F)C=C1	200,17	C9H9FO4
Z1068186288	CNC(=O)C1=NC=C(Br)C=C1	215,05	C7H7BrN2O
Z183864280	CCNC(=O)C1=CC(Br)=CN1	217,07	C7H9BrN2O
Z1653341133	CN(C(C)=O)C1=C(Br)C=CC=N1	229,08	C8H9BrN2O
Z1809367755	CC(C)CCC1=NNC(N)=C1	153,23	C8H15N3
Z1809367538	OC(CC1=CC(Cl)=CC=C1)C(O)=O	200,62	C9H9ClO3
Z1262398472	CC1=CC(=C(C)O1)C1=NN=C(N)O1	179,18	C8H9N3O2
Z1801307715	BrC1=CC2=C(OCCN2)C=C1	214,06	C8H8BrNO
Z1680940545	CC1CC(C)(C)CC(CO)(C1)NC(C)=O	213,32	C12H23NO2
Z1795818456	CC(CC(O)=O)N1CCCCC1=O	185,22	C9H15NO3
Z1778350515	CC(O)C1=NOC(=N1)C1=CC=CC=C1	190,20	C10H10N2O2
Z316170380	CN1C=CC(=CC1=O)C(O)=O	153,14	C7H7NO3
Z94602039	CCC1=C(SN=N1)C(O)=O	158,18	C5H6N2O2S
Z228586390	OCC1=CN2C=CC=CC2=N1	148,17	C8H8N2O
Z382906830	CCNC(=O)C1=C(C)C2=C(S1)C=CS2	225,32	C10H11NOS2
Z449368988	CC1=C(C(N)=O)C(N)=CC=C1	150,18	C8H10N2O
Z449369198	CC1=C(C=C(C=C1)C(O)=O)S(C)(=O)=O	214,24	C9H10O4S
Z445129464	CC(=O)NC1CCNC1	142,20	C7H14N2O
Z119815790	CC(C)C1=NN=C(NC(=O)C2CCC2)S1	225,31	C10H15N3OS
Z397585700	CC1=NC(=CC(=O)N1)C1=CC=C(N)C=C1	201,23	C11H11N3O
Z408255174	CS(=O)(=O)NCC(=O)N1CCCCC1	220,29	C8H16N2O3S
Z857667024	COCC1=NC(=CS1)C(O)=O	173,19	C6H7NO3S
Z168931250	CC1=NOC(CN2CCC(O)CC2)=C1	196,25	C10H16N2O2
Z134785326	CC(N1CCN(CC1)S(C)(=O)=O)C(N)=O	235,30	C8H17N3O3S
Z56887653	C[C@H](NC(C)=O)C1=NC2=C(N1)C=CC=C2	203,25	C11H13N3O
Z108544944	CN1C=CC(NC(=O)C2=CC=C(Cl)S2)=N1	241,69	C9H8ClN3OS
Z27167233	O=C(NC1=NN=C(S1)C1CC1)C1CCC1	223,29	C10H13N3OS
Z992717178	NC1=NC(=CC=C1)C(F)(F)F	162,12	C6H5F3N2
Z992717236	NC(=O)COC1=CN=CC=C1	152,15	C7H8N2O2
Z98976549	NC(=O)COC1=C(Cl)C=C(C=C1)C#N	210,62	C9H7ClN2O2
Z216777778	CN1C=C(Cl)C=C1C(=O)NC1=NN=CS1	242,68	C8H7ClN4OS
Z275127650	NCC1=CC2=C(N1)C=CC=C2	146,19	C9H10N2
Z1868316800	CC1=CN2C=CN=C(C(O)=O)C2=N1	177,16	C8H7N3O2
Z1473994889	CC(C)C(N1CCCS1(=O)=O)C(O)=O	221,27	C8H15NO4S
Z94598966	OCC1=NC2=C(C=CC=C2)C(=O)N1	176,18	C9H8N2O2
Z1266823190	CC(C)C1=NC2=C(CCN2)N1C	179,27	C10H17N3
Z2104548225	CN1CCCC1C1COCN1	170,26	C9H18N2O
Z1989522832	CC(O)CN1CCOC(C)C1	159,23	C8H17NO2
Z204781884	COC1CCN(CC1)C(C)C(=O)N(C)C	214,31	C11H22N2O2
Z238676600	CN1N=CC2=C1N=CN=C2N1CCC1	189,22	C9H11N5
Z1980876316	C[C@H]1CC[C@H](CNC2=NC(C)=NS2)N1C	226,34	C10H18N4S
Z2161542370	CC1(C)N(CC2=CN=NS2)CCNC1=O	226,30	C9H14N4OS
Z228590106	CC1=NN(CCC(O)=O)C(C)=C1Cl	202,64	C8H11ClN2O2
Z234897683	C1CC(CCN1)C1=CNC2=C1C=CC=N2	201,27	C12H15N3
Z1262327430	COC1=C(N)C=C2SC(C)=NC2=C1	194,25	C9H10N2OS
Z1603826937	Cl.COC1=C(F)C=C2CNCCC2=C1	217,67	C10H13ClFNO
Z1413218090	CC(C)C1=NOC(=C1)C(=O)N1CC(O)C1	210,23	C10H14N2O3
Z1333043518	OC(=O)CN1C=C2C=CC=CC2=N1	176,18	C9H8N2O2
Z1266854821	CN1CC(=O)NC2=C1C=CC(F)=C2	180,18	C9H9FN2O
Z228586964	O=C(CCC1CCCC1)N1CCNCC1	210,32	C12H22N2O
Z2213893368	O=C1NCCCNCC1=CC=CC=C1	204,27	C12H16N2O
Z2327131607	COC1=C2CC(N)CC2=CC=C1	163,22	C10H13NO
Z108567110	NC(=O)N1CCCC(C1)C(O)=O	172,18	C7H12N2O3
Z57728664	NC(=O)CCN1C(=O)OC2=C1C=CC=C2	206,20	C10H10N2O3
Z104869826	NC(=O)CNC1=C(Cl)C=C(F)C=C1	202,61	C8H8ClFN2O

Z44585798	CC1=CC=C(NC(=O)N2CCCC2)C=C1	204,27	C12H16N2O
Z221429944	COC1=CC2=C(C=C1)C=C(CO2)C(O)=O	206,20	C11H10O4
Z220565334	OC(=O)CC1=CC2=C(OCC2)C=C1	178,19	C10H10O3
Z220564246	CN1N=CC(C(O)=O)=C1C	140,14	C6H8N2O2
Z220564190	CC1=CC(=O)N2NC(=NC2=C1)C(F)(F)F	217,15	C8H6F3N3O
Z1741976084	CC1(C)C(=O)NC2=C1C=CC=C2	161,20	C10H11NO
Z1863617863	CCN1C=C(N)C(=N1)C(N)=O	154,17	C6H10N4O
Z1729281082	CC(O)C1=NN(CC2=NC=CC=C2)C=C1	203,25	C11H13N3O
Z1860991849	O=C1NC=CC2=C1CNCC2	150,18	C8H10N2O
Z1849011609	NC1=C(C#N)C(=NN1)C1CC1	148,17	C7H8N4
Z1889902522	CC(CC(O)=O)C1=CC2=C(N1)C=CC=C2	203,24	C12H13NO2
Z1889902451	NC1=NC(=CC=N1)C1CCNC1	178,24	C9H14N4
Z1889861358	CNC1=NN=C(C=C1)C(F)(F)F	177,13	C6H6F3N3
Z1889710303	CC1CC2=C(CN1)C=CC=C2N	162,24	C10H14N2
Z1889706343	CN1N=C(C=C1N)C1=CC(F)=CC(F)=C1	209,20	C10H9F2N3
Z1881599363	OC1COC2=C1C=CC(Cl)=C2	170,59	C8H7ClO2
Z1869801297	CC(C)OC1=CN=C(C=C1)C(O)=O	181,19	C9H11NO3
Z1868431107	CC1OCCC1(C)C(O)=O	144,17	C7H12O3
Z1222283852	CC1=CSC(=N1)N1CCCC(C1)C(O)=O	226,29	C10H14N2O2S
Z234898661	OC(=O)CCC1=CC(Cl)=CS1	190,64	C7H7ClO2S
Z1022691264	CC(C)(C(N)=O)C1=CC(Br)=CC=C1	242,12	C10H12BrNO
Z998307488	CNC(=O)C(C)C(N1C=C(Br)C=N1	246,11	C8H12BrN3O
Z786289060	ClC1=CN(CC2=C(C=CC=C2)C#N)N=C1	217,66	C11H8ClN3
Z26824740	CCC1=NN=C(NC(=O)C2CCCC2)S1	225,31	C10H15N3OS
Z1116960368	CC1CCC(CN1CC=C(C)C)C(N)=O	210,32	C12H22N2O
Z375694448	CC1COCN1C(=O)C1=CNC(=O)N1	211,22	C9H13N3O3
Z423217540	CNC(=O)C1=CN=C(S1)C1=CC=CC=C1	218,27	C11H10N2OS
Z287121492	COC1CCN(CC1)C(=O)NCC1CC1	212,29	C11H20N2O2
Z989260264	CN1CCC2=C(C1)C(=NC=N2)N1CCC1	204,28	C11H16N4
Z1575304447	OC1COC2=C1C=CC=C2	136,15	C8H8O2
Z2217052426	CC1C(O)CCCN1CC1=CC=CC=C1	205,30	C13H19NO
Z1569715418	NCC1=CC(OC2COC2)=NC=C1	194,23	C10H14N2O2
Z373768838	CCN1C=C(NC(=O)C2=CC=CS2)C=N1	221,28	C10H11N3OS
Z1172115961	CC1=NN=C2CCC(CN12)C(O)=O	181,20	C8H11N3O2
Z1172068249	CC1=CC=NC2=C(C=NN12)C(O)=O	177,16	C8H7N3O2
Z1171979272	OC(=O)C1=CC2=C(NC(=N2)C(F)F)C=C1	212,16	C9H6F2N2O2
Z354989594	CC(C)NC(=O)CN1CC(C)OCC1C	214,31	C11H22N2O2
Z177089660	CCN(CC1=CC=C(Cl)S1)C(=O)NC	232,73	C9H13ClN2OS
Z1188327367	CCN(C)C(=O)NCC1=CC(Br)=CC=C1	271,16	C11H15BrN2O
Z1661228897	CC1=NN=C(O1)C1=CC(Br)=CN=C1	240,06	C8H6BrN3O
Z1429880392	CN1N=C(C)C(C#N)=C1N	136,16	C6H8N4
Z2492800236		210,23	C10H14N2O3
Z2492774613	NC1=C(N=C(CC2=CC=CC=C2)O1)C#N	199,21	C11H9N3O
Z2492774455	O=C1C=CNC2=C1CCCC2	149,19	C9H11NO
Z2489418741	OC(=O)C1=CN(C2CC2)C(=O)C=C1	179,18	C9H9NO3
Z2489418705		141,21	C8H15NO
Z818732094	NC(C(O)=O)C1=C(Br)C=CC=C1	230,06	C8H8BrNO2
Z345570098	CN(CC1=C(Cl)C=CC=C1Cl)C(C)=O	232,10	C10H11Cl2NO
Z2472860092	OCC1CC2=C(CO1)C=CC=C2	164,20	C10H12O2
Z270828822	CN(C)C(C(O)=O)C1=CC=C(Cl)C=C1	213,66	C10H12ClNO2
Z2510258126	CN1C(=O)CC2=C1C=C(C=C2)C(O)=O	191,19	C10H9NO3
Z2167281359	CC1=C(SC(=N1)C1CCOC1)C(O)=O	213,25	C9H11NO3S
Z2510258228	OC(=O)C1=C(C=C1O1)C1CC1	152,15	C8H8O3
Z2510258200	CN1C=C(C(O)=O)C2=C1C=CC(F)=C2	193,18	C10H8FNO2
Z1982493938	CC1=C(N)C=C(C=C1)C1=NC(=O)NN1	190,21	C9H10N4O
Z1981870468	CC1=C(C(O)=O)C(F)=CC(Br)=C1	233,04	C8H6BrFO2
Z1551688335	CC(O)C(=O)NCC1=NC=CC=C1	180,21	C9H12N2O2
Z199534086	CC1OC2=C(OCC1C(O)=O)C=CC=C2	194,19	C10H10O4
Z1966565729	CN1N=NC2=C1C=CC(Br)=C2	212,05	C7H6BrN3
Z1891772277	CN1N=C(C)C2=C1N=C(C=C2)C(O)=O	191,19	C9H9N3O2
Z1956828432	C1CN2C(CN1)=NN=C2C1=CN=CC=C1	201,23	C10H11N5
Z1956828705	CC1=C(C)C(N)=CC(=C1)S(C)(=O)=O	199,27	C9H13NO2S
Z1328078283	CC1(C)CN(C(=O)NCC2CC2)C1(C)C	210,32	C12H22N2O
Z1948933973	OC(=O)C1=CON=C1C1CC1	153,14	C7H7NO3
Z1948934180	CC(C)OC1=C(C=CN=C1)C(O)=O	181,19	C9H11NO3
Z1947444027	NC1=C(C=CC=C1)C(O)C1=NC=CC=C1	200,24	C12H12N2O
Z734661922	CCNC(=O)C1=CC2=C(C=CC=C2)N1C	202,26	C12H14N2O

Z1946684524	CC1CCC(CC1)OCC(O)=O	172,22	C9H16O3
Z1945984086	OC(=O)CCC1=NC=CN=C1	152,15	C7H8N2O2
Z1270207942	NCC(O)C1=CC=C(Cl)S1	177,65	C6H8ClNOS
Z228585324	CC1=CC(CO)=C(C)N1C1CC1	165,24	C10H15NO
Z993967192	CC(N1CCCCC1=O)C(O)=O	171,20	C8H13NO3
Z404993336	CN1C=C(NC(=O)C2=NOC(C)=C2)C=N1	206,21	C9H10N4O2
Z237578996	CC(C)CNC1=C2C=NNC2=NC=N1	191,24	C9H13N5
Z17828979	CNC(=O)COC1=C(Br)C=CC=C1	244,09	C9H10BrNO2
Z56789829	O=C(NC1CCS(=O)(=O)C1)C1=CC=CO1	229,25	C9H11NO4S
Z56774274	NC(=O)CN1N=NC2=C1C=CC=C2	176,18	C8H8N4O
Z2692093659	C1CC1C1=NC2=C(CNCC2)C=N1	175,24	C10H13N3
Z2692093591	OC(=O)C1(O)CCC2=C(C1)C=CC(Br)=C2	271,11	C11H11BrO3
Z2690050348	NC(CC(O)=O)C1=CC(Cl)=CS1	205,66	C7H8ClNO2S
Z1653345710	CC(C)C(=O)N(C)C1=C(Br)C=CC=N1	257,13	C10H13BrN2O
Z1342879039	COC1=C(C=C(Cl)C(Cl)=C1)C(O)=O	221,03	C8H6Cl2O3
Z1834265808	COC1=C(N)C2=C(CCC2)C=C1	163,22	C10H13NO
Z1259041039	CC1CCC(N)(CC1)C(O)=O	157,21	C8H15NO2
Z1259040932	CC1=C(C=CC(F)=C1)C#N	135,14	C8H6FN
Z1258992717	O=C(NC1CCCN1)C1=CC=CC=C1	204,27	C12H16N2O
Z1232889846	CC(NS(C)(=O)=O)C1=C(Cl)C=C(F)C=C1	251,70	C9H11ClFNO2S
Z1258578221	CC(CN)C1=CC(C)=CC=C1	149,24	C10H15N
Z228588744	OC(=O)CNC(=O)C1=NC=CC=C1	180,16	C8H8N2O3
Z1250132697	OC(=O)C1=CC=C(C=C1)N1CC=CC1	189,21	C11H11NO2
Z1250132662		176,22	C11H12O2
Z1250132611	CC(C)NC1CCOCC1	143,23	C8H17NO
Z33545896	CS(=O)(=O)C1=CC(=CC=C1)C(N)=O	199,22	C8H9NO3S
Z929052328	CC(C)(NC(=O)C1=CSC(Br)=C1)C(O)=O	292,15	C9H10BrNO3S
Z1262237317	CS(=O)(=O)C1=C(F)C=C(N)C=C1	189,20	C7H8FNO2S
Z57275697	CC1=CC2=C(NC=C(C(O)=O)C2=O)C=C1	203,20	C11H9NO3
Z1262237202	CCC1=CC=C(C=C1)C1=NC(N)=NN=C1	200,25	C11H12N4
Z1259341106	CC1=CC(C(O)=O)=C(S1)C(O)=O	186,18	C7H6O4S
Z1259341078	CC1=CC(C)=C(C=C1)C1=NOC(N)=C1	188,23	C11H12N2O
Z1259340992	OC(=O)CC1CCOC2=C1C=CC=C2	192,21	C11H12O3
Z1259340995	O=C1CCCC2=C(N1)C=CS2	167,23	C8H9NOS
Z1259340009	CNC1(CCOCC1)C(O)=O	159,19	C7H13NO3
Z1259339936	CC(C)C1=NOC(=C1)C(O)=O	155,15	C7H9NO3
Z1259339892	FC1=C(NC2CCNCC2)C=CC=C1	194,25	C11H15FN2
Z57469736	CC1=CC=C(C=C1)C1=NON=C1N	175,19	C9H9N3O
Z1259339887	CS(=O)(=O)C1=CC=C(CCN)C=C1	199,27	C9H13NO2S
Z1259339747	C1CCCCN1N1CCOCC1	170,26	C9H18N2O
Z1259335898	CC1=C(F)C=CC(=C1)C(O)=O	154,14	C8H7FO2
Z1259335889	OC(=O)C1CC1C1=C(F)C=CC(F)=C1	198,17	C10H8F2O2
Z1259335801	OC1=NC(=NC=C1)C1CC1	136,15	C7H8N2O
Z1259335793	CC(C)C1=NC(O)=CC=N1	138,17	C7H10N2O
Z1259273395	CC1=C2NC=C(CCC(O)=O)C2=CC=C1	203,24	C12H13NO2
Z1259273129	CCN(C)C(O)C1=CC(=CC=C1)C(O)=O	207,23	C11H13NO3
Z1259273099	OC(=O)COC1=C(F)C=CC(F)=C1	188,13	C8H6F2O3
Z1259162080	OC(=O)C1CC1C1CCCC1	168,24	C10H16O2
Z1259161894	CC1=CC(C(O)=O)=C(F)C=C1	154,14	C8H7FO2
Z1259161842	CCC(C)C(=O)N1CCCC(C1)C(O)=O	213,28	C11H19NO3
Z1462145959	CC1=CC(NC2CCNC2=O)=CC(F)=C1	208,24	C11H13FN2O
Z2142244288	CCNC1=C(F)C=C(C=C1)S(C)(=O)=O	217,26	C9H12FN2O2S
Z1267882073	CNC1CCN(CC1)C1=NC=CC=N1	192,27	C10H16N4
Z1263811740	CC(=O)N1CCC(CN)CC1	156,23	C8H16N2O
Z1951532824	C(N1CCC[C@H]2OCC[C@H]12)C1=CSN=N1	225,31	C10H15N3OS
Z2219060251	CC1=NOC=C1CNC1=CC(F)=CC=C1	206,22	C11H11FN2O
Z137632340	FC1=CC=C(NCC2=CSC=N2)C=C1	208,25	C10H9FN2S
Z137740702	CN1C=C(CNC2=CC(F)=CC=C2)C=N1	205,24	C11H12FN3
Z2687203888	OC(=O)CC1(CC1)C1=CC=CC=C1	176,22	C11H12O2
Z2271007255	CCNC1=NC=C(C=N1)C(F)F	173,17	C7H9F2N3
Z2684296057	CCC1=NN(C(=O)C1)C1=NC=C(N)C=C1	204,23	C10H12N4O
Z1171979224	CC1=CC(=CC=C1)N1C=C(N=N1)C(O)=O	203,20	C10H9N3O2
Z57481220	OC(=O)C1=CC=C(CN2C=CC=C2)C=C1	201,23	C12H11NO2
Z1171978785	CN1N=NC2=C1C=CC(=C2)C(O)=O	177,16	C8H7N3O2
Z221226202	CC1CN(CCO1)C(=O)C1=CC(Cl)=CN1	228,68	C10H13ClN2O2
Z1165167999	CC(NC(=O)C1CCOCC1)C(O)=O	201,22	C9H15NO4
Z1162910738	NC(=O)C1(N)CCOCC1	144,17	C6H12N2O2

Z32364066	COCC(=O)NC1=C(Cl)C=C(F)C=C1	217,62	C9H9CIFNO2
Z373769120	CCN1C=C(NC(=O)C2=CC=CO2)C=N1	205,22	C10H11N3O2
Z1160899528	OC(=O)CC1OCCCC2=C1SC=C2	198,24	C9H10O3S
Z196120788	CC(O)CNC1=C2SC=CC2=NC=N1	209,27	C9H11N3OS
Z166702366	O=C(NC1=CN=CC=C1)N1CCCC1	191,23	C10H13N3O
Z1768160698	COCC1=NC(C)=C(S1)C(O)=O	187,21	C7H9NO3S
Z332722148	CN1C=CC(NC(=O)C2=COC(Br)=C2)=N1	270,09	C9H8BrN3O2
Z1271581412	CC1=NOC(CN2C=CC=C(C)C2=O)=N1	205,22	C10H11N3O2
Z1762997350	Cl.COC1=C(F)C(=CC=C1)C1CCNCC1	245,72	C12H17ClFNO
Z1762997277	CN(C)C1=C(C=NC=C1)C(O)=O	166,18	C8H10N2O2
Z1762658189	NC1=C(OC(F)F)C=CC(=C1)C(O)=O	203,15	C8H7F2NO3
Z1742055002	CNC1=NC=C(OC)C=N1	139,16	C6H9N3O
Z1696936039	O=C(NC1=NC=CN=C1)C1CC1C1CC1	203,25	C11H13N3O
Z1651637958	NC(=O)COC1=C(Br)C=C(F)C=C1F	266,04	C8H6BrF2NO2
Z1551999220	CC(CC1=CC=C(Br)C=C1)C(N)=O	242,12	C10H12BrNO
Z1649283124	CCC(C)N1CCNC(=O)C1C(C)C	198,31	C11H22N2O
Z286103228	CNC(=O)CCN1N=C(C)C=C1C	181,24	C9H15N3O
Z1262252971	OCCN1CCCCC1=O	157,21	C8H15NO2
Z1346370629	CC1CN(CCC1N)S(C)(=O)=O	192,28	C7H16N2O2S
Z1566599209	C[C@@H]1CN(CCN1)C1CCOCC1	184,28	C10H20N2O
Z1741966630	CC(C)(N)CN1CCCC1	142,25	C8H18N2
Z1245580425	CC1CCCCN1CCN	142,25	C8H18N2
Z1954803140	C1CN(CCO1)C1CCCNCC1	184,28	C10H20N2O
Z2677388736	COC1=C(SC=C1)S(=O)(=O)N1CC=CC1	245,31	C9H11NO3S2
Z2146513998	CC1=CC=C(CCC(O)=O)S1	170,23	C8H10O2S
Z1891775084	CNC1=NN=C2CCNCC2=C1	164,21	C8H12N4
Z1823337665	CC1=C(C=CO1)S(=O)CC1=CC=CC=C1	220,29	C12H12O2S
Z1741981630	NC12CC3CC(C1)CC(O)(C3)C2	167,25	C10H17NO
Z2111525701	CC1=C(C)C(CO)=C(O)N=N1	154,17	C7H10N2O2
Z2111524565	COC1=CC=C(C=C1)C1=C(N)ON=C1	190,20	C10H10N2O2
Z2092370890	NC1=C2CNC(=O)C2=CC=C1	148,17	C8H8N2O
Z2092370157	COC1=C(F)C(N)=C(C=C1)C(O)=O	185,15	C8H8FNO3
Z2082999988	NC1=CN=C(CCO)C=C1	138,17	C7H10N2O
Z1942253409	OC1CCC(CC1)C(=O)NC1CC=CC1	209,29	C12H19NO2
Z2106610741	OC(=O)C1=NN2CCOC2=C1	154,13	C6H6N2O3
Z2158595086	NC1=C(C=C(F)C(F)=C1)N1CCCCC1	212,24	C11H14F2N2
Z228574284	CN(C)C(CN)C1CCCC1	170,30	C10H22N2
Z1246465616	CC(CC1=C(C)ON=C1C)C(=O)N(C)C	210,28	C11H18N2O2
Z1501469877	CN1C=C(C=N1)C(N)CN	140,19	C6H12N4
Z1577369655	CC1=NC=C(CNC2CCOCC2)S1	226,34	C11H18N2OS
Z1250132788	CCC(NC)C1=CC=NC=C1	150,23	C9H14N2
Z1262237477	COC1=C(C=CC=C1)C(C)(C)CN	179,26	C11H17NO
Z168922792	COCCN1CCCC(O)C1	159,23	C8H17NO2
Z803153678	CC(N)COC1=C(C)C=CC=C1	165,24	C10H15NO
Z228570960	CC(C)C(CN)N1CCCC1	156,27	C9H20N2
Z1444214989	CC(C)(NC(=O)C1=CSC=N1)C(O)=O	214,24	C8H10N2O3S
Z1696844496	CN1C=C(C=N1)C(O)CN1CCNCC1	210,28	C10H18N4O
Z857667076	NCC1=NC(=CS1)C1=CC=CC=C1	190,26	C10H10N2S
Z910842756	CC(C)C1=NC(C(O)=O)=C(Cl)C=N1	200,62	C8H9ClN2O2
Z234897013	O=C1NC2=C(COCC2)C=C1C#N	176,18	C9H8N2O2
Z234896997	CCNC(=O)C1=CC=C2C(C)NCCN12	207,28	C11H17N3O
Z234896787	CC1=C2C(CCN)=CNC2=CC=C1	174,25	C11H14N2
Z29418402	ClC1=C(C=CC(NC(=O)C2CC2)=C1)C#N	220,66	C11H9ClN2O
Z55293743	CN(C)C(=O)NC1=CC=C(C)C=C1	178,24	C10H14N2O
Z57981094	CC1=C(CCC(O)=O)C(C)=NO1	169,18	C8H11NO3
Z227830198	CN(C)S(=O)(=O)C1=C(CN)C=CC=C1	214,28	C9H14N2O2S
Z45527644	CN(C)S(=O)(=O)C1=C(C)ON=C1C	204,24	C7H12N2O3S
Z33545306	CN(C)S(=O)(=O)C1=CC=C(C=C1)C(N)=O	228,27	C9H12N2O3S
Z970066372	CC1=CC=C(C=C1)S(=O)(=O)N1C=CC=N1	222,26	C10H10N2O2S
Z90507809	CC1CCCCC1NCC1=CN=CC=C1	204,32	C13H20N2
Z90539031	CC1CCC(CC1)NCC1=CC=NC=C1	204,32	C13H20N2
Z768399682	CC1CN(C(C)CO1)C(=O)C1=NSN=C1	227,28	C9H13N3O2S
Z373768898	CCN1C=C(NC(=O)C2CCCC2)C=N1	207,28	C11H17N3O
Z275727840	CC(N1CCCCC1)C1=NC(C)=NO1	209,29	C11H19N3O
Z134991794	CC(N)C(=O)NCC1=CC=CO1	168,20	C8H12N2O2
Z916847036	CC(N)C1=C(C)OC(C)=C1	139,20	C8H13NO
Z184825330	CCOC1=C(C=CC=N1)C(=O)N(C)C	194,23	C10H14N2O2

Z369936976	CN(CC1=NOC(C)=C1)C(=O)NC1CC1	209,25	C10H15N3O2
Z32014360	CN(C)(C=O)CC1=CC=CS1	169,24	C8H11NOS
Z416877194	CC1=NOC(CN2CCC(CO)CC2)=N1	211,27	C10H17N3O2
Z812517094	CN1C=CC2=C1C=C(N)C=C2	146,19	C9H10N2
Z763367884	CC(N)COC1=C(F)C=CC=C1	169,20	C9H12FNO
Z234897025	COC1=CC(N)=C(OC(F)F)C=C1	189,16	C8H9F2NO2
Z2327226136	CC1=C(C(N)=CC=C1)S(C)(=O)=O	185,24	C8H11NO2S
Z2327226154	CC(CC(O)=O)C1=CN(C)N=C1	168,20	C8H12N2O2
Z2235389984	CN1NC2=C(C=C(Br)C=N2)C1=O	228,05	C7H6BrN3O
Z2306625465	OC(=O)C1(CCC1)NC1CC1	155,20	C8H13NO2
Z57101324	CNC1=C2C=NNC2=NC=N1	149,16	C6H7N5
Z2301499922	COC1=CC(C(O)=O)=C(F)C(Cl)=C1	204,58	C8H6ClFO3
Z1954802631	OC(=O)[C@H]1CC[C@H](C1)C(O)=O	158,15	C7H10O4
Z2293604761	CN1N=CC2=C1CCCNC2=O	165,20	C8H11N3O
Z1891775475	C(CC1=CC=CC=C1)C1CNCCO1	191,27	C12H17NO
Z1229289858	NC(=O)N1CCC[C@H]1CO	144,17	C6H12N2O2
Z1223130943	CC(C)C1CCC(C)CCN1CC(N)=O	212,34	C12H24N2O
Z1267773736	CC(NC1=C(N)C=NC=C1)C1CCCO1	207,28	C11H17N3O
Z1266933958	CN1CCC2=C(C1)C=C(C#N)C(N)=N2	188,23	C10H12N4
Z1266933873	CC1=NC(=NC(N)=N1)C1=CC=CS1	192,24	C8H8N4S
Z1266823254	CC1=NN=C2CNCCN12	138,17	C6H10N4
Z1266823144	CCOCC1=NN=C(N)O1	143,15	C5H9N3O2
Z1263820357	CC(C)(C1=NN=C(N)S1)C1=CC=CC=C1	219,31	C11H13N3S
Z1263820310	C1CN(CCN1)C1=NC2=C(O1)C=CC=C2	203,25	C11H13N3O
Z1263714070	NC(=O)C1CNC2=C1C=CC=C2	162,19	C9H10N2O
Z1263602416	CS(=O)(=O)C1=C(Cl)C=C(N)C=C1	205,66	C7H8ClNO2S
Z2234185700	OC(=O)CC1=C(Br)C=CS1	221,07	C6H5BrO2S
Z2379767235	C1CC1C1=CS(C=N1)C1=NN=CN1	192,24	C8H8N4S
Z1437108487	CC1CCC(NCCO)C2=C1C=CC=C2	205,30	C13H19NO
Z2417926821	CC(C)CN1C=NN2C=CC=C2C1=O	191,23	C10H13N3O
Z90507767	CN1CCC(CC1)NCC1=CN=CC=C1	205,31	C12H19N3
Z1263811784	CCC(C)(N)C1=CC=CC=C1	149,24	C10H15N
Z1840712742	CC1OCCCC1C(=O)N1CC(CO)C1	213,28	C11H19NO3
Z1266933909	CC(N)C1=NC2=C(N1)C=CC(Cl)=C2	195,65	C9H10ClN3
Z1250132798	C1CNCC(C1)C1=NC=NC=C1	163,22	C9H13N3
Z90122149	CNC(C)C1=NC2=C(S1)C=CC=C2	192,28	C10H12N2S
Z1949075848	NC1CCC(C1)C(=O)N1CCCC1	182,27	C10H18N2O
Z1262252935	NCC1=CN=C(OC2=CC=CC=C2)C=C1	200,24	C12H12N2O
Z744843724	CCN(C)S(=O)(=O)C1=C(C)NN=C1C	217,29	C8H15N3O2S
Z1863624700	COC1CCN(CC1)C1=C(C)C=NC=C1	206,29	C12H18N2O
Z57161818	C(N1C=NC=N1)C1=CC=CC=C1	159,19	C9H9N3
Z1614439780	CN1C=CC=C1C(=O)N1CCC=C(F)C1	208,24	C11H13FN2O
Z1815390993	FC1=CN=C(CN2N=CSC2=O)C=C1	211,21	C8H6FN3OS
Z1619979835	CN1C=NC=C1CN1CCC=C(F)C1	195,24	C10H14FN3
Z1587273210	CC1=NC(CN2CCC=C(F)C2)=NO1	197,21	C9H12FN3O
Z1636210119	CC1=NSC=C1C(=O)N1CCC=C(F)C1	226,27	C10H11FN2OS
Z1815382056	CCC1=NC=CN1CC1=NC=C(F)C=C1	205,24	C11H12FN3
Z2017168803	C[C@H](CO)N(C)C1=C(F)C=CC=N1	184,21	C9H13FN2O
Z1796028750	NC(=O)C1(CC2=C(F)C=CC=C2)CC1	193,22	C11H12FNO
Z2273523339	C[C@H](NC1=NC=C(F)C=N1)C1CC1	181,21	C9H12FN3
Z281802048	COC1=NC(=NC=C1)N(C)C	153,19	C7H11N3O
Z2255142757	CN1C=CN=C1C1CC(N)CCO1	181,24	C9H15N3O
Z1262254353	CCC(=O)NC1CCNC1	156,23	C8H16N2O
Z28870646	CC1CCC2=C(C=CC=C2)N1C(C)=O	189,26	C12H15NO
Z2213892991	CC1(C)CC(CC(O)=O)C1	142,20	C8H14O2
Z1918536193	CN1C=C(OC2=C(Cl)C=NC=N2)C=N1	210,62	C8H7ClN4O
Z2067304833	CCNC1=C(C)N(N=C1)C1=CC=CC=C1	201,27	C12H15N3
Z2326990059	CNCC1=CC(Cl)=C(OC)C=C1	185,65	C9H12ClNO
Z2235790913	CC(C)OC1=C(N)C=C(Cl)C=N1	186,64	C8H11ClN2O
Z2301499709	C1CC(C1)C1CNCCO1	141,21	C8H15NO
Z172492286	CN1CCN(CCN)CC1	143,23	C7H17N3
Z2327884032	CC1CN(CCO)C(C)CN1	158,25	C8H18N2O
Z1354785445	O[C@H]1CN(CC(F)F)[C@H]1O	167,16	C6H11F2NO2
Z104442660	CC1OC2=C(NC1=O)C=C(N)C=C2	178,19	C9H10N2O2
Z89283375	OCC1=CC2=C(OC(CO2)C(Cl)=C1	214,65	C10H11ClO3
Z57756572	CN(C)C1=CC=C(C=C1)C#N	146,19	C9H10N2
Z85927317	CC1=C(Cl)C=C(NC(=O)CO)C=C1	199,63	C9H10ClNO2

Z85922627	OC(=O)CCC1=NC2=C(C=CC=C2)C=C1	201,23	C12H11NO2
Z85923150	CCS(=O)C1=C(C=CC=C1)C(O)=O	198,24	C9H10O3S
Z85923398	CCC1=NOC(C(C)=C1C(O)=O	155,15	C7H9NO3
Z85921034	CC1=NN(C(C)=C1CO)C1=CC=CC=C1	202,26	C12H14N2O
Z57980672	OC(=O)CN1CCCC1=O	143,14	C6H9NO3
Z56974908	OC(=O)CN1C(=O)OC2=C1C=CC=C2	193,16	C9H7NO4
Z818810474	CC1=CSC(=N1)N1CCCNCC1	197,30	C9H15N3S
Z433017950	CNC(=O)CN(C(C)=O)C1=C(Br)C=CS1	291,16	C9H11BrN2O2S
Z133755368	CN(CC(=O)N1CCOCC1)S(C)(=O)=O	236,29	C8H16N2O4S
Z382906588	CNC(=O)C1=C(C)C2=C(S1)C=CS2	211,30	C9H9NOS2
Z420008560	CC1=C(SC=N1)C(=O)NCC1=CC=CO1	222,26	C10H10N2O2S
Z31182072	NC(=O)C1CCCN(C1)C1=NC=CC=N1	206,25	C10H14N4O
Z419994690	CC1CCCN(C1)C(=O)C1=C(C)N=CS1	224,32	C11H16N2O5
Z422368058	CC1CN(CCO1)C(=O)C1=C(C)N=CS1	226,29	C10H14N2O2S
Z216777796	O=C(CN1C=CC=N1)NC1=NN=CS1	209,23	C7H7N5O5
Z140107416	CN(C(C)=O)CNC(=O)C1=CC(Br)=CN1	274,12	C9H12BrN3O2
Z752370852	OC(=O)CC1=CC(Br)=C(F)C=C1	233,04	C8H6BrFO2
Z237732034	CC1=C(N)C=C(C=C1N)C(O)=O	166,18	C8H10N2O2
Z235361315	CCC(=O)NC1=C(C)C(N)=CC=C1	178,24	C10H14N2O
Z32023832	CCNC(=O)C1=CC(=CC=C1)S(C)(=O)=O	227,28	C10H13N3O5
Z381785674	CN(C(C)=O)N1CCCC(C1)C(O)=O	200,24	C9H16N2O3
Z235354537	OCCN1C=C2CNCCC2=N1	167,21	C8H13N3O
Z133632670	CS(=O)(=O)N1CCCC(C1)C(O)=O	207,24	C7H13NO4S
Z355180744	CN(C)S(=O)(=O)N1CCC2=C(C1)C=CS2	246,34	C9H14N2O2S2
Z32016296	CNC(=O)C1=CC2=C(C=C1)N=CS2	192,24	C9H8N2O5
Z367678716	CC1=NNC(=O)C(C(O)=O)=C1C	168,15	C7H8N2O3
Z367678540	NCC(O)C1=C(F)C=CC=C1	155,17	C8H10FNO
Z367452368	CC1=C(C=NN1C1=NC=CC=C1)C(O)=O	203,20	C10H9N3O2
Z367452182	NC1=CC(=CC=C1)S(=O)(=O)C1CCCC1	225,31	C11H15N2O2S
Z2470036279	OC(=O)CC1OCC2=C1C=CC(Cl)=C2	212,63	C10H9ClO3
Z1716711827	CN(C)C1=C(Cl)C=C(C=N1)C(O)=O	200,62	C8H9ClN2O2
Z208331706	COC1=CC2=C(NC=C2)C=C1	147,18	C9H9NO
Z1741972926	OC(=O)C1=CSC(=N1)N1CCCCC1	212,27	C9H12N2O2S
Z1741982217	OC(=O)C1CCC2=C(C1)C=CC=C2	176,22	C11H12O2
Z2467454615	CS(=O)(=O)N1C=CC(N)=N1	161,18	C4H7N3O2S
Z2466331661	CC1=C(Br)C=C2NC(=O)NC2=N1	228,05	C7H6BrN3O
Z2465619864	CN1N=NC2=C1C=CN=C2	134,14	C6H6N4
Z2465619834	CN1C=C(C=N1)C1=C(OC=C1)C(O)=O	192,17	C9H8N2O3
Z68259725	OCC1=C(NC(=O)C2CC2)C=CC=C1	191,23	C11H13NO2
Z2429425665	CC1=NN=C(C=C1)C1=CC=C(CO)C=C1	200,24	C12H12N2O
Z360149094	CN1N=CC(=O)C2=C1C=CC=C2	160,18	C9H8N2O
Z2418194212	OC(=O)C1=CN(N=N1)C1CCC1	167,17	C7H9N3O2
Z2418193716	O=C1NCCCC2=C1C=NN2	151,17	C7H9N3O
Z2418193710	CN1C=CC=C1CCC(O)=O	153,18	C8H11NO2
Z1266823365	CCC1=NN2CC(N)CCC2=N1	166,23	C8H14N4
Z1263811750	CCC(N)C1=NC(C)=CS1	156,25	C7H12N2S
Z1020684212	CC(O)(CN)C1=CC=CC=C1	151,21	C9H13NO
Z1258948114	CCC(C)(N)C1=NC(C)=CS1	170,27	C8H14N2S
Z1263811761	CC(C)OC1=C(F)C=C(CN)C=C1	183,23	C10H14FNO
Z1269702204	COC1=NC=C(CO)C=C1	139,15	C7H9NO2
Z1354432973	COC1CCN(CCN)CC1	158,25	C8H18N2O
Z1675167270	CC1=NC=C(CCO)N=C1	138,17	C7H10N2O
Z54813718	CS(=O)(=O)N1CCC(CC1)C(O)=O	207,24	C7H13NO4S
Z31131631	COC1=C(C=CC=N1)C#N	134,14	C7H6N2O
Z1238477803	CC1=C(C)N(CCC(O)=O)C(=O)S1	201,24	C8H11NO3S
Z1222331427	OC(=O)C1=CC2=C(NCCC(=O)N2)C=C1	206,20	C10H10N2O3
Z285777804	CC(C)NC1=C(C=CC=C1)S(C)(=O)=O	213,30	C10H15NO2S
Z839522486	CC1=NOC(=C1)C1CCCN1	152,20	C8H12N2O
Z2060794587	O=C(C1CCOC1)N1CCN2N=CC=C12	207,23	C10H13N3O2
Z32015055	CN(C(C)=O)CC1=CC(F)=CC=C1	181,21	C10H12FNO
Z1258578164	CCC1=NC(C)=C(S1)C(C)NC	184,30	C9H16N2S
Z1267773577	CNC1CCCC2=C1SC(C)=N2	182,29	C9H14N2S
Z228587862	C1CNCCN(C1)C1=NC=CS1	183,27	C8H13N3S
Z220564284	NCCCC1=NN=C2CCCCCN12	180,26	C9H16N4
Z1333043406	CCC1=NC=NC(=C1)N1CCC(N)CC1	206,29	C11H18N4
Z360056130	COC1=C(Br)C=C(C=C1)[C@H](C)O	231,09	C9H11BrO2
Z1275599911	CC(=O)N1CCCC2(C1)CCCCC2	209,33	C13H23NO

Z2240999730	OC(=O)C1CC(O)(C1)C1CCCC1	198,26	C11H18O3
Z145119960	NC(=O)C1=NC=CC(=C1)N1CCCC1	191,23	C10H13N3O
Z2238508676	O=C1NC(C2=CC=NC=C2)=NO1	177,16	C8H7N3O2
Z1954804097	CN1N=C(C=C1C1=CN=CC=C1)C(O)=O	203,20	C10H9N3O2
Z1166114418	OC(=O)C1=CC2=C(CCCC2)N1	165,19	C9H11NO2
Z1463415030	CCC1=C(C)NC2=NC(C)=NN2C1=O	192,22	C9H12N4O
Z970076882	CN1N=C(C=C1C1=CC=CC=C1)C(O)=O	202,21	C11H10N2O2
Z2235810181	OC(=O)CC1COC2=C(O1)C=CC=C2	194,19	C10H10O4
Z2235810193	CCOC1=NC2=C(O1)C=CC(N)=C2	178,19	C9H10N2O2
Z354992234	CC1CN(CC2=C(Cl)SN=N2)C(C)CO1	247,74	C9H14ClN3OS
Z2255112293	OC(=O)C1(CCC1)C1CCC1	154,21	C9H14O2
Z1796678844	COC1=NC(CN2N=CSC2=O)=CC=C1	223,25	C9H9N3O2S
Z94599212	CCOC1=CC=C(C=C1)C1CCCN1	191,27	C12H17NO
Z1127932252	CNC(=O)CC1=C(C=CC=C1)C(F)(F)F	217,19	C10H10F3NO
Z1143401905	CNC(=O)C1=C(Br)C(=NN1)C(C)C	246,11	C8H12BrN3O
Z1250288840	CC(=O)N(CC(N)=O)C1=CC=C(C)C=C1	206,25	C11H14N2O2
Z1245537949	CC(C)CC(C)N1N=CC=C1N	167,26	C9H17N3
Z1939437573	CC1=C(C(C)=NO1)C1=CC=CC=C1	173,22	C11H11NO
Z234894327	NCC1=CC(=NC=C1)N1CCCC1	177,25	C10H15N3
Z1259339822	CC(CN)CC1=CC=CS1	155,26	C8H13NS
Z1269702487	CCN1CCC(N)CC1C	142,25	C8H18N2
Z991556980	CN(C)C1=NC(CN)=CS1	157,24	C6H11N3S
Z1258948093	CN1C=C(C=N1)C(C)C(N)	139,20	C7H13N3
Z1798265228	CC(O)CN(C)C1=C(C=CC=C1Cl)C#N	224,69	C11H13ClN2O
Z278210580	CCS(=O)(=O)N1CCC(N)CC1	192,28	C7H16N2O2S
Z1798264062	CC(O)CN(C)C1=C2C=COC2=CC=N1	206,25	C11H14N2O2
Z1185276742	CCOC1=C(Cl)C=C(C=N1)C(=O)N(C)C	228,68	C10H13ClN2O2
Z1591867242	CS(=O)(=O)N1CCN(CC1)C(=O)CO	222,26	C7H14N2O4S
Z1696844737	N[C@H](C(O)=O)C1=CC=C(F)C=C1	169,16	C8H8FNO2
Z1695922870	CCS(=O)(=O)C1=C(C=C(Cl)C=C1)C(O)=O	248,68	C9H9ClO4S
Z32016909	CNC(=O)C(C)NC(=O)C1=CC=CC=C1	206,25	C11H14N2O2
Z1679733364	O=C1N(CC2CC2)N=C2C=NC=CN12	204,23	C10H12N4O
Z1996939123	NC(C(N)=O)C1=CNC2=C1C=CC=C2	189,22	C10H11N3O
Z1095000458	CC(C)(O)CNC1=C(C#N)C(F)=CC=C1	208,24	C11H13FN2O
Z2028214375	COC1=C(C=C(Cl)C=C1N)C(=O)N(C)C	228,68	C10H13ClN2O2
Z2027049516	OCC1=CN(N=N1)C1=C(Br)C=CC=C1	254,09	C9H8BrN3O
Z1791180120	CN1N=C(C)C=C1C(=O)NC1=CN=NS1	223,25	C8H9N5OS
Z1741976022	BrC1=C2CNC(=O)C2=CC=C1	212,05	C8H6BrNO
Z2017843139	CN1C=C(C=N1)C1CCCN1	165,24	C9H15N3
Z1820273488	CC1=CSC=C1C(=O)NC1=CN=NS1	225,28	C8H7N3OS2
Z2010041964	COC1=NC(C)=CC(=C1)C#N	148,17	C8H8N2O
Z2010010272	OC(=O)C1=NC=C2CCCC2=C1	177,20	C10H11NO2
Z1822510252	CC1=C(CN2N=CSC2=O)N=CC=C1	207,25	C9H9N3OS
Z1623872182	CC(C)CC1=CC(=CC(=O)N1)C(O)=O	195,22	C10H13NO3
Z446250928	CN(C1CCS(=O)(=O)C1)C(=O)NCC=C	232,30	C9H16N2O3S
Z1603826964	CC1=CC(=CC(=O)N1)C(O)=O	153,14	C7H7NO3
Z1578014146	CNC1=C(OC)C=CC=N1	138,17	C7H10N2O
Z1575304381	CC1=CC2=C(N=C1)N(CC(O)=O)N=C2	191,19	C9H9N3O2
Z1508069143	O[C@H]1CC[C@H](CC1)NC1=NC=C(Cl)C=N1	227,69	C10H14ClN3O
Z1642389730	N#CC1=NC=CC(=C1)C1CC1	144,18	C9H8N2
Z1679724508	CC1CCCC(CN2C=CN=C2C#N)C1	203,29	C12H17N3
Z1610969401	CN1N=CC(CNC2=NN=CS2)=C1C	209,27	C8H11N5S
Z1269638507	NC1=CN(CC2=CC=C(Cl)C=C2)N=C1	207,66	C10H10ClN3
Z1699555768	CN1N=C(C)N=C1NCC1=CC=C(C)O1	206,25	C10H14N4O
Z415735006	C1CC2(CCN1)CCOCC2	155,24	C9H17NO
Z145120146	CCC1=C(SN=N1)C(N)=O	157,19	C5H7N3OS
Z1935338995	CC1(CNC2=CN=CC=C2)COC1	178,24	C10H14N2O
Z1262237209	NCC(O)CN1CCCC1=O	158,20	C7H14N2O2
Z1259339724	NC1(CO)CN2CCCC2	156,23	C8H16N2O
Z1245633173	CC(C)OC1=CC(=CC=C1)C(C)N	179,26	C11H17NO
Z1407801656	CC1CCCN(CC2(O)CCC2)C1	183,30	C11H21NO
Z51119298	CCOC1=C(C=CC=C1)C#N	147,18	C9H9NO
Z1695906714	CC1=NN(C=C1C(O)=O)C1CCOCC1	210,23	C10H14N2O3
Z1695729010	NC(C(O)=O)C1=C(Cl)C=CC=C1Cl	220,05	C8H7Cl2NO2
Z1546783878	CC1=C(C)N=C(NC2CCOC2)N=C1	207,28	C11H17N3O
Z19645843	NC(=O)COC1=C2N=CC=CC2=CC=C1	202,21	C11H10N2O2
Z317545418	CN1C=CC(=CC1=O)C(N)=O	152,15	C7H8N2O2

Z1333173819	OC[C@@H]1C[C@H](NC2=NC=C(Br)C=N2)C=C1	270,13	C10H12BrN3O
Z1675167189	COC1=CC2=C(NC=NC2=O)C=C1	176,18	C9H8N2O2
Z1434233645	CN1N=C(CC2CC2)C=C1N	151,21	C8H13N3
Z2230911781	NC1=NN=C(S1)C1CCOCC1	185,25	C7H11N3OS
Z1983458260	OC[C@@H]1C[C@H](NC2=C(Br)C=NC=C2)C=C1	269,14	C11H13BrN2O
Z2217033058	OC(=O)C1=CC(C#N)=C(N=C1)C(F)(F)F	216,12	C8H3F3N2O2
Z2217033040	CS(=O)(=O)C1=CN=C(N)C=C1	172,20	C6H8N2O2S
Z2217033072	COC1=CC=C(C=C1)C1=CN=C(N)N1C	203,25	C11H13N3O
Z2216711599	CCC1=NC=NC(CC)=C1C(O)=O	180,21	C9H12N2O2
Z1148747945	CC(=O)NC1=C(C)C=NC=C1	150,18	C8H10N2O
Z2527856105	OCC1=NN2C=C(Br)C=NC2=N1	229,04	C6H5BrN4O
Z1509609013	OC1CCCC2=C1C=C(C(C(O)=O)C(=O)N2	209,20	C10H11NO4
Z2517219338	CC1(C)OCC2CC12C(O)=O	156,18	C8H12O3
Z2512942891	O=C1NCCCC1C1CCCCC1	181,28	C11H19NO
Z401537596	CCC1=NC(C)=C(S1)C(O)=O	171,21	C7H9NO2S
Z164680268	CC1OC2=C(NC1=O)C=CC=C2	163,18	C9H9NO2
Z99600452	CC1=CC(C)=C(C(N)=O)C(=O)N1	166,18	C8H10N2O2
Z29672917	CC1=NN=C(NC(=O)C2=CC=C(Br)O2)S1	288,12	C8H6BrN3O2S
Z50147845	CC1=NN(C2CCS(=O)(=O)C2)C(=O)C1	216,26	C8H12N2O3S
Z168362656	CN1C(C)=CC=C1C(N)=O	138,17	C7H10N2O
Z56921840	OC(=O)CC1=CC2=C(OCCO2)C=C1	194,19	C10H10O4
Z56911972	CC1=C(C)C(OCC(O)=O)=CC=C1	180,20	C10H12O3
Z45527663	CNS(=O)(=O)C1=C=CC=C(F)C=C1	189,20	C7H8FNO2S
Z56899213	CC1=CC(OCC(O)=O)=C(Cl)C=C1	200,62	C9H9ClO3
Z56891397	CC1=CC=C(S1)C(=O)NCC(O)=O	199,22	C8H9NO3S
Z56891216	O=C(CC(=O)N1CCCC1)N1CCCC1	210,28	C11H18N2O2
Z56870732	O=S(=O)(N1CCNCC1)C1=CC=CC=C1	226,29	C10H14N2O2S
Z56858239	CS(=O)(=O)C1=CC(N)=C(Cl)C=C1	205,66	C7H8ClNO2S
Z56852724	CC12CC3CC(C)(C1)CC(O)(C3)C2	180,29	C12H20O
Z56823032	CC1=C(Cl)C=CC(OCC(O)=O)=C1	200,62	C9H9ClO3
Z56788608	NC1=C(C=CC(=C1)C(F)(F)F)C(O)=O	205,14	C8H6F3NO2
Z56792153	CN1C(C)=CC(C(O)=O)=C1C	153,18	C8H11NO2
Z56754093	[Li+].NC(CC1=CNC2=C1C=CC=C2)C([O-])=O	210,16	C11H11LiN2O2
Z56756861	CC1=NC(C#N)=C(O1)N1CCOCC1	193,21	C9H11N3O2
Z116453054	C=CCNC(=O)C1CCS(=O)(=O)C1	203,26	C8H13NO3S
Z1428158225	OCC1=CN=C(C=C1)N1CCOCC1	194,23	C10H14N2O2
Z1428159815	CC1=CC(C)=C(N1)C(O)=O	139,15	C7H9NO2
Z1421527684	OC(=O)CN1C=C(N=N1)C1=CC=CC=C1	203,20	C10H9N3O2
Z1132044191	CN1CCCC(CCO)C1	143,23	C8H17NO
Z1416203195	CC(C)OC1=NC=CC(=C1)C(O)=O	181,19	C9H11NO3
Z1413780465	O=C1CC2(CCOC2)CN1	141,17	C7H11NO2
Z1407004178	COC1=C(OC)C=C2C=CCCC2=C1	191,23	C11H13NO2
Z1404660409	OC(=O)CC1CCCCO1	144,17	C7H12O3
Z1381287296	CC(C)OC1=C(N)C=C(C=C1)C(O)=O	195,22	C10H13NO3
Z959151850	O[C@H]1CCC2=C1C=CC(Cl)=C2	168,62	C9H9ClO
Z1375682862	CNC1=NN=C(C=C1)C1=CC=CC=C1	185,23	C11H11N3
Z1359429584	CN1C=C(Br)C=C(N)C1=O	203,04	C6H7BrN2O
Z1359429546	OC(CC1CCCCN1)C1=CC=CS1	225,35	C12H19NOS
Z1343518214	COC1CN(C1)S(=O)(=O)N1CCCC1	220,29	C8H16N2O3S
Z237375076	COC1=C(OC)C=C(C=C1)C1CCCN1	207,27	C12H17NO2
Z228584850	C1COC2=C(N1)C=CC=C2	135,17	C8H9NO
Z51119297	COC1=C(C=CC=C1)C#N	133,15	C8H7NO
Z839522560	OC(=O)COC1CCCC1	144,17	C7H12O3
Z57102389	COC1=C(CC(C)N)C=CC=C1	165,24	C10H15NO
Z1217910541	CC(C)(CN)C1=CC=CC=C1	149,24	C10H15N
Z1190318571	CCOC1=CC(CN)=CC=C1	151,21	C9H13NO
Z1342128874	C(CC1=CC=CC=C1)N1C=NC=N1	173,22	C10H11N3
Z54464104	CCOC1=CC(=CC=C1)C#N	147,18	C9H9NO
Z992422546	COC1=CC=C(C=C1)C1CCNC1	177,25	C11H15NO
Z927525866	NCCC(=O)N1CCCC2=C(C1)C=CS2	210,30	C10H14N2OS
Z28879653	CC(NC(=O)C1CCCO1)C1=CC=CS1	225,31	C11H15NO2S
Z927854532	NCCC(=O)N1CCCCC1	156,23	C8H16N2O
Z204695214	FC1=C(CN2CCCC2)C=C(C=C1)C#N	204,25	C12H13FN2
Z1348288726	CC1=CN=C(OCC2=NC=CC=C2)C=C1	200,24	C12H12N2O
Z343737504	CC1CN(C(C)CO1)C(=O)C1=CC=CO1	209,25	C11H15NO3
Z265488240	CC1CC(C)CN(CC2=NC(C)=NO2)C1	209,29	C11H19N3O
Z31255398	OCC1CCCN(C1)C1=NC=CC=N1	193,25	C10H15N3O

Z2235681150		142,20	C8H14O2
Z2168515541	CC(C)(O)C1=NC=CC=N1	138,17	C7H10N2O
Z2168542068	CC1=C(N=CC=C1)C(C)(C)CN	164,25	C10H16N2
Z1887715429	OC1CN(CC2=CC=C(CI)S2)CC1O	233,71	C9H12ClNO2S
Z1796688128	FC1=CC(CN2N=CSC2=O)=CC(F)=C1	228,22	C9H6F2N2OS
Z2017694733	CN1N=CN=C1C1COCCN1	168,20	C7H12N4O
Z254580986	CN(C)C(=O)C1=NOC(=C1)C1=CC=CS1	222,26	C10H10N2O2S
Z907784200	CCNC(=O)C1=CC(F)=C(C=C1)N(C)C	210,25	C11H15FN2O
Z916759702	CC(C)NC(=O)C1=CN=C(C)S1	184,26	C8H12N2OS
Z432808946	OC1CCCN(CC2=CSC(Br)=C2)C1	276,19	C10H14BrNOS
Z420007172	CC(C)NC(=O)C1=C(C)N=CS1	184,26	C8H12N2OS
Z406451888	CNC(=O)CCC1=C(CI)C(CI)=CC=C1	232,10	C10H11Cl2NO
Z133751890	CC(NS(C)=O)=O)C1=C(C)C=CC(C)=C1	227,32	C11H17NO2S
Z875490688	CC1=NC(=CS1)C(=O)NCC1CCC1	210,30	C10H14N2OS
Z54825231	CC(C)NC(=O)C1=C(C)N=C(C)S1	198,28	C9H14N2OS
Z26824802	CCC1=NN=C(NC(=O)C2CC2C)S1	211,28	C9H13N3OS
Z140088802	CNC(=O)CNC(=O)C1=C(C)OC(C)=C1	210,23	C10H14N2O3
Z1272948929	CC1=NC(=CS1)C1=CC(=CC=C1)C(O)=O	219,26	C11H9NO2S
Z1272739859	CC1=C(N)C(=CC(Br)=C1)C(O)=O	230,06	C8H8BrNO2
Z1318356961	CC(C)N1C=C(C#N)C(N)=N1	150,19	C7H10N4
Z1318356924	CCC1=CC(=O)C2=C(N1)C=CC(F)=C2	191,21	C11H10FNO
Z642326330	CCN(C)C(=O)NC1=CC=C(C)C=C1	192,26	C11H16N2O
Z1318147486	COC1=C(N)C=C(C)C=N1	138,17	C7H10N2O
Z1318147477	OC(=O)C1=CC=C(C=C1)N1CCCC1	205,26	C12H15NO2
Z1318147472	CC(O)CC1=NC2=C(C=CC=C2)C=C1	187,24	C12H13NO
Z1172202072	CC(CO)NC1=C(C=CC=N1)C#N	177,21	C9H11N3O
Z274553582	CC(CC(O)=O)N1C=NC=N1	155,16	C6H9N3O2
Z224209256	CCC(=O)N(C)C1=C(C=CC=C1)C(O)=O	207,23	C11H13NO3
Z227823068	OC(=O)C1=CC(NC2CCCC2)=NC=C1	206,25	C11H14N2O2
Z228588852	COC1=CC2=C(OCC(=C2)C(O)=O)C=C1	206,20	C11H10O4
Z1276745158	OCC1=CC2=C(CCC2)C=C1	148,21	C10H12O
Z2186895525	CCC1=NN(C)C=C1C#N	135,17	C7H9N3
Z1203252645	CN(C(C)=O)C1=CN=CC=C1	150,18	C8H10N2O
Z2692095260	COCC1(C)CNCCO1	145,20	C7H15NO2
Z1610314560	OCCNC1CCOCC1	145,20	C7H15NO2
Z2182115562	CC1(C)CNC1C1=CN=CC=C1	162,24	C10H14N2
Z274787916	CC1CC2=C(O1)C=CC(CO)=C2	164,20	C10H12O2
Z1276496838	CN(C)C1=NC2=C(C=CC=C2)C(CN)=C1	201,27	C12H15N3
Z1103351268	CC(C)(O)CNC1CCOCC1	173,26	C9H19NO2
Z318711254	CN(CCO)C1=NC(C)=CC(C)=N1	181,24	C9H15N3O
Z1413780552	COCC1=NN2CC(N)CCC2=N1	182,23	C8H14N4O
Z1955566419	CC1=CC(=O)C(OCC2=NC=CS2)=CO1	223,25	C10H9NO3S
Z2067000095	N[C@H]1CC[C@H](CC1)NC1=NC=CC=C1	191,28	C11H17N3
Z2065788064	OC(=O)C1=C2CCCC2=CO1	152,15	C8H8O3
Z2065788326	OCCC1=CN2C=CC=CC2=N1	162,19	C9H10N2O
Z2065464249	COC1=C(Br)C=C(C(O)=O)C(N)=C1	246,06	C8H8BrNO3
Z2065464302	NC1=NN2CCCC2=C1	137,19	C7H11N3
Z2065464238	OC(=O)C1=CC(NC(=O)C2CC2)=NC=C1	206,20	C10H10N2O3
Z1820272539	CC1=CC(C)=C(O1)C(=O)NC1=CN=NS1	223,25	C9H9N3O2S
Z2050688202	CC(C)C1=C(C=CN1)C(O)=O	153,18	C8H11NO2
Z1896596077	CNC1=NC2=C(C=C(CI)C=C2)C(=C1)C#N	217,66	C11H8ClN3
Z2048189261	CC(C)C1COCC(=O)N1	143,19	C7H13NO2
Z2044768809	CC1=CC=C(C=C1)N1CCNCC1=O	190,25	C11H14N2O
Z1791178999	O=C(NC1=CN=NS1)C1CCC=CC1	209,27	C9H11N3OS
Z1848954486	N#CC1=CSC(CNC2=NC=CN=C2)=C1	216,26	C10H8N4S
Z1848950527	CC1=CC=C(CNC2=C(F)C=NC=C2)O1	206,22	C11H11FN2O
Z1741966151	CS(=O)(=O)NCC1CCNCC1	192,28	C7H16N2O2S
Z1791179552	O=C(NC1=CN=NS1)C1CCCC1	211,28	C9H13N3OS
Z1820275462	CC1=C(C=CC=N1)C(=O)NC1=CN=NS1	220,25	C9H8N4OS
Z1271843019	CN(C)C1=CC(C)=C(C=C1)C#N	160,22	C10H12N2
Z1270640441	OC(=O)CCN1C=CC=C1	139,15	C7H9NO2
Z1270446348	CC1=CC=C(O1)C(N)CC(O)=O	169,18	C8H11NO3
Z1270446318	CC(C(O)=O)C1=CC=C(Br)S1	235,10	C7H7BrO2S
Z1270443614	CCC(C)(N)C1=NC(=O)C(C)=C(C)N1	195,27	C10H17N3O
Z1270403496	OC(=O)C1(CC1)C(=O)NC1CC1	169,18	C8H11NO3
Z1270312106	Cl.FC(F)(F)C1=NNC2=C1CNCC2	227,62	C7H9ClF3N3
Z255149896	CC1CC(C)N2N=CC=C2N1	151,21	C8H13N3

Z1268152350	C1CCC(NC1)C1=CCN=C1	151,21	C8H13N3
Z31725250	OCCNC(=O)C1=CC=CC=C1	165,19	C9H11NO2
Z1267881753	OC1CNC(C1)C1CCCCC1	169,27	C10H19NO
Z1262246218	NC1=CN(CC(=O)NC2CCCC2)N=C1	208,27	C10H16N4O
Z1262246220	NC1=CN=C(N=C1)C1CC1	135,17	C7H9N3
Z2658863616	CN1N=CC=C1C(O)C1CCNCC1	195,27	C10H17N3O
Z2630877631	COC1=C2N=C(N)C=CC2=CC=C1	174,20	C10H10N2O
Z2588063784	CC1=NC2=C(N1)C=C(F)C(=C2)C(O)=O	194,17	C9H7FN2O2
Z1741966131	OC(=O)CC1NC(=O)C2=C1C=CC=C2	191,19	C10H9NO3
Z2587654820	OC(=O)C1=CC(=NO1)C1CCNCC1	196,21	C9H12N2O3
Z2583036222	OCC1=CNC(CC2=CC=CC=C2)=N1	188,23	C11H12N2O
Z2234185679	CN1C(=O)N2CCCCC2=C1C(O)=O	196,21	C9H12N2O3
Z2106593034	CCN1C=C(C(O)=O)C(=N1)C1CC1	180,21	C9H12N2O2
Z2106598235	CNC(=O)C1=CC(=NN1C)C(O)=O	183,17	C7H9N3O3
Z2106594244	CCN1N=C(N)C=C1C(O)=O	155,16	C6H9N3O2
Z1741968837	CC1=CC(Cl)=C(C=C1)C(O)=O	170,59	C8H7ClO2
Z2510259497	OC(=O)C1=NC=C(Cl)C(=C1)C1CC1	197,62	C9H8ClNO2
Z2106596435	COC1=C(SC=C1C)C(O)=O	172,20	C7H8O3S
Z2235681686	COC1=C(C#N)C(F)=CC(=C1)C(O)=O	195,15	C9H6FNO3
Z2510259319	CC(N1CCNC1=O)C(O)=O	158,16	C6H10N2O3
Z2510259419	CCC1=NOC=C1C(O)=O	141,13	C6H7NO3
Z2510258108	CC1(CCC2=C1C=CC=C2)C(O)=O	176,22	C11H12O2
Z1741968426	CC1=C(C=CC=C1F)C(O)=O	154,14	C8H7FO2
Z1863941693	OCC1CN(C1)C1=NC=CC=C1	164,21	C9H12N2O
Z2412196601	CC1=CC(C)=C(CCO)N=C1	151,21	C9H13NO
Z2045701767	NC(=O)CN1CCC2=C(C1)C=C(Br)C=C2	269,14	C11H13BrN2O
Z2380439813	OC(=O)C1=CN2CCCCC2=C1	165,19	C9H11NO2
Z2379802743	CN1C=C(NC1=O)C(O)=O	142,11	C5H6N2O3
Z1020680530	CNCC1(O)CCC2=C1C=CC=C2	177,25	C11H15NO
Z183854878	CNC(=O)C1CCC=CC1	139,20	C8H13NO
Z2350906816	CC1=C(C=CC(=C1)C(O)=O)N1C=CC=N1	202,21	C11H10N2O2
Z2327883817	CC1=C(NC1(=O)N1)C(O)=O	142,11	C5H6N2O3
Z1509609880	COC1=C(C=C(Br)C=C1)C1(CC1)C(O)=O	271,11	C11H11BrO3
Z2327883913	CN1CC(NC1=O)C(O)=O	144,13	C5H8N2O3
Z1033301244	CC(C)N1C=CN=C1CO	140,19	C7H12N2O
Z86430593	O=C(NC1CCS(=O)(=O)C1)C1=CC=CS1	245,31	C9H11NO3S2
Z1262691705	CC1=C(C=CC(=C1)C#N)N1C=NC=N1	184,20	C10H8N4
Z1262398566	CNC(=O)CN1C=NC(N)=N1	155,16	C5H9N5O
Z1262398499	CC(C(O)=O)C1=C(C=CC=C1)C(F)(F)F	218,18	C10H9F3O2
Z1262398379	CC1=NN2CC(N)CCC2=N1	152,20	C7H12N4
Z2680629344	CC1=NNC(N)=C1C1=CC(C)=CC=C1	187,25	C11H13N3
Z2680629322	COC1=C2N=C(N)C=CC2=C(Cl)C=C1	208,65	C10H9ClN2O
Z2677009987	CC1(C)CC(C(O)=O)C(C)(C)O1	172,22	C9H16O3
Z2679906821	O=C1NCCC2=C1NC=N2	137,14	C6H7N3O
Z2678251339	CC1(CC1)C1=NSC(N)=N1	155,22	C6H9N3S
Z1204332192	CC1=CC(OC(F)F)=C(S1)C(N)=O	207,19	C7H7F2NO2S
Z1889709700	OC(=O)C1=CN(N=C1)C1CC1	152,15	C7H8N2O2
Z1262254315	CCOC1=C2CNCCC2=NC=N1	179,22	C9H13N3O
Z1262254306	CC1=CN2CC(N)CCC2=N1	151,21	C8H13N3
Z1262254299	Cl.Cl.C1CNCC(C1)C1=NC=CS1	241,17	C8H14Cl2N2S
Z1741814701	CCC1CN(CCN)CCO1	158,25	C8H18N2O
Z1824028566	OC[C@H]1CCCN1CC1=CC=C(Br)O1	260,13	C10H14BrNO2
Z1259339814	OCC1CCC2=C1C=CC=C2	148,21	C10H12O
Z2111525346	O=C1NCCCN1CC1=CC=CC=C1	190,25	C11H14N2O
Z2050688001	COC1=C(Cl)C=C2NC=CC2=C1	181,62	C9H8ClNO
Z2044768696	CN1CC(=O)NC2=C1C=C(Br)C=C2	241,09	C9H9BrN2O
Z2027049497	OC(=O)C1=NNC(CC2=CC=CC=C2)=C1	202,21	C11H10N2O2
Z1896598998	CNC1=C2C=CC=CC2=NC(=N1)C(F)F	209,20	C10H9F2N3
Z1982689193	COC1=C(C=CC=C1)C1=C(N)C=CC=N1	200,24	C12H12N2O
Z1945707487	O=C1CC2CCCN2C2=C(N1)C=CC=C2	202,26	C12H14N2O
Z1881598945	COC1=C(C=C(C=C1)C(O)=O)C1CC1	192,21	C11H12O3
Z1868316875	CN1C(=O)OC2=C1C=CC(CO)=C2	179,18	C9H9NO3
Z1827897989	CC1=C(N)C=C(C=C1)N1C=CC=N1	173,22	C10H11N3
Z1824334032	CCOC1=CC=C(C=C1)C1=CCN=C1N	203,25	C11H13N3O
Z1815157395	CN1CCC2=C1C=CC(=C2)C(O)=O	177,20	C10H11NO2
Z1318171181	CN(CCO)C1=CC=C(F)C=C1	169,20	C9H12FNO
Z1337753275	OCCN1CCCC1C1=CC(F)=CC=C1	209,26	C12H16FNO

Z636447806	C1C1=CC=C(CNC2=NC=CC=C2)S1	224,71	C10H9CIN2S
Z940781276	BrC1=C(CNC2=NC=CC=N2)SC=C1	270,15	C9H8BrN3S
Z153217142	CC(=C)CN1N=NC2=C(C=CC=C2)C1=O	201,23	C11H11N3O
Z458900954	CC(C)S(=O)(=O)C1=CC=C(C=C1)C(N)=O	227,28	C10H13NO3S
Z2583384752	OC1CCOC2(CCOCC2)C1	172,22	C9H16O3
Z1552027336	CC1=CC(=C(CN)C=C1)S(C)(=O)=O	199,27	C9H13NO2S
Z1552027084	CC1=C(C=NN1C1CCOCC1)C(O)=O	210,23	C10H14N2O3
Z1551463531	NC1=NOC(COC2=CC=C(F)C=C2)=N1	209,18	C9H8FN3O2
Z1536942816	OC(=O)CN1C=NC(=N1)C1=CC=CC=C1	203,20	C10H9N3O2
Z220616874	CN1N=C(C)C2=C1SC(=C2)C(O)=O	196,22	C8H8N2O2S
Z1501468148	CC1=NC2=C(NC=C(C#N)C2=O)C=C1	185,19	C10H7N3O
Z1495385160	CN(C)C1=C(N)C=CC(C)=N1	151,21	C8H13N3
Z1203840176	CC(N1CC[C@H](O)C1)C1=CC=C(F)C=C1	209,26	C12H16FNO
Z1465461599	OC1(CCCC1)C1=CC=CC=C1	148,21	C10H12O
Z133718524	CS(=O)(=O)N1CCNC(=O)C1	178,21	C5H10N2O3S
Z1463254711	C[C@H](O)C1=CC(=CC=C1)C#N	147,18	C9H9NO
Z1309454334	N[C@H]1CC[C@H](CC1)N1CCCS1(=O)=O	218,32	C9H18N2O2S
Z1416203541	CC1CCC(=O)N1CC1=CC=CC=C1	189,26	C12H15NO
Z1255526837	COC1=CC(=CC=C1)C#CCO	162,19	C10H10O2
Z90504166	CC1CCC(CC1)NCC1CCCO1	197,32	C12H23NO
Z1259087027	CC1=CC(O)CC(C)C1	140,23	C9H16O
Z1336428394	CS(=O)(=O)C1CCC(O)C1	164,22	C6H12O3S
Z1587237771	CN(CC1=NC=CN=C1)C1=NC=CC=C1	200,25	C11H12N4
Z52665456	C=CCN1CCN(CC1)C1=NC=CC=N1	204,28	C11H16N4
Z228588982	NCCN1CCCCC1	142,25	C8H18N2
Z1267882018	CC1=C(CN)OC2=C1C=CC=C2	161,20	C10H11NO
Z57756573	N#CC1=CC=C(C=C1)N1CCCC1	172,23	C11H12N2
Z956073828	CS(=O)(=O)N1CCCC1CN1CCCC1	232,34	C10H20N2O2S
Z1747831414	OCC1CCCN1C(=O)C1=CC(Br)=CS1	290,18	C10H12BrNO2S
Z1924626474	CC1=C(C=C(F)C=C1)C1=NN=C(N)S1	209,24	C9H8FN3S
Z1741972095	COC1=C(Cl)C=CC(N)=C1	157,60	C7H8ClNO
Z1898799515	CC1=NC2=C(N1)C=CC=C2F	150,16	C8H7FN2
Z1889975631	CN1N=C(C(F)F)C2=C1SC(=C2)C(O)=O	232,20	C8H6F2N2O2S
Z744593170	NC1=NN=C(O1)C1CC2=C(O1)C=CC=C2	203,20	C10H9N3O2
Z373775692	CN1C=C(NC(=O)C2=CC=C(Cl)S2)C=N1	241,69	C9H8ClN3O5
Z57728689	OC(=O)CCN1C(=O)SC2=C1C=CC=C2	223,25	C10H9NO3S
Z372500344	CC1=C(SC=C1)C(=O)NC1=CCN=C1	207,25	C9H9N3O5
Z373775856	CN1C=C(NC(=O)C2=CC=CO2)C=N1	191,19	C9H9N3O2
Z57346035	CC1=CC(NC(=O)C2=CC=CS2)=NO1	208,24	C9H8N2O2S
Z85887064	OC(=O)CNC(=O)C1=CC(F)=CC(F)=C1	215,16	C9H7F2NO3
Z32014170	CN(C)C(=O)CNC(=O)C1=CC=C(Br)O1	275,10	C9H11BrN2O3
Z1259335845	OC(=O)C1CC(C1)C1=CC=C(F)C=C1	194,21	C11H11FO2
Z1259273114	NC(C(O)=O)C1=CC(Cl)=CC=C1	185,61	C8H8ClNO2
Z1259162044	Cl.FC1=CC(CN2CCNCC2=O)=CC=C1	244,69	C11H14ClFN2O
Z1259162021	CC1CC(=O)N(C)C2=C(N1)C=CC=C2	190,25	C11H14N2O
Z1250100761	NCC1=CC=C(C=C1)C1=CC=NC=C1	184,24	C12H12N2
Z1245537799	NC1=CC(CN2C=CC=N2)=CC=C1	173,22	C10H11N3
Z1143333160	CC(C)C1=NNC(C(=O)N(C)C)=C1Br	260,14	C9H14BrN3O
Z1171979231	CC1=NN(C=C1)C1=CC(=CC=C1)C(O)=O	202,21	C11H10N2O2
Z68249055	CNC(=O)C1(CC1)C1=CC=C(Cl)C=C1	209,67	C11H12ClNO
Z790348314	FC1=CC2=C(C=C1)N=C(NC2=O)C1CC1	204,20	C11H9FN2O
Z28880832	CC(NC(=O)C1=CC=CO1)C1=CC=CS1	221,27	C11H11NO2S
Z425484910	CC1=CC(=O)NC(=N1)C1=CC(N)=CC=C1	201,23	C11H11N3O
Z1900549400	CC1=CN=C(CNC2=C(F)C=CC=N2)O1	207,21	C10H10FN3O
Z2054373621	CO[C@H]1C[C@H](N(C1)C1CCCC1)C(N)=O	212,29	C11H20N2O2
Z1601232164	FC1=C(F)C=C(NCC2=CSN=N2)C=C1	227,23	C9H7F2N3S
Z871834842	NCC1CCN(CC1)C1CCOCC1	198,31	C11H22N2O
Z2447618800	CCN(C(=O)C(C)N)C1=CC=C(F)C=C1	210,25	C11H15FN2O
Z1667545918	CC(=O)NCC1=CN=CS1	156,20	C6H8N2OS
Z1419216922	CN(C)C(=O)C1=CC2=C(SC=C2)C=C1	205,28	C11H11NO5
Z275170288	CN1C=C(Br)C(=N1)C(O)=O	205,01	C5H5BrN2O2
Z2205958920	CC1=NSC(NC2CC2)=C1C(O)=O	198,24	C8H10N2O2S
Z2197092708	CC1=CC2=C(C=C1)N=C(N)N2	147,18	C8H9N3
Z2188171939	COC1=CC2=C(C=C1)C(N)=NO2	164,16	C8H8N2O2
Z2182115389	NC(=O)[C@H]1CCO[C@@H](C1)CCNCC1	198,27	C10H18N2O2
Z2177031060	FC(F)C1=NC2=C(C=C(Cl)C=C2)C(=O)N1	230,60	C9H5ClF2N2O
Z2177031006	OCC1(CCN1)C1=CC=CC=C1	177,25	C11H15NO

Z1899665464	C1C1=CC=C(CN2N=CC=CC2=O)C=C1	220,66	C11H9CIN2O
Z2168496123	COCC1(CCOCC1)C(O)=O	174,20	C8H14O4
Z2168282707	CN1N=NC2=C1CC(C2)C(O)=O	181,20	C8H11N3O2
Z2168282799	OC(C(O)=O)C1=C(F)C=C(Cl)C=C1	204,58	C8H6ClFO3
Z85517151	CC1=CC=C(S1)C(=O)NC1=CC=NC=C1	218,27	C11H10N2O5
Z32024593	CCNC(=O)C1CCCC1	141,21	C8H15NO
Z31479594	CC(C)C(NC(C)=O)C(=O)N1CCCC1	212,29	C11H20N2O2
Z32064488	C=CCNC(=O)C1=CC2=C(C=C1)N=CS2	218,27	C11H10N2O5
Z111479616	OC(=O)CN1C(=O)SC2=C1C=CC=C2	209,22	C9H7NO3S
Z30841099	BrC1=CC(=CN=C1)C(=O)NC1CC1	241,09	C9H9BrN2O
Z57745260	C1CCN(C1)C1=C2N=CN2=NC=N1	189,22	C9H11N5
Z140637338	COCC(=O)NC1=CC=C(C=C1)C#N	190,20	C10H10N2O2
Z262222238	CC1=C(C(O)=O)C(=NO1)C1=CC=CC=C1	203,20	C11H9NO3
Z57040473	NC1=CC=NN1CC1=CC=CO1	163,18	C8H9N3O
Z1193326527	CN1C=C(CN2C=C(Br)C=N2)C=N1	241,09	C8H9BrN4
Z1396758266	CC1(C)CN(CCS1=O)C1=NC=CN=C1	225,31	C10H15N3O5
Z991187420	Cl.C(N1CCCC1)C1=CN2C=CC=NC2=N1	238,72	C11H15ClN4
Z1169950314	CC1CC1C1=NC(=NO1)C1=CN=CC=C1	201,23	C11H11N3O
Z1245633121	CN1N=CC2=C1CCCC2N	151,21	C8H13N3
Z239081196	CC(N)C(N1CCCC1)C1=CC=CC=C1	204,32	C13H20N2
Z1262252990	CC1=C(C=CC=C1)C(C)(C)CN	163,26	C11H17N
Z1313429074	COC1(C)CC(N)C1(C)C	143,23	C8H17NO
Z1318147319	CC(CN)NC1=CC=CC=C1	150,23	C9H14N2
Z1146147705	CC(=O)NCC1=CC=C(Br)C=C1	228,09	C9H10BrNO
Z1346385372	CC1=CC(=CC=C1)C1=NON=C1N	175,19	C9H9N3O
Z1346385327	OC(=O)CCC1=NC2=C(N1)C=CC=C2F	208,19	C10H9FN2O2
Z740170614	CNS(=O)(=O)C1=CSC(=C1)C(O)=O	221,25	C6H7NO4S2
Z1340444601	CC(=O)N1CCC(C1)C(O)=O	157,17	C7H11NO3
Z1220685184	CN(CC(N)=O)C1=CC(C)=C(Br)C=C1	257,13	C10H13BrN2O
Z1335722261	CCS(=O)(=O)C1=NC2=C(S1)C=C(N)C=C2	242,31	C9H10N2O2S2
Z340632658	CC(=O)NCC1=CC(Br)=CC=C1	228,09	C9H10BrNO
Z1268436514	CC1=CC(=CC(C)=C1OCC(N)=O)C#N	204,23	C11H12N2O2
Z1333043367	CN1N=CC2=C1N=C(C)C=C2C(O)=O	191,19	C9H9N3O2
Z133742684	CC(NS(C)(=O)=O)C1=CC=C(Cl)C=C1	233,71	C9H12ClNO2S
Z1357774220	CC(=O)NC1=NC(C(O)=O)=C(Br)C=C1	259,06	C8H7BrN2O3
Z1354487571	COCC1=NC2=C(O1)C=CC(N)=C2	178,19	C9H10N2O2
Z1815149156	CN(C)C1(CN)CC2=C(C1)C=CC=C2	190,29	C12H18N2
Z1814381728	CC1=CCC(CC1)C(O)=O	140,18	C8H12O2
Z1614607478	OC(=O)C1(CC1)C(=O)NC1=CC=CC=C1	205,21	C11H11NO3
Z31408238	O=C(NCC1=CC=CO1)C1=CC=CS1	207,25	C10H9NO2S
Z25117855	NC(=O)COC1=C(F)C=C(Br)C=C1	248,05	C8H7BrFNO2
Z439257438	CN1N=C(N)C2=C1CCC2	137,19	C7H11N3
Z415636582	CC1=CC=C(C=C1)N1C=C(N=N1)C(O)=O	203,20	C10H9N3O2
Z274797730	BrC1=CN=C(N=C1)N1CCNCC1	243,11	C8H11BrN4
Z32367696	O=C(NC1CC1)C1=CC2=C(C=C1)N=CS2	218,27	C11H10N2O5
Z26283147	NC(=O)COC1=CC(F)=C(F)C=C1	187,15	C8H7F2NO2
Z728935218	NC(=O)C1=CC(Cl)=C(N=C1)N1CCCC1	225,68	C10H12ClN3O
Z401435400	CC(NS(C)(=O)=O)C1=C(F)C=CC(F)=C1	235,25	C9H11F2NO2S
Z594970990	O=C(NCC1=CC=CS1)C1=NSN=C1	225,28	C8H7N3OS2
Z649822028	CC1=C(SC=N1)C(=O)NCC1=NNC=C1	222,27	C9H10N4OS
Z108544658	CN1C=CC(NC(=O)C2=CC=C(Br)O2)=N1	270,09	C9H8BrN3O2
Z332753086	BrC1=CC(=CS1)C(=O)N1CCNC(=O)C1	289,15	C9H9BrN2O2S
Z235785166	OC(=O)CN1CCC2=C(C1)C=CS2	197,25	C9H11NO2S
Z85886787	OC(=O)CNC(=O)C1CCCC1	157,17	C7H11NO3
Z992716974	CC(C(O)=O)C1=C(C)ON=C1C	169,18	C8H11NO3
Z275163834	OC(=O)C1=CC=C(CN2C=C(Cl)C=N2)O1	226,62	C9H7ClN2O3
Z992716784	CC1=NN=C2C=CC(=CN12)C(O)=O	177,16	C8H7N3O2
Z29672816	CC1=NN=C(NC(=O)C2=CN=CC=C2)S1	220,25	C9H8N4OS
Z108545268	CN1C=CC(NC(=O)C2=CC=C(Br)S2)=N1	286,15	C9H8BrN3OS
Z680882022	CCN1N=CC2=C1N=C(C)C=C2C(O)=O	205,22	C10H11N3O2
Z57912417	CC1=C(N)C=C(C=C1)C(N)=O	150,18	C8H10N2O
Z193091370	CS(=O)(=O)N1CCCC1C(N)=O	192,23	C6H12N2O3S
Z434632738	CN1C=C(NC(=O)C2=C(Br)C=CS2)C=N1	286,15	C9H8BrN3OS
Z211302168	NC1=C(N=CC=N1)C(=O)N1CCCCC1	206,25	C10H14N4O
Z729725920	CC1=NOC(NC(=O)C2CCC=CC2)=N1	207,23	C10H13N3O2
Z339569398	O=C(NC1CCS(=O)(=O)C1)N1CCCC1	232,30	C9H16N2O3S
Z1783461887	CN1C=NN(CCC2=CC=CS2)C1=O	209,27	C9H11N3OS

Z1694794721	CN1C=NN=C1NC(=O)C1=CC=C(C)O1	206,21	C9H10N4O2
Z1102357527	O=C(NC1CCC(=O)NC1)C1=CSC=N1	225,27	C9H11N3O2S
Z211003642	OC(=O)C1CCN1C(=O)C1=CC=CC=C1	205,21	C11H11N3O3
Z383822506	OC1=C(C=CC=N1)C(=O)NCC1CCCC1	206,25	C11H14N2O2
Z803129884	CN1C=C(C(O)=O)C(=N1)C1=CN=CC=C1	203,20	C10H9N3O2
Z1262246184	NC1=CC2=C(C=C1)N=C(S2)C1CC1	190,26	C10H10N2S
Z2372280348	CN1C(=O)NCC11CCNCC1	169,23	C8H15N3O
Z29693757	O=C(NCC1=CC=CS1)C1CC1	181,25	C9H11NOS
Z1222331974	CCOC1=NC(=CC=C1)N1CCNCC1	207,28	C11H17N3O
Z839818900	CC(N1CCCC(O)C1)C1=NN=C(C)O1	211,27	C10H17N3O2
Z1891775791	FC1=CN=C(N=C1)N1CCNCC1	182,20	C8H11FN4
Z744843682	OC(=O)C1=CC=CN1CC1=CC=CS1	207,25	C10H9NO2S
Z1139751314	NC1(CC(C1)C1=CC=CC=C1)C(O)=O	191,23	C11H13NO2
Z1626921271	CC1CC(CC(=O)N1)C(O)=O	157,17	C7H11NO3
Z1443588488	CC1=C(N)C=C(CN2CCCC2)C=C1	190,29	C12H18N2
Z1415893841	C1CNC2=C(NC1)N=CC=C2	149,20	C8H11N3
Z1354416054	NC1=CC2=C(C=C1)N=C(O2)C1CC1	174,20	C10H10N2O
Z1272670423	CCC1=NN=C(O1)C1=CC=C(N)C=C1	189,22	C10H11N3O
Z1270207933	O=C1CC2(CN1)CCCCC2	153,23	C9H15NO
Z2227687433	O=C1NC(=NC2=C1CCC2)C1CC1	176,22	C10H12N2O
Z2327131587	CC1C(N)CC2=C1C=CC=C2	147,22	C10H13N
Z199471388	CC(=O)NC1=NN=C(S1)C1=CC=NC=C1	220,25	C9H8N4O5
Z33598681	CC1CCC(CC1)NC(=O)CNC(C)=O	212,29	C11H20N2O2
Z57299924	CC(C)CN1C(CO)=NC2=C1C=CC=C2	204,27	C12H16N2O
Z45527714	CNS(=O)(=O)C1=C(Cl)C=CC=C1	205,66	C7H8ClNO2S
Z220564330	COC1=CC(=CC(OC)=C1Br)C(O)=O	261,07	C9H9BrO4
Z220383490	COC1=CC2=C(C=C1)N=C(C=C2)C(O)=O	203,20	C11H9NO3
Z31212209	CC1=C(C)C2=C(S1)N=CN=C2NCCO	223,29	C10H13N3OS
Z220533930	COC1=CC(C(O)=O)=C(Br)C=C1	231,05	C8H7BrO3
Z217102814	N#CC1=CN=C(C=C1)N1CCOCC1	189,22	C10H11N3O
Z1860991862	CC1=CC(=O)C2=C(N1)C(F)=C(F)C=C2	195,17	C10H7F2NO
Z1860991543	OC(=O)C1COC2=C1C=C(Cl)C=C2	198,60	C9H7ClO3
Z1889902486	OC(=O)C1CCCC2=C1N=CN2	166,18	C8H10N2O2
Z1898825882	CC1=C(Br)C=CC(N)=C1F	204,04	C7H7BrFN
Z1817048016	NC(=O)N1CCCC2(CCCC2)CC1	210,32	C12H22N2O
Z1868430549	CC1=C(CC(O)=O)C=CS1	156,20	C7H8O2S
Z1868430535	CC(=O)N1CC(C1)C(O)=O	143,14	C6H9NO3
Z1127124482	O[C@H]1CCN(C1)C1=C2SC=CC2=NC=N1	221,28	C10H11N3OS
Z288780094	CN1C(C)=CC=C1C(=O)NCC1CC1	192,26	C11H16N2O
Z199538186	C1CN(CCN1)C1=CC=NC=C1	163,22	C9H13N3
Z56869298	CN1N(C(=O)C(N)=C1C)C1=CC=CC=C1	203,25	C11H13N3O
Z1166180298	CC1CN(C)CCN1C(=O)C1=CN=NS1	226,30	C9H14N4OS
Z340495298	CC(C)N(C1CC1)C(=O)C1=NOC(C)=C1	208,26	C11H16N2O2
Z279850696	COCC(=O)NC1=C(F)C=CC=C1F	201,17	C9H9F2NO2
Z2216711746	NC1=NC=C(C=C1)C1CCC1	148,21	C9H12N2
Z1245580414	CCOC1=C(N)C=CC=N1	138,17	C7H10N2O
Z1569715489	CC1(CCC(O)=O)CCC(=O)N1	171,20	C8H13NO3
Z1551469282	C1CCC2(C1)COCCN2	141,21	C8H15NO
Z31183312	CN(CC1=CC=CO1)C1=NC=CC=N1	189,22	C10H11N3O
Z1262395901	CC1=NN=C(C=C1)N1CCCC1CO	193,25	C10H15N3O
Z1183468884	OCC1=CN2C=CN=C2C(Cl)=C1	182,61	C8H7ClN2O
Z998307088	CC(C(=O)N(C)C)C1=C(Cl)C=CC=C1Cl	246,13	C11H13Cl2NO
Z319845694	CC(C)C(=O)NC1CCCC2=C1C=CO2	207,27	C12H17NO2
Z369044210	CC1COCCN1CC1=C(Cl)SN=N1	233,71	C8H12ClN3OS
Z1266823292	CC(N)C1=CC(C)=CC(C)=C1	149,24	C10H15N
Z1262254168	CC1=CC(NCC2CCNC2)=NC=C1	191,28	C11H17N3
Z1255406112	N#CC1=CC2=C(COCCO2)N=C1	162,15	C8H6N2O2
Z2507919883	CC1=NC(N)=C(C#N)C(C)=C1	147,18	C8H9N3
Z2492774517	CC(C)CC1=NC(C#N)=C(N)O1	165,20	C8H11N3O
Z2492774641		141,21	C8H15NO
Z2492774577	CC(CC(O)=O)N1C=CC(C)=N1	168,20	C8H12N2O2
Z2492774555	CN(C)C1=C(N)C=C(C)N=N1	152,20	C7H12N4
Z1945710573	CC1(CC1)C1=CSC(=N1)C1=CC=NN1	205,28	C10H11N3S
Z335451356	CC1=CC(=CC=C1)C(N)CC(O)=O	179,22	C10H13NO2
Z2472860086	COC1=C(Cl)C=C(C2CC2)C(N)=C1	197,66	C10H12ClNO
Z2472860018	CC1=C(NC(=O)C2=C1C=CC=C2)C(O)=O	203,20	C11H9NO3
Z2471547970	FC(F)(F)C1=C2OCC(=O)NC2=CC=C1	217,15	C9H6F3NO2

Z2510258174	CC1=C(CC(O)=O)SC(=N1)C1CC1	197,25	C9H11NO2S
Z1982493954	CC1=NC(C2CC2)=C(N)C=N1	149,20	C8H11N3
Z1981870462	CN1C=CC(C(O)=O)=C1C	139,15	C7H9NO2
Z1973465452	NC1=C(CO)C=CC(Br)=C1	202,05	C7H8BrNO
Z914115824	CN(C)C1=CN=C(NC(C)=O)C=C1	179,22	C9H13N3O
Z1948934309	CC(C)C1=NC=C(N)C=N1	137,19	C7H11N3
Z1232688349	N#CC1=C(NC2CCC=CC2)N=CC=N1	200,25	C11H12N4
Z1838000858	CN1N=CN=C1S(=O)(=O)CC1CC1	201,24	C7H11N3O2S
Z1992316392	O=C1CN2CCCC2CN1	140,19	C7H12N2O
Z1259041014	OC(=O)C1COC2=C1C=CC=C2	164,16	C9H8O3
Z1516187297	COC1=C(C#N)C(F)=CC=C1	151,14	C8H6FNO
Z291280256	OC(=O)C1=CC2=C(NC(=O)CCC2)C=C1	205,21	C11H11NO3
Z2692095047	CN1C=CC(=N1)C1=NC(=CS1)C#N	190,22	C8H6N4S
Z2692093609	CN1C=NN=C1C1=CC(Br)=C(C)C=C1	252,12	C10H10BrN3
Z2692093569	OC(=O)C1=C(Br)C(=CC=C1F)C(F)(F)F	287,01	C8H3BrF4O2
Z2692093940	CCC1=C(N)N=CC(Cl)=C1	156,61	C7H9ClN2
Z2092555279	CCC1(O)CCN(C1)C1=NC=C(F)C=C1	210,25	C11H15FN2O
Z1259155983	CN(C)C1=C(N)C=NC=C1	137,19	C7H11N3
Z1259155970	COC1=C(N)C(=CC=N1)N(C)C	167,21	C8H13N3O
Z1820007629	CCC1=NC2=C(C=CC=C2)N1CCN	189,26	C11H15N3
Z98976533	OCCOC1=C(Cl)C=C(C=C1)C#N	197,62	C9H8ClNO2
Z1395852355	CC1=CSC(CN2CCS(=O)CC2)=N1	230,34	C9H14N2OS2
Z1837073461	CCC(C)N1N=CC(C(O)=O)=C1C	182,22	C9H14N2O2
Z1231613812	NC(=O)C1=C(F)C=C(OC(F)F)C=C1F	223,13	C8H5F4NO2
Z1836338758	COC1=C(Br)C=NC(C)=C1	202,05	C7H8BrNO
Z1513499619	O=C1CN(CCN1)C1=C(C=CN=C1)C#N	202,22	C10H10N4O
Z1750884927	CN1C=NN=C1NC(=O)C1=CSN=C1C	223,25	C8H9N5OS
Z1827111442	O=C1C=CNC(CCC2=CC=CC=C2)=N1	200,24	C12H12N2O
Z1824511371	OCC1(CCCCC1)C1=CC=CC=C1	176,26	C12H16O
Z1258992644	OC1C(=O)NC2=C1C=CC=C2	149,15	C8H7NO2
Z57900343	COC1=C(C)C=C(C=C1)C#N	147,18	C9H9NO
Z1258992472	OCC1=CC2=C(C(NN=N2)C=C1	149,15	C7H7N3O
Z1258932991	CCN1N=NC(C(O)=O)=C1CC	169,18	C7H11N3O2
Z1255523429	CC1=C(C(N)=NN1)C1=CC(Br)=CC=C1	252,12	C10H10BrN3
Z1251219820	CC(C)N1C=CC(CO)=N1	140,19	C7H12N2O
Z1250132686		214,62	C10H8ClFO2
Z1250132683	CN(C)C(=O)NC1=CC(=CC=C1)C(O)=O	208,22	C10H12N2O3
Z1250132389	OCC1=CN=C(O1)C1=CC=CS1	181,21	C8H7NO2S
Z1250132330	CC(C)N1C=CC=C1C(O)=O	153,18	C8H11NO2
Z1262237272	CC(CC1=C(C)N(C)N=C1C)C(O)=O	196,25	C10H16N2O2
Z275128648	NC1=NN(CC2=CC=CC=C2)C=C1	173,22	C10H11N3
Z1259341102	CC1=C(OC(CO)=O)C=CC=C1Cl	200,62	C9H9ClO3
Z1259341103	OC(=O)C1=C(F)C=C(OC(F)F)C=C1F	224,11	C8H4F4O3
Z71176798	CC(C)NC1=C(C=CC=N1)C(O)=O	180,21	C9H12N2O2
Z1259339977	CC(C)(C(O)=O)C1=CC=CS1	170,23	C8H10O2S
Z1229798311	CC(=O)NC1=C(C(O)=O)C(F)=CC=C1	197,17	C9H8FNO3
Z1259335904	CN(C)C(=O)C1=C(C=CC=C1)C(O)=O	193,20	C10H11NO3
Z1259162097	CC(O)(CC1=CC=CC=C1)C(O)=O	180,20	C10H12O3
Z235448344	OC1CCOC2=C1C=C(Br)C=C2	229,07	C9H9BrO2
Z1259161906		192,21	C11H12O3
Z228589672	COC1=C(N)C(C(O)=O)=C(Cl)C=C1	201,61	C8H8ClNO3
Z2689031646	OCC1=CC2=C(OC(CO2)C(Br)=C1	259,10	C10H11BrO3
Z2689031546	CC(C)C1=NOC=C1C(O)=O	155,15	C7H9NO3
Z1460222863	CC1=CC(F)=C(NC2CCNC2=O)C=C1	208,24	C11H13FN2O
Z1613884267	CC1=C(C=CO1)C(=O)N1CCC=C(F)C1	209,22	C11H12FN2O2
Z2687735108	CNC1=NC(=CC=N1)C1=C(C)N=C(C)S1	220,29	C10H12N4S
Z1432018343	C[C@@H](CO)NC1=C(F)C=C(Cl)C=N1	204,63	C8H10ClFN2O
Z1267881987	CC(CN)OC1=CC=C(C)C=C1	165,24	C10H15NO
Z1545196101	CC1=NNC=C1CNC1=C(F)C=CC=C1	205,24	C11H12FN3
Z1480753089	FC1=C(NCC2=CN=CS2)C=CC=C1	208,25	C10H9FN2S
Z1354370966	FC1=C(N=CC(Cl)=C1)N1CCNC(=O)C1	229,64	C9H9ClFN3O
Z2687203970	O=C1NCCC2=C1C=CS2	153,20	C7H7NOS
Z2687203908		183,25	C10H17NO2
Z2687203705	NC1=C(Cl)C=C2CCCC2=C1	167,64	C9H10ClN
Z1203191681	CC(=O)NCC1=NC=CN1	139,16	C6H9N3O
Z1481102552	FC1=CN=C(NCC2=CC=CS2)N=C1	209,24	C9H8FN3S
Z1840519037	CNS(=O)(=O)C1=C(F)C=C(OC)C=C1	219,23	C8H10FNO3S

Z192952702	CN(C)S(=O)(=O)C1=CC(F)=CC(F)=C1	221,22	C8H9F2NO2S
Z923951640	CS(=O)(=O)NCC1=C(F)C=C(F)C=C1	221,22	C8H9F2NO2S
Z1171978800	OC(=O)C1=C(OC(F)F)C=CS1	194,15	C6H4F2O3S
Z1171978897	CCC1=NC=C(S1)C(O)=O	157,19	C6H7NO2S
Z118690766	O=C(NC1CCS(=O)(=O)C1)C1CC1	203,26	C8H13NO3S
Z135505014	CNC(=O)C1C2CC3CC(C2)CC1C3	193,29	C12H19NO
Z1167043933	COC1=CC(NC2CCNCC2)=CC=C1	206,29	C12H18N2O
Z227840048	CN(C)S(=O)(=O)C1=C(SC=C1)C(O)=O	235,27	C7H9NO4S2
Z899154150	NC(=O)CN1C=CC(=O)C2=C1C=CC=C2	202,21	C11H10N2O2
Z381479818	O=C(NC1=CC=CC=C1)C1COCCO1	207,23	C11H13NO3
Z126992654	CN(CCO)C1=C2C=CC=CC2=NC=N1	203,25	C11H13N3O
Z62455180	C=CCNC1=C2C=CC=CC2=NC=N1	185,23	C11H11N3
Z139937454	CCNC(=O)C1=CN=C2SC=CN2C1=O	223,25	C9H9N3O2S
Z1160899478	OC1CC(C(O)=O)C2=C1C=CC=C2	178,19	C10H10O3
Z1768428950	COC(C)C1=NC(=CS1)C(O)=O	187,21	C7H9NO3S
Z1768428787	OC(=O)C1CC11CCS(=O)(=O)CC1	204,24	C8H12O4S
Z1768160457	CC1=C(C)N2C(S1)=NC=C(C(O)=O)C2=O	224,23	C9H8N2O3S
Z1768160454	OC(=O)CCC1=CC2=C(CCC2)C=C1	190,24	C12H14O2
Z1762658220	COC1=C(N)C(C(O)=O)=C(Br)C=C1	246,06	C8H8BrNO3
Z1742054999	CN(C)C1=NOC(=N1)C1CCNCC1	196,25	C9H16N4O
Z1603605397	CC1=C(SC=C1)C(=O)NC1(CC1)C(O)=O	225,26	C10H11NO3S
Z1737940684	CC(N)(C(O)=O)C1=CC(F)=CC=C1	183,18	C9H10FN2O2
Z1718361702	CC(C)CCN1N=CC(C#N)=C1N	178,24	C9H14N4
Z26794305	CC(=O)NC1=CC2=C(NC(=O)N2)C=C1	191,19	C9H9N3O2
Z1499061380	CN1CCCC(C)(CO)C1	143,23	C8H17NO
Z2326079238	CC1CCC(C)(C)N1C(=O)COC(F)F	221,25	C10H17F2NO2
Z85926259	CC(N1N=CC=C1N)C1=CC=CS1	193,27	C9H11N3S
Z1259087078	CC(CN)CN1C=CC=N1	139,20	C7H13N3
Z2234185640	CC(C)(CC1CCCN1)C(N)=O	184,28	C10H20N2O
Z1340493763	COCC(C)(N)C1=CC=CC=C1	165,24	C10H15NO
Z2358147253	FC1=CNC(=C1)C(=O)NCC1CC11CC1	208,24	C11H13FN2O
Z1522339024	CNC(=O)CN1CCC(=CC1)C(F)(F)F	222,21	C9H13F3N2O
Z2111525761	OCCC1=NN=C(O1)C1=CC=CC=C1	190,20	C10H10N2O2
Z2111525135	NC1=NC2=C(C(CCC2)N)C=C1	149,20	C8H11N3
Z365255930	CN1CC(CC1=O)C(N)=O	142,16	C6H10N2O2
Z2092370954	CCN(C)C(=O)C1=CC(N)=CC=C1	178,24	C10H14N2O
Z1203329531	CC(=O)NCC1(O)CCCC1	157,21	C8H15NO2
Z2034643365	CC#CCN1C=NC(=N1)C1=NC=CS1	204,25	C9H8N4S
Z1431002634	NC1(CCO)CCOCC1	145,20	C7H15NO2
Z44548922	CC(N)C(=O)N1CCCCC1	156,23	C8H16N2O
Z1258578160	CNC1=NNC(=C1)C(C)C	139,20	C7H13N3
Z1273312142	CCOC1=C(C=CC=C1F)C(=O)N(C)C	211,24	C11H14FN2O2
Z280816320	CC(C1CC1)N(C)C(=O)C1=CC(C)=NO1	208,26	C11H16N2O2
Z1406872867	CC1CCCC(CCO)C1	142,24	C9H18O
Z1696946116	CC1CCOC1C(=O)NC1=NC=CN=C1	207,23	C10H13N3O2
Z1723549409	CC(C)C1CCCC(N)C1	141,26	C9H19N
Z1723549378	CC(C)C1(C)CC1C(O)=O	142,20	C8H14O2
Z1238477874	C1CCC(NC1)C1=CC=CO1	151,21	C9H13NO
Z193075552	CC(N(C)S(C)(=O)=O)C1=CC=C(F)C=C1	231,29	C10H14FNO2S
Z1171716847	NCC1CCCN(CC2=CN=CC=C2)C1	205,31	C12H19N3
Z56346996	CCN1N=NC2=C1C=CC(=C2)C(O)=O	191,19	C9H9N3O2
Z103726028	CN(C)CC1=NN=C(O1)C1=CC=C(Br)O1	272,10	C9H10BrN3O2
Z31195264	CC(NC1=NC=CC=N1)C1=CC=CC=C1	199,26	C12H13N3
Z234896505	CC1=C(C)C=C(C=C1)C1=NC(N)=NN=C1	200,25	C11H12N4
Z234896483	CCC(N)(C(O)=O)C1=CC(Cl)=CC=C1	213,66	C10H12ClNO2
Z102895082	COC1=C(OC)C2=C(C=C1)C=NNC2=O	206,20	C10H10N2O3
Z234895477	CN(C)C1=CC(=NC=C1)C(O)=O	166,18	C8H10N2O2
Z26824643	CCC1=NN=C(NC(=O)C2=CC=CO2)S1	223,25	C9H9N3O2S
Z16114793	CNC(=O)COC1=C(Cl)C=CC(C)=C1	213,66	C10H12ClNO2
Z18391402	NC(=O)COC1=C(Cl)C=C(F)C=C1	203,60	C8H7ClFNO2
Z234853588	CCOCC1=C(N)N=C(C)N=C1	167,21	C8H13N3O
Z369263636	CC(NS(C)(=O)=O)C1=C(C)N(C)N=C1	217,29	C8H15N3O2S
Z1483951257	CC(C)N1CCCCC1CN	156,27	C9H20N2
Z90507087	C(NC1CCCCC1)C1=NC=CC=C1	204,32	C13H20N2
Z435369108	CN(CC1=CC(Br)=CS1)C(=O)C1CC1	274,18	C10H12BrNOS
Z314446712	CCN(C1CC1)C(=O)C1=CC=CS1	195,28	C10H13NOS
Z355728146	CCNC(=O)CN1CC(C)OCC1C	200,28	C10H20N2O2

Z19755216	CN(C)C(=O)COC1=CC(F)=CC=C1	197,21	C10H12FNO2
Z647442662	CC1=NOC(CN2CCCC2CO)=N1	211,27	C10H17N3O2
Z104652094	CC1=CSC(=O)N1CCN1CCOCC1	228,31	C10H16N2O2S
Z2327226256	COC1=C(OC)C(Cl)=C(C=C1)C#N	197,62	C9H8ClNO2
Z1348316421	N#CC1=NC=C(C=C1)N1CCOCC1	189,22	C10H11N3O
Z2326990066	COC1=C(N)N=CC(Cl)=C1	158,59	C6H7ClN2O
Z2309759377	NC1=C(Br)C=CC(CO)=C1	202,05	C7H8BrNO
Z2306627089	FC1=C(F)C2=C(NCCO2)C=C1	171,15	C8H7F2NO
Z2301499876	COC1=CC(OC)=C(Cl)C(N)=C1	187,62	C8H10ClNO2
Z2301499896	CC1=CC2=C(C=CN=C2N)C=C1	158,20	C10H10N2
Z1741966337	CN1C=C(N)C(=N1)C(N)=O	140,15	C5H8N4O
Z2106597800	CC1=CN(N=C1)C1=CC=C(C=C1)C#N	183,21	C11H9N3
Z2301438405	CCC1=CC(=O)NN=C1C1=CC=CC=C1	200,24	C12H12N2O
Z728940672	FC1=CC2=C(C=C1)N=CN=C2NC1CC1	203,22	C11H10FN3
Z2293608204	CC1=NN(C=C1)C1=CC=C(C=C1)C#N	183,21	C11H9N3
Z959330822	CC(CC1=CN(C)N=C1)C(O)=O	168,20	C8H12N2O2
Z680889192	CN1NC(=O)C2=C1N=CC(Br)=C2	228,05	C7H6BrN3O
Z2293605544	OC(=O)C1=CC2=C(C(COC2)N1	167,16	C8H9NO3
Z1267881663	O=C1CCCN1CC1=CC=C(C=C1)C#N	200,24	C12H12N2O
Z1266933854	CC(N)C(O)C1=CC=C(F)C=C1	169,20	C9H12FNO
Z1266854954	CC1=C(C)C2=C(NN=C2N)N=N1	163,18	C7H9N5
Z1266854829	OC(C1CCNCC1)C1=CC=C(F)C=C1	209,26	C12H16FNO
Z228585842	CN1CCN(CC1)C(=O)CO	158,20	C7H14N2O2
Z1263820262	CC(C)N1C=NC2=C1C=CC(=C2)C(O)=O	204,23	C11H12N2O2
Z1263602424	COC1=CC(C2=NN=C(N)O2)=C(Br)C=C1	270,09	C9H8BrN3O2
Z1263602410	CN1C(=O)OC2=C1C=CC(N)=C2	164,16	C8H8N2O2
Z1741962470	CN1N=C(C=C1N)C1CC1	137,19	C7H11N3
Z367452370	Cl.CN(C)C(=O)C1CCNCC1	192,69	C8H17ClN2O
Z1815733624	CC1=NC(=NC=C1)N1CC(C)(O)C1	179,22	C9H13N3O
Z1956351798	CC(O)CNC1CCCC2=NN(C)C=C12	209,29	C11H19N3O
Z56928625	CNCC1=CC=C(OC)C=C1	151,21	C9H13NO
Z1428018544	CN(C1CCCC1)C1=C(N)C=CC=C1	190,29	C12H18N2
Z57039604	NCC(N1CCCC1)C1=C(Cl)C=CC=C1	224,73	C12H17ClN2
Z1442183892	CC(O)C1=C(C=CC=C1F)N1C=CC=N1	206,22	C11H11FN2O
Z2234631193	CN(C)S(=O)(=O)C1=C(C=CC=C1)C(O)=O	229,25	C9H11NO4S
Z1974660264	CC(=O)N[C@@H]1C[C@H]1C1=CC(F)=C(Cl)C=C1	227,66	C11H11ClFNO
Z1619978933	CC1=NN=C(CN2CCC=C(F)C2)S1	213,27	C9H12FN3S
Z1783230611	CNC(=O)C1(CC2=CC=C(F)C=C2)CC1	207,25	C12H14FNO
Z1251753693	CNC(=O)C1CC1C1=C(Cl)C=CC=C1F	227,66	C11H11ClFNO
Z1619985466	FC1=CCCN(CCN2C=CN=C2)C1	195,24	C10H14FN3
Z2034475738	CN(CC(C)(C)O)C1=NC=C(F)C=C1	198,24	C10H15FN2O
Z1900627254	FC1=CCCN(C1)C1=NC=CN=C1	179,20	C9H10FN3
Z1689442171	FC1=CCCN(C1)C(=O)N1CCOCC1	214,24	C10H15FN2O2
Z1481145839	FC1=CN=C(N=C1)N1CC2CCCC2C1	207,25	C11H14FN3
Z1395929370	OCCN1CCOC2=C1C=C(F)C=C2	197,21	C10H12FNO2
Z758198920	CC(=O)N1CCOC2=C(C1)C=CC=C2	191,23	C11H13NO2
Z1741980282	COC1=C(CO)C=CC=N1	139,15	C7H9NO2
Z1824334043	CNCC1=C(N)C=CC(Br)=C1	215,09	C8H11BrN2
Z1759803490	CCN1C=NN=C1C1CN(CC)CCO1	210,28	C10H18N4O
Z2240988377	CCN1CCN(CC(C)C)N)CC1	185,32	C10H23N3
Z1741815708	CC1(C)CCCN1CCN	142,25	C8H18N2
Z19025264	NC(=O)CN1C(=O)C=NC2=C1C=CC=C2	203,20	C10H9N3O2
Z107728826	OCC(=O)NC1=CC2=C(OCCO2)C=C1	209,20	C10H11NO4
Z26824739	CCC1=NN=C(NC(=O)C2CCC2)S1	211,28	C9H13N3OS
Z104341242	OC(=O)C1CCS(=O)(=O)C1	164,18	C5H8O4S
Z99601600	CC1=CC(C)=C(NC(=O)CO)C(C)=C1	193,25	C11H15NO2
Z234893819	NC1=C2C(=O)NCC2=CC=C1	148,17	C8H8N2O
Z90663557	NC(=O)CC1=CN2C=CC=CC2=N1	175,19	C9H9N3O
Z85934875	CNC(=O)CN1CCNCC1	157,22	C7H15N3O
Z89283364	OC(=O)C1=CC2=C(OCCCO2)C=C1	194,19	C10H10O4
Z85917566	O=C1CCC2=C(N1)C=CC=C2	147,18	C9H9NO
Z57984669	CC1=NC(=CS1)C1=CC(N)=CC=C1	190,26	C10H10N2S
Z57056172	CC1=CC=C(CC(=O)N2CCCC2)C=C1	203,29	C13H17NO
Z823287468	OC(=O)CC1=CSC(=N1)C1=CC=C(Cl)S1	259,72	C9H6ClNO2S2
Z815264064	CCOC1=NC(C(O)=O)=C(Cl)C=C1	201,61	C8H8ClNO3
Z228588764	COC1=C2OCC(=CC2=CC=C1)C(O)=O	206,20	C11H10O4
Z17834203	NC(=O)COC1=CC(Cl)=CC(Cl)=C1	220,05	C8H7Cl2NO2

Z31490566	O=C(NCC1CCCC1)C1=CC=CS1	211,28	C10H13NO2S
Z744843398	CC1=CN(CC(O)=O)N=C1	140,14	C6H8N2O2
Z85893775	CC(C)C(=O)N1CCCC(C1)C(O)=O	199,25	C10H17NO3
Z85525304	CC1=CC=C(S1)C(=O)NC1=NC=CC=C1	218,27	C11H10N2O5
Z354263674	CC1=CN2N=C(NCC=C)SC2=N1	194,26	C8H10N4S
Z57000601	CC1=C2C=CC=CC2=NC(N)=C1C#N	183,21	C11H9N3
Z235352163	OC(=O)C1=CC=CN1CC1=CC=CC=C1	201,23	C12H11NO2
Z90165620	CC(NC1=NC=CC=C1)C1=CC=CO1	188,23	C11H12N2O
Z85886770	OC(=O)CNC(=O)C1=C(F)C=C(F)C=C1	215,16	C9H7F2NO3
Z235341985	CC(C)CN1N=CC2=C1NC(=O)C=C2C	205,26	C11H15N3O
Z169512032	CC(=O)NC(C1CCCC1)C(O)=O	185,22	C9H15NO3
Z223814814	CN1N=CC2=C1N=CN=C2N1CCCC1	203,25	C10H13N5
Z381061402	COC1=CC(N)=C(C=C1)C(O)=O	167,16	C8H9NO3
Z144495968	CN(C)C(=O)C1=CN=C2SC=CN2C1=O	223,25	C9H9N3O2S
Z372853960	NC(=O)C1(N)CCCCC1	156,23	C8H16N2O
Z367678518	OC(=O)CNC(=O)C1=CC=NC=C1	180,16	C8H8N2O3
Z367452204	OC(=O)CCC1=CC(F)=C(F)C=C1	186,16	C9H8F2O2
Z367451024	CN(C)C1=NC=C(C=C1)C(O)=O	166,18	C8H10N2O2
Z183417690	CC1=NC(C)=C(S1)C(=O)NC1CC1	196,27	C9H12N2O5
Z26251905	CC1=C(C)C=C2N(CC(N)=O)C=NC2=C1	203,25	C11H13N3O
Z52305549	CNC(=O)CNC(=O)C1=CC(Br)=CN=C1	272,10	C9H10BrN3O2
Z320136522	COC1=C(CO)C=C(Br)C=C1CO	247,09	C9H11BrO3
Z1271630862	CCOC1=C2C=CNC2=CC=C1	161,20	C10H11NO
Z2466617844	CC1=NC2=C(C=CC=C2)C11CCNCC1	200,29	C13H16N2
Z2106596953	CCN1N=CC2=C1C(=O)NC=N2	164,17	C7H8N4O
Z2429425516	CCC1=CC2=C(O1)C=CNC2=O	163,18	C9H9NO2
Z1720581929	NCC1(O)CCC2=C1C=CC(F)=C2	181,21	C10H12FNO
Z1272272409	C[C@H](NC1=NC(C)=NS1)C1=NC=CC=C1	220,29	C10H12N4S
Z1263811594	CC(CN)OC1=C(C)C=CC=C1	165,24	C10H15NO
Z1263811616	CC(C)(CN)C1=CC=C(F)C=C1	167,23	C10H14FN
Z1266823369	NC1CCC2=NC=NN2C1	138,17	C6H10N4
Z1544648160	CN(C)C(=O)C1CCCC1C(=O)N(C)C	212,29	C11H20N2O2
Z1222278743	CC1CCN(CC1)C1=NC=C(CN)C=C1	205,31	C12H19N3
Z1359429502	CC1C(O)CC2=C1C=CC=C2	148,21	C10H12O
Z1416200837	CC(N)C1=NOC(=N1)C1=CC=CC=C1	189,22	C10H11N3O
Z1250132764	CC1=C(C)N=C(S1)C(C)(C)N	170,27	C8H14N2S
Z1258578133	CCC(C)C1=NOC(=C1)C(O)=O	169,18	C8H11NO3
Z1350579414	CCC1=NC(=NO1)C1CCCN1	167,21	C8H13N3O
Z1340493791	CCC1CNCN1CC(C)O	172,27	C9H20N2O
Z228584490	CC(C)N(C)C(=O)C1=CC=C(CN)C=C1	206,29	C12H18N2O
Z1262237397	NCC1CCN(C1)C1=CC=C(CI)C=C1	210,71	C11H15ClN2
Z1428019337	CC1CN(CCN1)C(C)=O	142,20	C7H14N2O
Z139565496	CN1CCCCC1CCO	143,23	C8H17NO
Z57162030	OC(=O)CC1CCS(=O)(=O)C1	178,20	C6H10O4S
Z228474600	CC(N1C(=O)OC2=C1C=CC=C2)C(O)=O	207,19	C10H9NO4
Z210803656	CN1N=C(C)C(CCC(O)=O)=C1C	182,22	C9H14N2O2
Z89264974	COC1=CC(F)=C(C=C1)C(O)=O	170,14	C8H7FO3
Z1020680330	NCC1(O)CC2=C(C1)C=CC=C2	163,22	C10H13NO
Z1250080911	CC1=NN=C(N1)C1=CC(=CC=C1)C#N	184,20	C10H8N4
Z1222331846	CNC(C(O)=O)C1=C(F)C=CC(F)=C1	201,17	C9H9F2NO2
Z1416171278	OC(=O)CC1CCC(=O)NC1	157,17	C7H11NO3
Z2218585938	CC(C)OC1=C(N)C=C(C)C=N1	166,22	C9H14N2O
Z241287306	CN(C1CCCC1)C(=O)C1CCC1	181,28	C11H19NO
Z1269702201	CC(CN)OC1=CC=C(Cl)C=C1	185,65	C9H12ClNO
Z1269702301	CN(C)C1CCC2=C(C=CC=C2)C1N	190,29	C12H18N2
Z1267882047	CC(N)C(C)OC1=C(F)C=CC=C1	183,23	C10H14FNO
Z1267773513	CNC1CCCC1S(C(=O)=O)=O	177,26	C7H15NO2S
Z2216303521	NCC(CO)C1CCCCC1	157,26	C9H19NO
Z1273048529	CC1=CC=C(C=C1)C1OCCCC1CN	205,30	C13H19NO
Z1613492358	CC(O)CCN1C=CC=N1	140,19	C7H12N2O
Z137402504	CC1=CC(CNC2=C(CI)C=CC=C2)=NO1	222,67	C11H11ClN2O
Z85893824	CC(C)CC(=O)N1CCCC(C1)C(O)=O	213,28	C11H19NO3
Z137654490	CCC1CCCN1CC1=C(Cl)SN=N1	245,77	C10H16ClN3S
Z2242946632	NC1=CC2=C(CNC2)C=C1	134,18	C8H10N2
Z2235831699	CC(C)NC(=O)C1=NN(C)C=C1N	182,23	C8H14N4O
Z1739363149	CS(=O)(=O)N1CCOC(C1)C1CC1	205,27	C8H15NO3S
Z90504557	OCCNC1CCCCC1	143,23	C8H17NO

Z2238508528	COC1=NC2=C(CCN2)C=C1	150,18	C8H10N2O
Z1509441055	CN(C)C1=C(Br)C=NC(N)=C1	216,08	C7H10BrN3
Z2236735311	NC1=NC(=CN=N1)C(F)(F)F	164,09	C4H3F3N4
Z2236735605	CN1NC(=CC1=O)C(O)=O	142,11	C5H6N2O3
Z2067123286	C1C1=C(CN2C=CSC2=O)SC=C1	231,71	C8H6ClNOS2
Z1255361336	O=C1CCC2=C(CCN1)C=CC=C2	175,23	C11H13NO
Z1198163513	OC(=O)CCC1CCC(=O)N1	157,17	C7H11NO3
Z2235810166	CN1C(=CC=C1C(O)=O)C#N	150,14	C7H6N2O2
Z2235810123	CC1=NC2=C(CCC(O)C2)N1	152,20	C8H12N2O
Z2235810223		194,19	C10H10O4
Z2235810203	CC1=C2CCNC2=NC=C1	134,18	C8H10N2
Z1891775483	CC1(C)CNCC(C)(C)O1	143,23	C8H17NO
Z1365534373	CN1C=CC(C)=C(N)C1=O	138,17	C7H10N2O
Z2255113012	OC(=O)C1CN(C1)C(=O)C1CCCCC1	211,26	C11H17NO3
Z2004563941	CC(O)C1=CN(N=C1)C1CCCC1	180,25	C10H16N2O
Z1076481138	C(NC1CCCC1)C1=NC=CN1	179,27	C10H17N3
Z426210734	N#CC1=CC=C(OCC2CCOC2)C=C1	203,24	C12H13NO2
Z1250089987	OCCN1N=CC2=C1C=CC=C2	162,19	C9H10N2O
Z1245735303	CC(O)C1=C(C)N=C(C)S1	157,23	C7H11NOS
Z1245646677	OCC1=CN(CC2=CC=C(Br)C=C2)N=C1	267,13	C11H11BrN2O
Z100642432	CN(C)C(=O)C1=C(Br)C=C(F)C=C1	246,08	C9H9BrFNO
Z247511056	CC(=O)N(CCN)=O)C1=CC=CC=C1	192,22	C10H12N2O2
Z104647358	NC(=O)CNC1=CC=C(Cl)C=C1	184,62	C8H9ClN2O
Z104549838	CC1=CC(NCC(N)=O)=C(C)C=C1	178,24	C10H14N2O
Z1245537957	NCCNC1=C2C=CSC2=NC=N1	194,26	C8H10N4S
Z1983132602	CS(=O)(=O)C1(CO)CCC1	164,22	C6H12O3S
Z1101755952	CC1CCCN(C1)C(=O)C1=CSC=N1	224,32	C11H16N2OS
Z133729826	CC(NS(C)(=O)=O)C1=CC(Cl)=CC=C1	233,71	C9H12ClNO2S
Z1956875677	NCC(CO)C1CCOC1	145,20	C7H15NO2
Z1262254296	CC(N)C1=CC(NC(C)=O)=CC=C1	178,24	C10H14N2O
Z1263529802	COC1=C(C(C)N)C(F)=CC=C1	169,20	C9H12FNO
Z1295585445	CCC(N)C1CCOCC1	143,23	C8H17NO
Z1362754412	COC(C)C1=NC(CN)=CS1	172,25	C7H12N2OS
Z197266168	OCCN1CCCCC1	143,23	C8H17NO
Z1838995460	COC1=CC(CN2C=CC=N2)=C(Cl)C=C1	222,67	C11H11ClN2O
Z1655141307	CN1C(C)=NC(C(N)=O)=C1N	154,17	C6H10N4O
Z1649893034	CCC1=NC(=CO1)C(O)=O	141,13	C6H7NO3
Z1606822433	CC1=NC(CNC2=NC(C)=NO2)=CS1	210,26	C8H10N4OS
Z1705831819	CC1=NC2=NC(C(C(N)=O)=CN2C=C1	190,21	C9H10N4O
Z1661748238	CC(C)NC(=O)CN1N=CSC1=O	201,24	C7H11N3O2S
Z1698549667	NC(CC(O)=O)C1=C(F)C=C(F)C=C1	201,17	C9H9F2NO2
Z1696824152	NC1=NNC(=O)C1C1=CC=CC=C1	175,19	C9H9N3O
Z1696824078	OC(=O)C1=C2N=C(NC2=CC=C1)C1CC1	202,21	C11H10N2O2
Z2004547594	CC1(C)CC(=O)NC2=C1C=CC=C2	175,23	C11H13NO
Z1741967102	C1C1=CC(=CC=C1)C1CNCCN1	196,68	C10H13ClN2
Z1998637006	OCC1CCCC2=C1N=CC=C2	163,22	C10H13NO
Z1741977642	CCC1=CC=C(C=C1)C1CNCCN1	190,29	C12H18N2
Z2028214420	CC1(C)NC(=O)CCC1N	142,20	C7H14N2O
Z2027896796	CC(C)CN1C(N)=NC=C1C(F)(F)F	207,20	C8H12F3N3
Z1896595030	CNC1=C2C=C(OC)C=CC2=NC(C)=N1	203,25	C11H13N3O
Z1820276480	CN1C=C(Cl)C=C1C(=O)NC1=CN=NS1	242,68	C8H7ClN4OS
Z1623872049	CC1=C(C(O)=O)C(=O)NC=C1	153,14	C7H7NO3
Z319550626	CN(C)S(=O)(=O)C1=CN(C)C(=C1)C(O)=O	232,25	C8H12N2O4S
Z1614605132	O=C1NCCN2N=CC=C12	137,14	C6H7N3O
Z1165945108	CC(O)CN(C)C1=NC=C(Br)C=N1	246,11	C8H12BrN3O
Z1582263013	CCC1(O)CCC(N)CC1	143,23	C8H17NO
Z1575311908	CCNC1=NC=C(C=C1)C(O)=O	166,18	C8H10N2O2
Z1575082073	CC1=NC2=C(N1)N=CC=C2C	147,18	C8H9N3
Z1569708695	CS(=O)(=O)C1=CSC(=C1)C(O)=O	206,23	C6H6O4S2
Z1552026926	CCC1(CO)CCNCC1	143,23	C8H17NO
Z145985740	CC1=NOC(=C1)C(=O)NC1=CN=CC=C1	203,20	C10H9N3O2
Z1333173490	OC[C@H]1C[C@H](NC2=NC=C(Cl)C=N2)C=C1	225,68	C10H12ClN3O
Z32016410	CNC(=O)C1=CC=CC=C1	135,17	C8H9NO
Z94598702	NC(C1=CC=CS1)C1=CC=C(F)C=C1	207,27	C11H10FNS
Z1238477848	NCC1=C(F)C=CC(Br)=C1	204,04	C7H7BrFN
Z2028236605	C1CC2(CN1)CCOC2	141,21	C8H15NO
Z1924550188	NCC1=C(F)C=C(C=C1)C1=CC=CO1	191,21	C11H10FNO

Z1266823177	CC(C)C(N)C1=NN=C2CCCN12	180,26	C9H16N4
Z1217910552	COC1=CC(OC)=CC(CN)=C1	167,21	C9H13NO2
Z1444766645	CC(=O)N1CCOCC1C(O)=O	173,17	C7H11NO4
Z1267773518	CC1=C(C=CC=C1)C(N)C1CC1	161,25	C11H15N
Z1262252887	CC(N)C1CCN(C)CC1	142,25	C8H18N2
Z54633859	CN(CCO)C1=NC=CC=C1	152,20	C8H12N2O
Z445904810	COCCNC(=O)N1CCC1	158,20	C7H14N2O2
Z993991216	CS(=O)(=O)CC1=CC(CN)=CC=C1	199,27	C9H13NO2S
Z228474642	NCCC1=CN(N=C1)C1=CC=CC=C1	187,25	C11H13N3
Z1695906872	CCC1=C(C=C(C=C1)C(O)=O)C#N	175,19	C10H9NO2
Z1695709455	CS(=O)(=O)C1=CC(N)=C(F)C=C1	189,20	C7H8FNO2S
Z33545997	NC(=O)CN1C(=O)COC2=C1C=CC=C2	206,20	C10H10N2O3
Z2235681451	CCN1C(CO)=NC2=C1C=CC(OC)=C2	206,25	C11H14N2O2
Z2235681460	OCC1(CNC(=O)C1)C1=NC=CC=C1	192,22	C10H12N2O2
Z2235386824	CCN1N=NC(C)=C1CO	141,17	C6H11N3O
Z1562963009	C(N1CCN(CC1)C1CC1)C1=CSN=N1	224,33	C10H16N4S
Z2235330282	CC1CC2=C(N1)C=CN=C2	134,18	C8H10N2
Z2001240785	CC(=O)NC1=C(C)N=C2C=CC=CC2=C1	200,24	C12H12N2O
Z2218555527	CC1=CC(=O)C(C)=C(C)N1	137,18	C8H11NO
Z2574360326	CN1C=C(CCC(O)=O)N=N1	155,16	C6H9N3O2
Z2568758040	OC(=O)C1=CC=C(NC2=NCCC2)C=C1	204,23	C11H12N2O2
Z2568757968	CN1CCC2=C(C=CC=C2N)C1=O	176,22	C10H12N2O
Z1270392259	NC(=O)C1(CCC1)C(O)=O	143,14	C6H9NO3
Z2568751754	CN1C=NC(=CC1=O)C(O)=O	154,13	C6H6N2O3
Z2526439792	COC(C1CCCCC1)C(O)=O	172,22	C9H16O3
Z2526439760	NC1(CCC1)C1=CC=NC=C1	148,21	C9H12N2
Z2522939860	CC1=C(CO)C=C(O1)C(O)=O	156,14	C7H8O4
Z2584270329	OC(=O)CC1=CC2=C(NC=C2)C=C1	175,19	C10H9NO2
Z2522503334	CC1(CCN1=O)C(O)=O	143,14	C6H9NO3
Z2522503273	OCC1=CC2=C(S1)C=NC=C2	165,21	C8H7NOS
Z26414122	COC1=NC=C(NC(=O)C2CC2C)C=C1	206,25	C11H14N2O2
Z104378192	COC1=C(Br)C=C(C=C1)C(C)N	230,11	C9H12BrNO
Z94601317	CC1=NN(C(C)=C1)C1=CC=C(CO)C=C1	202,26	C12H14N2O
Z96092819	CC1=NOC(N)=C1C(O)=O	142,11	C5H6N2O3
Z172492258	NC1=C(Cl)C=C2OCCOC2=C1	185,61	C8H8ClNO2
Z166605386	OC(=O)CC1=COC(=N1)C1=CC=CC=C1	203,20	C11H9NO3
Z90662846	CC1=C(SC(=N1)C1=CC=CS1)C(O)=O	225,28	C9H7NO2S2
Z94602022	CCS(=O)(=O)C1=CC2=C(OC(C)=N2)C=C1	225,26	C10H11NO3S
Z57756597	COC1=C(OC)C(Cl)=CC(=C1)C#N	197,62	C9H8ClNO2
Z92741624	OC1CS(=O)(=O)CC1NCC1=CC=CO1	231,27	C9H13NO4S
Z118438292	CNC1=C(C#N)C(C)=NS1	153,20	C6H7N3S
Z44585773	ClC1=CC(NC(=O)N2CCCC2)=CC=C1	224,69	C11H13ClN2O
Z32016122	CNC(=O)CNC(=O)C1=CC=C(Br)C=C1	271,11	C10H11BrN2O2
Z56840113	OC(=O)CNC(=O)C1=CC=C(Cl)C=C1	213,62	C9H8ClNO3
Z19739846	NC(=O)COC1=CC=C(C=C1)C#N	176,18	C9H8N2O2
Z56973918	CCN1N=C(C=CC1=O)C(O)=O	168,15	C7H8N2O3
Z56960250	CCNCC1COC2=C(O1)C=CC=C2	193,25	C11H15NO2
Z53834532	CCOC1=CC=C(C=C1)C#N	147,18	C9H9NO
Z31434237	CN1CCN(CC1)C(=O)C1=CC=C(Br)O1	273,13	C10H13BrN2O2
Z56899132	OC(=O)CNC(=O)C1=CC=CO1	169,14	C7H7NO4
Z56899019	OC(=O)CCC(=O)N1CCOCC1	187,20	C8H13NO4
Z56896220	OC(=O)CNC(=O)C1=CC=C(F)C=C1	197,17	C9H8FNO3
Z28136791	CC(=O)NC1=C(Cl)C=CC(Cl)=C1	204,05	C8H7Cl2NO
Z30849291	COC1=C(OC)C=C(NC(C)=O)C=C1	195,22	C10H13NO3
Z3220055146	CC1=C(C#N)C(C)=CC(=O)N1	148,17	C8H8N2O
Z1258519591	NCC1=NOC(=C1)C1=CC=CC=C1	174,20	C10H10N2O
Z1416200883	COC1=CC(N)=C(C=C1)C#N	148,17	C8H8N2O
Z1416200895	NC1=NN=C2CCNCC2=C1	150,19	C7H10N4
Z1317589334	BrC1=CN=C(NC2CCS(=O)C2)N=C1	276,15	C8H10BrN3OS
Z1407007419	CC(C)(O)C1=NC2=C(S1)C=CC=C2	193,26	C10H11NO5
Z1407007417	CC1=CC2=C(NCCN2)N=C1	149,20	C8H11N3
Z1407007506	C1NCC1C1=NC2=C(N1)C=CC=C2	173,22	C10H11N3
Z1405445908	CN(C)C1=C(N)C=NC=N1	138,17	C6H10N4
Z196118762	OCCNC1=CC=C(C=C1)C#N	162,19	C9H10N2O
Z220616774	COC1=C(F)C=C(C=C1)C(C)O	170,18	C9H11FO2
Z295848548	C(N1CCOCC1)C1=NC(=NO1)C1CC1	209,25	C10H15N3O2
Z86242586	CN(C)C1=C(C=CC=N1)C#N	147,18	C8H9N3

Z1318357723	NC1CCN(CC1)C1CCCCC1	182,31	C11H22N2
Z1250132434	CNC1=C(OC)C=C(F)C=C1	155,17	C8H10FNO
Z1003207278	CNS(=O)(=O)CC1CCCCC1	191,29	C8H17NO2S
Z295124002	CNC(C)C1=CC=C(OC)C=C1	165,24	C10H15NO
Z343738014	CC1CN(C(C)CO1)C(=O)C1=CC=CS1	225,31	C11H15NO2S
Z2234631237	CC(N)(C(O)=O)C1=CC=C(Br)C=C1	244,09	C9H10BrNO2
Z1396280317	CC(=O)N1CCN(CC1)C1CCOC1	198,27	C10H18N2O2
Z2235681143	NC1CCOC(C1)C1=CC=NC=C1	178,24	C10H14N2O
Z1262255346	NCC1=CC2=C(OCC2)C=C1	149,19	C9H11NO
Z641408164	CC(N1CCCC1)C1=NC(=NO1)C1CC1	207,28	C11H17N3O
Z1443588587	NC1CCOC2(CCCC2)C1	155,24	C9H17NO
Z169226638	CC(=O)NCCN1CCCCC1	184,28	C10H20N2O
Z2235409400	CC1CCCC1(C)C(O)=O	142,20	C8H14O2
Z1685106505	CN1C=CN=C1C1=NOC(=N1)C1CCC1	204,23	C10H12N4O
Z644971758	NC(=O)CN1CCCC1C1CCCCC1	210,32	C12H22N2O
Z50145871	CCC1=NN(C(=O)C1)C1=CC=CC=C1	188,23	C11H12N2O
Z168766620	COCC(=O)NC1=CC(F)=CC(F)=C1	201,17	C9H9F2NO2
Z19733482	CN(C)C(=O)COC1=C(C)C=CC=C1	193,25	C11H15NO2
Z32013275	CN(C)C(=O)C1=CC(F)=CC(F)=C1	185,17	C9H9F2NO
Z32372098	COCC(=O)NC1=CC(F)=C(F)C=C1	201,17	C9H9F2NO2
Z54739316	CN1C=CC=C1C(=O)NC1CCCC1	192,26	C11H16N2O
Z144495580	CN(C)C(=O)C1=CSC(=N1)C1=CC=CS1	238,32	C10H10N2OS2
Z16164828	NC(=O)COC1=C2C=CSC2=NC=N1	209,22	C8H7N3O2S
Z1272096656	OC(=O)C1C2CCCCC12	140,18	C8H12O2
Z1272096654	CN(C)C1=NC2=C(C=CC=C2)C(=C1)C#N	197,24	C12H11N3
Z1271843050	COC1=C2C=CC=CC2=NC=C1C#N	184,20	C11H8N2O
Z266487838	CC1=NOC(CNC2=CC=C(C)C=C2)=C1	202,26	C12H14N2O
Z133729708	CC(NS(C)(=O)=O)C1=C(CI)C=CC=C1	233,71	C9H12ClNO2S
Z1297772359	CC(N)C(O)C1=C(F)C=CC=C1F	187,19	C9H11F2NO
Z1295543908	CC1NC2=C(NC1=O)C=CC=C2	162,19	C9H10N2O
Z382594240	CN(C)C(=O)N1CCN(CC(C)=C)CC1	211,31	C11H21N3O
Z2685356778	CC(C)C1=NC=C(C(N1C)C1=CN=CC=C1	201,27	C12H15N3
Z1268153230	CCC1=CN=C(CCN)S1	156,25	C7H12N2S
Z1255460290	CC1=NC(CCO)=NC=C1	138,17	C7H10N2O
Z2034678675	CNC1=C(CI)C=C(CI)C(=C1)C(N)=O	219,07	C8H8Cl2N2O
Z1918236928	CN1C=C(OCC2=C(C)SC(C)=C2)C=N1	222,31	C11H14N2OS
Z2065616401	NCC1=CC2=C(N=C1)C(F)=CC=C2	176,19	C10H9FN2
Z2065464300	CC(O)C1=C(F)C=CC(N)=C1	155,17	C8H10FNO
Z1259273081	COC1=CC(=CC=C1)C(N)C(O)=O	181,19	C9H11NO3
Z1827602749	CC1CCOC1C(=O)NC1=CN=NS1	213,26	C8H11N3O2S
Z1840852315	CC(O)C(=O)NC1=CC2=C(SN=C2)C=C1	222,26	C10H10N2O2S
Z338089614	FC1=CC(F)=C(CNC(=O)C2CC2)C=C1	211,21	C11H11F2NO
Z1855630367	CC(NC1=CC(C)=C(Br)C(C)=C1)C(N)=O	271,16	C11H15BrN2O
Z1899690168	CC1=CC(=O)N(CC2=NC=CC=C2)N=C1	201,23	C11H11N3O
Z1791179790	CCC1=CC=C(O1)C(=O)NC1=CN=NS1	223,25	C9H9N3O2S
Z57229049	CC(NC(=O)C1=CC=CC=C1)C(O)=O	193,20	C10H11NO3
Z85915745	CC(=O)NC1=C(C=CC(Cl)=C1)C(O)=O	213,62	C9H8ClNO3
Z220542622	OC(=O)C1=CNC(=C1)C(=O)N1CCCC1	208,22	C10H12N2O3
Z85895198	CN(CC(O)=O)C(=O)C1=CC=C(F)C=C1	211,19	C10H10FNO3
Z56827660	OC(=O)CNC(=O)C1=CC(Cl)=CC=C1	213,62	C9H8ClNO3
Z1269638513	CCC(CO)N1CCNCC1	158,25	C8H18N2O
Z1268152406	CC1=NC(NC2CCNCC2)=CC=C1	191,28	C11H17N3
Z1268152319	NC1=NN=C(C=C1)C1CC1	135,17	C7H9N3
Z1267886876	NC1=C(C=C2CCCCC2=N1)C(O)=O	192,22	C10H12N2O2
Z1267882601	CC1=NNC=C1CNC1=CC=CC=C1	187,25	C11H13N3
Z1262254288	Cl.CC(N)C1=C(C)C=CC(C)=C1	185,70	C10H16ClN
Z1262254244	NC1=CC2=C(OCC2)C=C1	149,19	C9H11NO
Z1262250855	NC(=O)[C@H]1CC2=C(N1)C=CC=C2	162,19	C9H10N2O
Z2630881496	OC(=O)C1=C(F)C=CC(=C1)C(F)F	190,12	C8H5F3O2
Z1573270315	CC1=C(F)C=CC(NCC2=CSN=N2)=C1	223,27	C10H10FN3S
Z2588063738	O=C1NCCCCCNC2CCCC12	210,32	C12H22N2O
Z2588063517	OCC1CCC2=NC=NN12	139,16	C6H9N3O
Z2588039584	CN1NC(=O)C2=C1C=CC=C2	148,17	C8H8N2O
Z1148797578	N#CC1=CC=C(NC2CCC2)C=C1	172,23	C11H12N2
Z2574909837	COC1=CC(=CC=C1)C1(O)CCC1	178,23	C11H14O2
Z2584270333	COC1=C(C=CC=C1)C1=NNC(CO)=C1	204,23	C11H12N2O2
Z2106594936	OC(=O)C1=NN2C(=C1)N=CC=C2C1CC1	203,20	C10H9N3O2

Z2106600566	CCC(N1C=C(C)C=N1)C(O)=O	168,20	C8H12N2O2
Z2510970259	CCC(C)N1N=C(N)C=C1C(O)=O	183,21	C8H13N3O2
Z2106593001	CN1C=C(C=N1)C1=NN(CC(O)=O)C=C1	206,21	C9H10N4O2
Z2510259409	COC1=C(C(O)=O)C2=C(C=CC=C2)N=C1	203,20	C11H9NO3
Z2510259525	COC(C(O)=O)C1=CN(C)N=C1	170,17	C7H10N2O3
Z275210998	CC1=NC=C(CC(O)=O)S1	157,19	C6H7NO2S
Z1258540488	OC(=O)C1CC2(C1)CCOCC2	170,21	C9H14O3
Z2106593030	CN1C=C(C(O)=O)C(=N1)C1CC1	166,18	C8H10N2O2
Z2510259477	OC(=O)C1CCC2=C(C1)C=NC=N2	178,19	C9H10N2O2
Z1891772658	CO[C@H]1C[C@H](N(C1)C(C)=O)C(O)=O	187,20	C8H13NO4
Z2412196607	CC1=C(N=C(O)S1)C(O)=O	159,16	C5H5NO3S
Z2380439289	C1CC2(C1)NCCC1=C2NC=N1	163,22	C9H13N3
Z2380439748	CCC1=NC2=C(S1)C=C(N)C=C2	178,25	C9H10N2S
Z57744712	CN(C)S(=O)(=O)N1CCOCC1	194,25	C6H14N2O3S
Z2350907441	OCC1=NN2CCCC2=C1	138,17	C7H10N2O
Z2350907411	OCC=CC1=CC(Br)=CN=C1	214,06	C8H8BrNO
Z2346401046	NC1=C(N=C(C=C1)C(F)(F)F)C(O)=O	206,12	C7H5F3N2O2
Z2335647002	CC1(C)NC(=O)CC1C1=CC=CC=C1	189,26	C12H15NO
Z927319568	CC1=C(C=CO1)C(=O)NC1CCNCC1	208,26	C11H16N2O2
Z1263529586	CC(C)NC(=O)C1=CC(CN)=CC=C1	192,26	C11H16N2O
Z1263529584	CCC(N)C1=NC2=C(N1)C=CC=C2	175,24	C10H13N3
Z166966904	CNC(=O)CN1C(C)=CC2=C1C=CC=C2	202,26	C12H14N2O
Z1262398421	NC1=C(C)C=CC(CO)=C1	157,60	C7H8CINO
Z275169946	CCN1N=CC(C)=C1C(O)=O	174,58	C6H7CIN2O2
Z2679906799	CCN1C(C)=NC2=C1C(Br)=CN=C2	240,10	C9H10BrN3
Z2678251351	O=C1CC2CCC(CN1)S2(=O)=O	189,23	C7H11NO3S
Z2677307838		193,25	C11H15NO2
Z1258519590	COC1=C(C=C(C)C=C1)C1=NNC(N)=C1	223,66	C10H10CIN3O
Z1396419547	CC1CCCC1NCCO	143,23	C8H17NO
Z1837772594	C=CCC1(CCC1)C(=O)N1CCCC1	193,29	C12H19NO
Z1874954907	CCC(C)N1N=CC(N)=C1C	153,23	C8H15N3
Z99599002	COC1=CC=C(C=C1)C(N)C(C)C	179,26	C11H17NO
Z1863597297	NCCC1=C(C=CC=C1C)N1CCCC1	224,73	C12H17CIN2
Z1860991728	NC1CCCC(C1)C1=CC=CC=C1	175,28	C12H17N
Z1694504496	CC1CN(C)CCC1NC1=CN(C)N=C1	208,31	C11H20N4
Z1738061802	O=C1SC=NN1CC1=CSC(=N1)C1CC1	239,31	C9H9N3OS2
Z1682035317	CC1CN(CC2=NNC=C2)C(C)(C)CO1	209,29	C11H19N3O
Z1815156517	CCN1N=CC=C1CCO	140,19	C7H12N2O
Z1703431439	CC(O)C1CCCN(CC2=CC=CS2)C1	225,35	C12H19NOS
Z1801361776	CC1=C(CN)C=CC(=C1)C(F)(F)F	189,18	C9H10F3N
Z372974252	CC1COCCN1C(=O)C1=CC(C)=CN1	228,68	C10H13CIN2O2
Z1509566268	FC(F)(F)C1=C=CC2=C(C=C1)C(=O)NC=C2	213,16	C10H6F3NO
Z1636723439	CNC(=O)C1CNCCO1	144,17	C6H12N2O2
Z1688142576	O=C1CCN(C2CC2)C2=C(N1)C=CC=C2	202,26	C12H14N2O
Z2026151591	CNC1=CC2=C(C=CC=C2)C(=O)N1	174,20	C10H10N2O
Z1741970224	CC1=NC2=C(O1)C=CC(=C2)C(O)=O	177,16	C9H7NO3
Z1889861361	OCC1=CN2=C1C(F)=CC=C2	165,17	C9H8FNO
Z1743510287	CC1(CNC2=NN=CS2)CCOCC1	213,30	C9H15N3OS
Z1795818295	CC1(CC2=CC=CC=C2)CCNC1=O	189,26	C12H15NO
Z56755628	CN(C)CC1CCCCC1O	157,26	C9H19NO
Z1902703066	NC1=NC=CC(CN2CCC=C(F)C2)=C1	207,25	C11H14FN3
Z1533185622	CC#CCN1C=NC(=CC1=O)C1CCC1	202,26	C12H14N2O
Z1994443056	CCN(C1CCNC1=O)C1CCCC=C1	208,31	C12H20N2O
Z1262691698	NCC1=CC(CO)=CC=C1	137,18	C8H11NO
Z56007122	CCNCC(=O)N1CCCCC1	184,28	C10H20N2O
Z1695729061	CC1=C(C=CC(CN)=C1)S(C)(=O)=O	199,27	C9H13NO2S
Z1318147459	NCCC1=NN=C(O1)C1=CC=CC=C1	189,22	C10H11N3O
Z136583730	CC1=NOC(=C1)C(=O)NC1=CC=NC=C1	203,20	C10H9N3O2
Z1551476075	COCC1(O)CCNCC1	145,20	C7H15NO2
Z1551463490	CC1=C(C=NN1C1=CC=NC=C1)C(O)=O	203,20	C10H9N3O2
Z1551463575	O=C1CN2C=CN=C2CN1	137,14	C6H7N3O
Z45509011	O=S(=O)(N1CCCC1)C1=CC=CS1	217,30	C8H11NO2S2
Z1446850417	OCC1(CCC1)NC1=NC=C(C=C1)C#N	203,25	C11H13N3O
Z1511495090	CC(CC(O)=O)C1=C(C)NN=C1C	182,22	C9H14N2O2
Z1266823274	NC(C1CC1)C1=CC=C(F)C=C1	165,21	C10H12FN
Z2301527375	NCC1(CN)CCCC1	142,25	C8H18N2
Z2162668942	CN1N=CC(C)=C1CN1CCC=C(F)C1	209,27	C11H16FN3

Z1483956890	CC1=C(C=CC(=O)N1)C(O)=O	153,14	C7H7NO3
Z1470841574	OC(=O)C1=C(ON=C1)C1CC1	153,14	C7H7NO3
Z1465463133	CC(C)OC1=CC(=CN=C1)C(O)=O	181,19	C9H11NO3
Z1459946718	CN1C=CN=C1C1=NN=C(N)O1	165,16	C6H7N5O
Z1446854992	CN(C)C1=NC2=C(O1)C=CC(=C2)C(O)=O	206,20	C10H10N2O3
Z33547038	NC(=O)CN1C=NC2=C(C=CC=C2)C1=O	203,20	C10H9N3O2
Z228463904	C1C1=CC=C(CN2C=NC(=N2)C#N)C=C1	218,64	C10H7CIN4
Z234853686	CC(CN1CCOCC1)C(O)=O	173,21	C8H15NO3
Z221226038	CC1CN(CCO1)C(=O)C1=CC(C)=NO1	210,23	C10H14N2O3
Z1259087073	CC(C)OC1=NC=C(CN)C=C1	166,22	C9H14N2O
Z1428018975	CCC1CN(CCC1N)S(=O)(=O)C(C)C	234,36	C10H22N2O2S
Z1335657495	CC(C)C1=NN=C(CN)S1	157,24	C6H11N3S
Z1357774582	COC1=CC(=CC(OC)=C1)C1CCNC1	207,27	C12H17NO2
Z1222331569	COC1=CC(=C(CN)C=C1)C(F)(F)F	205,18	C9H10F3NO
Z1266823348	CC(N)CN1CCN(C)CC1	157,26	C8H19N3
Z1139246057	CNC1CCCN(C1)C1=NN=CC=C1	192,27	C10H16N4
Z1245664706	NCC1=CC(F)=CC(F)=C1	143,14	C7H7F2N
Z1250132688	CCC1=C(N=CO1)C(O)=O	141,13	C6H7NO3
Z1245664618	CC(N)CCC1=CC=CC=C1	149,24	C10H15N
Z235582068	CNCC1=NC=CN1C(F)F	161,16	C6H9F2N3
Z1235963371	CC(C)(N)C1=CC(CI)=CC=C1	169,65	C9H12CIN
Z32014274	CN(C)C(=O)C1=C(Br)C=CC=C1	228,09	C9H10BrNO
Z314447664	CCN(C1CC1)C(=O)C1=CC=C(CI)S1	229,72	C10H12CINOS
Z1262237349	NCC1=CC(F)=C(F)C=C1	143,14	C7H7F2N
Z432590156	CCS(=O)(=O)C1=CC2=C(OCCO2)C=C1	228,26	C10H12O4S
Z381729066	CC(C)NC(=O)C1=NNC=C1	153,19	C7H11N3O
Z339866212	CN(CCO)C(=O)NC1=CC(CI)=CC=C1	228,68	C10H13CIN2O2
Z1945708064	CC1(C)CCCCC1C(O)=O	156,23	C9H16O2
Z1741975545	CC1=NC2=C(O1)C=C(C=C2)C(O)=O	177,16	C9H7NO3
Z1945695970	CC1=C(N=C(N)N=C1)C1=CC=CC=C1	185,23	C11H11N3
Z1945695971	CN1N=C(N=C1N)C1=CC=CS1	180,23	C7H8N4S
Z1729205124	COC1=CC(CI)=C(CN2C=CN=N2)C=C1	223,66	C10H10CIN3O
Z1203884549	CN(C)S(=O)(=O)C1=CNC=N1	175,21	C5H9N3O2S
Z1446900057	CCOC1=C(F)C=C(C=C1)C#N	165,17	C9H8FNO
Z1895742107	OCC1=NN=C2CCCCN12	153,19	C7H11N3O
Z1895583434	CN1N=CC2=C1NC=CC2=O	149,15	C7H7N3O
Z1889997417	CN1N=C(C(C1=O)C1CCCC1	166,22	C9H14N2O
Z1889996025	COC1=C(CC(O)=O)C=C(Br)C=N1	246,06	C8H8BrNO3
Z1889975639	CC1=C(F)C=CC(=C1)N1C=C(CO)N=N1	207,21	C10H10FN3O
Z133622412	CS(=O)(=O)NC1(CCCCC1)C(O)=O	221,27	C8H15NO4S
Z133263888	CC(=O)NC1=C(C=CC(F)=C1)C(O)=O	197,17	C9H8FNO3
Z594038164	NC(C(C)=O)C1=C(CI)C=C(CI)C=C1	220,05	C8H7Cl2NO2
Z44590817	O=C(NC1=CC=CC=C1)N1CCOCC1	206,25	C11H14N2O2
Z140637360	COCC(=O)NC1=CC(CI)=C(C=C1)C#N	224,64	C10H9CIN2O2
Z228463936	C1C1=CC(CN2C=NC(=N2)C#N)=CC=C1	218,64	C10H7CIN4
Z1245633383	CC1=CNC(=O)N1C1=CC=C(C)C=C1	188,23	C11H12N2O
Z164670582	CC1=NC(=CS1)C1=CC2=C(NCC2)C=C1	216,30	C12H12N2S
Z183932940	CC1=NC(C)=C(S1)C(=O)NCC=C	196,27	C9H12N2OS
Z438067480	CCC(=O)NCC1=NN=C2CCCCN12	208,27	C10H16N4O
Z335929200	OCCN1C=NC2=C(C=CC(CI)=C2)C1=O	224,64	C10H9CIN2O2
Z751928454	CC1=NNC=C1CNC1=CC=C(F)C=C1	205,24	C11H12FN3
Z2379767448	CC(C)C1=CSC(=N1)C1=C(N)SN=N1	226,32	C8H10N4S2
Z177087622	CNC(=O)N1CCC2=C(C1)C=CC=C2	190,25	C11H14N2O
Z1346370700	OCC1=CC(OC(F)F)=CC=C1	174,15	C8H8F2O2
Z2467541171	OC1CCCC1CCCC1	140,23	C9H16O
Z2216711594	NC1=NC(=NC=N1)C(F)(F)F	164,09	C4H3F3N4
Z2213893378	OC(=O)CCC1=NOC=C1	141,13	C6H7NO3
Z2205958575	OCC1(CCNCC1)C1=CC=CC=C1	191,27	C12H17NO
Z2182115476	COC1=C2N=CC=CC2=CC(N)=C1	174,20	C10H10N2O
Z1172115931	OC(=O)C1CCC2=NN=CN2C1	167,17	C7H9N3O2
Z826117806	CC(=O)NC1CC1C1=CC=CC=C1	175,23	C11H13NO
Z2168541837	CCC1=C(N2C=C(CI)C=CC2=N1)C(O)=O	224,64	C10H9CIN2O2
Z2168499582	OC(=O)C1=C(F)C=C(C=C1F)C(F)(F)F	226,10	C8H3F5O2
Z2168282689	CC1(C)OC2=C(NC1=O)C=C(C=C2)C#N	202,21	C11H10N2O2
Z29693704	O=C(NCC1=CC=CS1)C1=NC=CC=C1	218,27	C11H10N2OS
Z28775462	CCC(=O)NCC1=NC2=C(S1)C=CC=C2	220,29	C11H12N2OS
Z31490388	C1C1=CC=C(S1)C(=O)NCC1CCCO1	245,72	C10H12CINO2S

Z45511384	CC1CCCN(C1)S(=O)(=O)C1=CC=CS1	245,36	C10H15NO2S2
Z31602909	BrC1=CC=C(O1)C(=O)N1CCNC(=O)C1	273,09	C9H9BrN2O3
Z86948962	CC1=CC(NC(=O)C2=CC=C(Br)O2)=NO1	271,07	C9H7BrN2O3
Z219095946	N#CC1=CN=C(C=C1)N1CCCC1	173,22	C10H11N3
Z317046512	CCOC1=C(C=CC=N1)C#N	148,17	C8H8N2O
Z277468448	C1CCN(CC1)C1=C2N=CNC2=NC=N1	203,25	C10H13N5
Z19736616	NC(=O)COC1=CC(Br)=CC=C1	230,06	C8H8BrNO2
Z432813996	BrC1=C(SC=C1)C(=O)NCC1CCCO1	290,18	C10H12BrNO2S
Z422343286	CC1=C(SC=N1)C(=O)NCC1CCCO1	226,29	C10H14N2O2S
Z1893465070	OCC1CCC(N1)C(F)(F)F	169,15	C6H10F3NO
Z1342206610	CC1=NC=CN1CC1CCC1	165,24	C9H15N3
Z275170236	CN1N=C(C)C(CN)=C1C	139,20	C7H13N3
Z228584858	NC(CN1CCCC1)C1=CC=CC=C1	190,29	C12H18N2
Z1258578427	CN1C=CC=C1C(O)CN	140,19	C7H12N2O
Z1276496834	CC1=C(C)C(C)=C(N1)C(O)=O	153,18	C8H11NO2
Z1259339728	CC1=CC2=C(NCCO2)C=C1	149,19	C9H11NO
Z1245634050	CN(C)CC1=CC(CO)=CC=C1	165,24	C10H15NO
Z1250132784	CCC(N)C1=NC=C(C)S1	156,25	C7H12N2S
Z1259273100	COC1=C(C=CC=C1)C(N)C(O)=O	181,19	C9H11NO3
Z1350606483	NC(=O)N1CCCCC1C(O)=O	172,18	C7H12N2O3
Z1350606423	COC1=CC(=CC=C1)C1=NON=C1N	191,19	C9H9N3O2
Z57820217	CNS(=O)(=O)C1=C(OC)C=CC(Cl)=C1	235,68	C8H10ClNO3S
Z1342208412	CC1=C(F)C=C(F)C(=C1)C(O)=O	172,13	C8H6F2O2
Z255306774	CC(=O)NCC(O)C1=CC=CC=C1	179,22	C10H13NO2
Z1333873233	OC1CCC2=C1C=C(F)C=C2	152,17	C9H9FO
Z54814038	CS(=O)(=O)NCC1=C(Cl)C=CC=C1	219,68	C8H10ClNO2S
Z228589664	CC1=CC(N)=C(C(O)=O)C(C)=C1	165,19	C9H11NO2
Z1324054906	COCC1(C)CNC(=O)C1	143,19	C7H13NO2
Z1324054904	CC1=C(C=CC=C1)C(N)CC(O)=O	179,22	C10H13NO2
Z1815157608	NC1=NN(C2CCCC2)C(=C1)C(O)=O	195,22	C9H13N3O2
Z1815156017	CN1C=CC2=C1C(N)=CC=C2	146,19	C9H10N2
Z1815155418	CC1=C(C)C(C(O)=O)=C(Cl)S1	190,64	C7H7ClO2S
Z1815155476	OC(=O)CS(=O)C1=CC=C(Cl)C=C1	218,65	C8H7ClO3S
Z1815155460	CC(=O)NC1=C(N=CC=C1)C(O)=O	180,16	C8H8N2O3
Z1814381814	COC1=CC(C)=C(C=C1)C(C)C(O)=O	194,23	C11H14O3
Z1665934308	CCC1=C(F)C(=NC=N1)N1CC(CO)C1	211,24	C10H14FN3O
Z1278605667	CC1CCC(C)N(C1)C(=O)NC1CC1	196,29	C11H20N2O
Z1791224447	O=C1NCCC1C1=CN=CC=C1	162,19	C9H10N2O
Z1791182212	NCC1=C(OC2=C1C=CC=C2)C(N)=O	190,20	C10H10N2O2
Z1787355592	CC(C)C1=CC(=O)N(C)N1	140,19	C7H12N2O
Z1787355945	OC(=O)C1(CC2=C(F)C=CC=C2)CC1	194,21	C11H11FO2
Z1787158625	CC(=O)NC1CCC(N)CC1	156,23	C8H16N2O
Z805551440	CN(C)S(=O)(=O)C1=CN=C1	175,21	C5H9N3O2S
Z1778350445	CC1=C(C=NN1)C1=NN=C(N)S1	181,22	C6H7N5S
Z98996956	NC(=O)CN1C(=O)OC2=C1C=CC(Cl)=C2	226,62	C9H7ClN2O3
Z237599214	CCC(O)C1=NC2=C(C=CC=C2)N1CC	204,27	C12H16N2O
Z431947156	CC1=C(C)C=C(C#N)C(=O)N1	148,17	C8H8N2O
Z431947158	CC1=CC=C(C(O)=O)C(=O)N1	153,14	C7H7NO3
Z92433384	CNC(=O)C(C)OC1=C(F)C=C(F)C=C1	215,20	C10H11F2NO2
Z425449750	NC(=O)CN1C=C(N)C=N1	140,15	C5H8N4O
Z425389656	CC1=CC(C(O)=O)=C(C)N1C1=NC=CS1	222,26	C10H10N2O2S
Z65558737	OC(=O)COC1=CC(Cl)=C(Cl)C=C1	221,03	C8H6Cl2O3
Z406680118	CC1=NN(CC1)C1=CC=C(C=C1)C(O)=O	204,23	C11H12N2O2
Z234894117	CC1=CC=C(S1)C1=NN=C(N)O1	181,21	C7H7N3OS
Z398556904	CC1=CC=C(O1)C1=NC(=CS1)C(O)=O	209,22	C9H7NO3S
Z397585712	BrC1=CN=C(C=C1)N1CCNCC1	242,12	C9H12BrN3
Z384360874	BrC1=CNC(=C1)C(=O)NCC1CCOC1	273,13	C10H13BrN2O2
Z234894711	C1C1=CN=C(C=C1)N1CCNCC1	197,67	C9H12ClN3
Z18390836	CN(C)C(=O)COC1=C(Cl)C=C(F)C=C1	231,65	C10H11ClFNO2
Z381474098	O=C(NC1=NC=CC=C1)C1COCCO1	208,22	C10H12N2O3
Z409508902	CC1COCCN1C(=O)NC1=NN=CS1	228,27	C8H12N4O2S
Z992716962	OCC1=CN2C=C(Cl)C=C(Cl)C2=N1	217,05	C8H6Cl2N2O
Z275255230	OC(=O)C1=CC=C(CN2C=C(Br)C=N2)O1	271,07	C9H7BrN2O3
Z27633535	CC(NC(=O)C1CCC1)C1=NC=CC=C1	204,27	C12H16N2O
Z29672864	CC1=NN=C(NC(=O)C2=CC=CC=C2)S1	219,26	C10H9N3OS