

No.	Molweight	Formula	SMILES	IUPAC_Name	Amount [mg]	State
1.	417.5	C19H19N3O4S2	CC(=O)c1ccc(cc1)N1CCN(CC1)S(=O)(=O)c1ccc2[nH]c(=O)sc2c1	6-[(4-(4-acetylphenyl)piperazin-1-yl)sulfonyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
2.	443.46	C18H16F3N3O3S2	FC(F)(F)c1ccc(cc1)N1CCN(CC1)S(=O)(=O)c1ccc2[nH]c(=O)sc2c1	6-[(4-(3-(trifluoromethyl)phenyl)piperazin-1-yl)sulfonyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
3.	403.52	C19H21N3O3S2	CCn1c2ccc(cc2sc1=O)S(=O)(=O)N1CCN(CC1)c1ccccc1	3-ethyl-6-[(4-phenylpiperazin-1-yl)sulfonyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
4.	518.62	C24H27FN4O4S2	Fc1cccc1N1CCN(CC1)S(=O)(=O)c1ccc2n(CCC(=O)N3CCCC3)c1ccc2c1	6-[(4-(2-fluorophenyl)piperazin-1-yl)sulfonyl]-3-[3-oxo-3-(pyrrolidin-1-yl)propyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
5.	514.66	C25H30N4O4S2	O=C(CCN1c2ccc(cc2sc1=O)S(=O)(=O)N1CCN(CC1)c1ccccc1)N1CCCC1	3-[3-oxo-3-(piperidin-1-yl)propyl]-6-[(4-phenylpiperazin-1-yl)sulfonyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
6.	516.63	C24H28N4O5S2	O=C(CCN1c2ccc(cc2sc1=O)S(=O)(=O)N1CCN(CC1)c1ccccc1)N1CCOCC1	3-[3-(morpholin-4-yl)-3-oxopropyl]-6-[(4-phenylpiperazin-1-yl)sulfonyl]-2,3-dihydro-1,3-benzothiazol-2-one		5 Powder
7.	348.406	C20H24NO4O2	Cc1ccc(CNCC2c3c(C)nn(c4cccc4)c3[nH]c2=O)c1	3-methyl-5-(((5-methylfuran-2-yl)methyl)amino)methyl]-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
8.	402.498	C24H26N4O2	CC(C)Oc1cccc1CNCc1cc2c(C)nn(c3cccc3)c2[nH]c1=O	3-methyl-1-phenyl-5-(((2-(propan-2-yl)oxy)phenyl)methyl)amino)methyl]-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
9.	352.369	C19H17FN4O2	Cc1nn(c2ccc(F)cc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	1-(4-fluorophenyl)-5-((furan-2-ylmethyl)amino)methyl]-3-methyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
10.	422.46	C23H23FN4O3	COc1ccc(CNCc2cc3c(C)nn(c4ccc(F)cc4)c3[nH]c2=O)ccc1OC)c1	5-(((3,5-dimethoxyphenyl)methyl)amino)methyl)-1-(4-fluorophenyl)-3-methyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
11.	460.64	C27H32N4OS	Cc1cccc(N=C2Sc3nc4c(C)c(C)ccc4cc3CN2CCN2CCOCC2)c1C	(2E)-N-(2,3-dimethoxyphenyl)-8,9-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
12.	460.64	C27H32N4OS	CCc1cccc1N=C1Sc2nc3c(C)c(C)ccc3cc2CN1CCN1CCOCC1	(2E)-N-(2-ethylphenyl)-8,9-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
13.	460.64	C27H32N4OS	CCc1ccc(cc1)N=C1Sc2nc3c(C)c(C)ccc3cc2CN1CCN1CCOCC1	(2E)-N-(4-ethylphenyl)-8,9-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
14.	492.64	C27H32N4O3S	COc1ccc(N=C2Sc3nc4c(C)c(C)ccc4cc3CN2CCN2CCOCC2)c(OC)c1	(2E)-N-(2,4-dimethoxyphenyl)-8,9-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
15.	460.64	C27H32N4O3S	CCc1cccc1N=C1Sc2nc3cc(C)cc(C)c3cc2CN1CCN1CCOCC1	(2E)-N-(2-ethylphenyl)-6,8-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
16.	460.64	C27H32N4O3S	CCc1ccc(cc1)N=C1Sc2nc3cc(C)cc(C)c3cc2CN1CCN1CCOCC1	(2E)-N-(4-ethylphenyl)-6,8-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
17.	492.64	C27H32N4O3S	COc1ccc(N=C2Sc3nc4c(C)c(C)ccc4cc3CN2CCN2CCOCC2)c(OC)c1	(2E)-N-(2,4-dimethoxyphenyl)-6,8-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
18.	492.64	C27H32N4O3S	CCc1ccc(N=C2Sc3nc4c(C)ccc(C)c4cc3CN2CCN2CCOCC2)c(OC)c1	(2E)-N-(2,4-dimethoxyphenyl)-6,9-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
19.	446.61	C26H30N4O3S	Cc1cccc(c1)N=C1Sc2nc3cc(C)c(C)ccc3cc2CN1CCN1CCOCC1	(2E)-7,8-dimethyl-N-(3-methylphenyl)-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
20.	460.64	C27H32N4O3S	Cc1ccc(C)c(c1)N=C1Sc2nc3cc(C)c(C)ccc3cc2CN1CCN1CCOCC1	(2E)-N-(2,5-dimethylphenyl)-7,8-dimethyl-3-[2-(morpholin-4-yl)ethyl]-2H,3H,4H-[1,3]thiazino[6,5-b]quinolin-2-imine		5 Powder
21.	492.63	C28H32N2O4S	COc1ccc(cc1)S(=O)(=O)N1CC2CC(C)N2C1C1CCCC1C1CCCC(OC)C1	3-(4-methoxybenzenesulfonyl)-9-((3-methoxyphenyl)(phenyl)methyl)-3,9-diazabicyclo[4.2.1]nonane		5 Powder
22.	480.6	C27H29FN2O3S	COc1cccc(c1)C(N1C2CCC1CN(C)C2)S(=O)(=O)c1ccc(F)cc1c1ccccc1	3-(4-fluorobenzenesulfonyl)-9-((3-methoxyphenyl)(phenyl)methyl)-3,9-diazabicyclo[4.2.1]nonane		5 Powder
23.	400.54	C22H28N2O3S	CCc1cccc(c1)C(N1C2CCC1CN(C)C2)S(=O)(=O)c1ccc1c1ccccc1	3-methanesulfonyl-9-((3-methoxyphenyl)(phenyl)methyl)-3,9-diazabicyclo[4.2.1]nonane		5 Powder
24.	376.46	C22H28N2O2S	CC(C)(C)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	3-tert-butyl-5-((furan-2-ylmethyl)amino)methyl]-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
25.	464.95	C25H25ClN4O3	CC(C)(C)c1nn(c2ccc(Cl)cc2)c2[nH]c(=O)c1c(CNCc3cccc3OCC3)cc12	5-(((2H-1,3-benzodioxol-5-yl)methyl)amino)methyl)-3-tert-butyl-1-(4-chlorophenyl)-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
26.	410.9	C22H23ClN4O2	CC(C)(C)c1nn(c2ccc(Cl)cc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	3-tert-butyl-1-(4-chlorophenyl)-5-(((furan-2-ylmethyl)amino)methyl)-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
27.	450.97	C25H27ClN4O2	CCc1cccc1CNc1cc2c(nnc3ccc(Cl)cc3)c2[nH]c1=O)c1C(C)C(C)C	3-tert-butyl-1-(4-chlorophenyl)-5-(((2-methoxyphenyl)methyl)amino)methyl)-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
28.	368.82	C19H17ClN4O2	Cc1nn(c2ccc(Cl)cc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	1-(4-chlorophenyl)-5-(((furan-2-ylmethyl)amino)methyl)-3-methyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
29.	454.96	C27H23ClN4O2	Cc1ccc(cc1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	5-(((4-chlorophenyl)methyl)amino)methyl)-3-(4-fluorophenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
30.	480.524	C28H24N4O4	COc1ccc(cc1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3ccc4OCC4c3)cc12	5-(((2H-1,3-benzodioxol-5-yl)methyl)amino)methyl)-3-(4-methoxyphenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
31.	450.542	C28H26N4O2	COc1ccc(cc1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3ccc(C)cc3)cc12	3-(4-methoxyphenyl)-5-(((4-methylphenyl)methyl)amino)methyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
32.	458.92	C26H20ClFN4O	Fc1ccc(cc1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	5-(((2-chlorophenyl)methyl)amino)methyl)-3-(4-fluorophenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
33.	454.505	C27H23FN4O2	COc1cccc1CNc1cc2c(nnc3cccc3)c2[nH]c1=O)c1ccc(F)cc1	3-(4-fluorophenyl)-5-(((2-methoxyphenyl)methyl)amino)methyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
34.	510.55	C29H26N4O5	COc1ccc(cc1)OC)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3ccc4OCC4c3)cc12	5-(((2H-1,3-benzodioxol-5-yl)methyl)amino)methyl)-3-(3,4-dimethoxyphenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
35.	456.502	C26H24N4O4	CCc1ccc(cc1)OC)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	3-(3,4-dimethoxyphenyl)-5-(((furan-2-ylmethyl)amino)methyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
36.	458.92	C26H20ClFN4O	Fc1cccc(c1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3cccc3)cc12	5-(((2-chlorophenyl)methyl)amino)methyl)-3-(3-fluorophenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
37.	468.488	C27H21FN4O3	Fc1cccc(c1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3ccc4OCC4c3)cc12	5-(((2H-1,3-benzodioxol-5-yl)methyl)amino)methyl)-3-(3-fluorophenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
38.	458.92	C26H20ClFN4O	Fc1cccc(c1)c1nn(c2cccc2)c2[nH]c(=O)c1c(CNCc3ccc(C)cc3)cc12	5-(((4-chlorophenyl)methyl)amino)methyl)-3-(3-fluorophenyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
39.	454.505	C27H23FN4O2	COc1cccc1CNc1cc2c(nnc3cccc3)c2[nH]c1=O)c1ccc(F)c1	3-(3-fluorophenyl)-5-(((2-methoxyphenyl)methyl)amino)methyl)-1-phenyl-1H,6H,7H-pyrazolo[3,4-b]pyridin-6-one		5 Powder
40.	344.43	C18H20N2O3S	CC(C)(C)NC(=O)CN1c2cccc2-c2cccc2S1(=O)=O	N-tert-butyl-2-(8,8-dioxo-8-?-thia-9-azatricyclo[8.4.0.0?]?tetradeca-(14),2(7),3,5,10,12-hexaen-9-yl)acetamide		5 Powder
41.	344.43	C18H20N2O3S	CNC(C)C(=O)CN1c2cccc2-c2cccc2S1(=O)=O	2-(8,8-dioxo-8-?-thia-9-azatricyclo[8.4.0.0?]?tetradeca-(14),2(7),3,5,10,12-hexaen-9-yl)-N,N-diethylacetamide		5 Powder
42.	316.38	C16H16N2O3S	CNC(=O)CN1c2ccc(C)cc2-c2cccc2S1(=O)=O	N-methyl-2-(13-methyl-8,8-dioxo-8-?-thia-9-azatricyclo[8.4.0.0?]?tetradeca-(14),2(7),3,5,10,12-hexaen-9-yl)acetamide		5 Powder
43.	366.4	C16H14N8OS	CCOc1cccc1-n1nnnc1Sc1nnn1-c1ccccc1	1-(2-ethoxyphenyl)-5-(((1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl)-1H-1,2,3,4-tetrazole		5 Powder
44.	377.47	C18H19NO4S2	COc1ccc(C2Sc3c3c(C)c(C)ccc3CS2)c(OC)c1c1[N+](=O)[O-]=O	2-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)-4-methoxy-6-nitrophenol		5 Powder
45.	258.36	C13H10N2S2	Cc1ccc(cc1)-c1csc2nc[nH]c(=S)c12	5-(4-methylphenyl)-3H,4H-thieno[2,3-d]pyrimidine-4-thione		5 Powder
46.	323.396	C19H21N3O2	COCC1cc(=O)c2c(nnc3cccc3)c2[nH]1)C1CCCC1	3-cyclopentyl-6-(methoxymethyl)-1-phenyl-1H,4H,7H-pyrazolo[3,4-b]pyridin-4-one		5 Powder
47.	368.48	C25H24N2O	O=C(N1CCCN(CC1)C1c2cccc2-c2cccc2)c1ccccc1	1-benzoyl-4-(9H-fluoren-9-yl)-1,4-diazepane		5 Powder
48.	397.49	C21H23N3O3S	CC1CCCC(C1)NC(=O)c1ccc(NC2=NS(=O)(=O)c1ccc23)cc1 [t:6]	4-((1,1-dioxo-1-?-2-benzothiazol-3-yl)amino)-N-(3-methylcyclohexyl)benzamide		5 Powder
49.	398.48	C20H22N4O3S	CN1CCCN(CC1)C(=O)c1ccc(NC2=NS(=O)(=O)c3cccc23)cc1 [t:6]	3-[(4-(4-methyl-1,4-diazepan-1-carbonyl)phenyl)amino]-1-?-2-benzothiazole-1,1-dione		5 Powder
50.	272.32	C14H12N2O2S	Cc1ccc(NC2=NS(=O)(=O)c3cccc23)cc1 [t:6]	3-[(4-methylphenyl)amino]-1-?-2-benzothiazole-1,1-dione		5 Powder
51.	373.2	C15H10Cl2N8	Cl(C)Cl(c1nnn1-c1ccccc1)c1nnn1-c1ccccc1	5-(dichloro(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)methyl)-1-phenyl-1H-1,2,3,4-tetrazole		5 Powder
52.	332.371	C17H16N8	Cc1cccc1-n1nnnc1Cc1nnn1-c1ccccc1C	1-(2-methylphenyl)-5-(((1,2-methylphenyl)-1H-1,2,3,4-tetrazol-5-yl)methyl)-1H-1,2,3,4-tetrazole		5 Powder
53.	273.35	C15H15NO2S	CN1c2c(C)ccc(C)c2-c2cccc2S1(=O)=O	9,11,14-trimethyl-8-?-thia-9-azatricyclo[8.4.0.0?]?tetradeca-(14),2(7),3,5,10,12-hexaene-8,8-dione		5 Powder
54.	302.45	C17H18O5S2	Cc1cc2CSC(SCc2cc1C)c1ccccc1O	2-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)phenol		5 Powder
55.	283.31	C14H9N3O2S	O=C(Nc1nc(=O)c2cccc2s1)c1ccccc1	N-(4-oxo-4H-pyrido[3,2-e][1,3]thiazin-2-yl)benzamide		5 Powder
56.	282.32	C15H10N2O2S	O=C(Nc1nc2cccc2c(=O)s1)c1ccccc1	N-(4-oxo-4H-3,1-benzothiazin-2-yl)benzamide		5 Powder
57.	296.34	C16H12N2O2S	Cc1ccc(cc1)C(=O)Nc1nc2cccc2c(=O)s1	4-methyl-N-(4-oxo-4H-3,1-benzothiazin-2-yl)benzamide		5 Powder
58.	344.39	C17H16N2O4S	CCOC(=O)CN(C1=NS(=O)(=O)c2cccc12)c1ccccc1 [t:7]	ethyl 2-((1,1-dioxo-1-?-2-benzothiazol-3-yl)(phenyl)amino)acetate		5 Powder
59.	304.38	C14H12N2O2S2	CCc1cc(C)nc(SC2=C(S(=O)(=O)c3cccc23)n1 [t:8]	3-[(4,6-dimethylpyrimidin-2-yl)sulfonyl]-1-?-benzothioephene-1,1-dione		5 Powder
60.	313.36	C11H7NO4S3	O=c1oc2ccc(NS(=O)(=O)c3ccc3)cc2s1	N-(2-oxo-2H-1,3-benzoxathiol-5-yl)thiophene-2-sulfonamide		5 Powder
61.	363.42	C15H9NO4S3	O=c1oc2cc(cc(NS(=O)(=O)c3cccc3)c3cccc23)s1	N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)thiophene-2-sulfonamide		5 Powder
62.	395.43	C21H17NO5S	COc1ccc(cc1)OC)c1OC)c1nc2sc(cc3cccc3)c2c(=O)o1	5-phenyl-2-(3,4,5-trimethoxyphenyl)-4H-thieno[2,3-d][1,3]oxazin-4-one		5 Powder
63.	379.43	C21H17NO4S	COc1ccc(cc1)OC)-c1csc2nc(oc(=O)c12)-c1ccccc1C	5-(3,4-dimethoxyphenyl)-2-(2-methylphenyl)-4H-thieno[2,3-d][1,3]oxazin-4-one		5 Powder
64.	383.39	C20H14FNO4S	CCc1ccc(cc1)OC)-c1csc2nc(oc(=O)c12)-c1ccccc1F	5-(3,4-dimethoxyphenyl)-2-(2-fluorophenyl)-4H-thieno[2,3-d][1,3]oxazin-4-one		5 Powder
65.	269.32	C14H11N3OS	CCc1ccc(Nc2nc(=O)c3ccccc3s2)cc1	2-[(4-methylphenyl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one		5 Powder
66.	355.4	C13H9NO5S3	CC(=O)N(c1ccc2cc(=O)sc2c1)S(=O)(=O)c1ccccc1	N-(2-oxo-2H-1,3-benzoxathiol-5-yl)-N-(thiophene-2-sulfonyl)acetamide		5 Powder
67.	280.32	C10H8N4O2S2	Cc1nnc(NC2=NS(=O)(=O)c3cccc23)s1 [t:6]	3-[(5-methyl-1,3,4-thiadiazol-2-yl)amino]-1-?-2-benzothiazole-1,1-dione		5 Powder
68.	388.48	C16H12N4O2S3	O=S1(=O)N=C(Nc2nnc(SCc3cccc3)s2)c2cccc12 [t:3]	3-[(5-benzylsulfanyl)-1,3,4-thiadiazol-2-yl]amino]-1-?-2-benzothiazole-1,1-dione		5 Powder

69.	425.5	C15H15NO4S3	O=C(CSc1nnc(NC2=NS(=O)=O)c3cccc23)s1)N1COCOCC1 [t:9]	3-[(5-[(2-(morpholin-4-yl)-2-oxoethyl)sulfanyl]-1,3,4-thiadiazol-2-yl)amino]-1,7,2-benzothiazole-1,1-dione	5	Powder
70.	342.37	C16H14N4O3S	Cn1c2ccc(NC3=NS(=O)=O)c4cccc34cc2n(C)c1=O [t:7]	3-[(1,3-dimethyl-2-oxo-2,3-dihydro-1H-1,3-benzodiazol-5-yl)amino]-1,7,2-benzothiazole-1,1-dione	5	Powder
71.	423.516	C27H25N3O2	CCc1ccc(cc1)-c1nnc2c1cn(Cc1cccc1)c1cc(OC)c(OC)cc21	5-benzyl-3-(4-ethylphenyl)-7,8-dimethoxy-5H-pyrazolo[4,3-c]quinoline	5	Powder
72.	369.85	C23H16ClN3	C1c1ccc(Cn2cc3c(nnc3c3cccc23)-c2cccc2)cc1	5-[(4-chlorophenyl)methyl]-3-phenyl-5H-pyrazolo[4,3-c]quinoline	5	Powder
73.	353.4	C23H16FN3	Fc1cccc1Cn1cc2c(nnc2c2cccc12)-c1cccc1	5-[(2-fluorophenyl)methyl]-3-phenyl-5H-pyrazolo[4,3-c]quinoline	5	Powder
74.	353.4	C23H16FN3	Fc1cccc(Cn2cc3c(nnc3c3cccc23)-c2cccc2)c1	5-[(3-fluorophenyl)methyl]-3-phenyl-5H-pyrazolo[4,3-c]quinoline	5	Powder
75.	389.381	C23H14F3N3	Fc1cccc(Cn2cc3c(nnc3c3cc(F)cc(F)c23)-c2cccc2)c1	6,8-difluoro-5-[(3-fluorophenyl)methyl]-3-phenyl-5H-pyrazolo[4,3-c]quinoline	5	Powder
76.	451.526	C28H25N3O3	COc1cccc1Cn1cc2c(nnc2c2c3COCCO3c3c12)-c1ccc(C)c(C)c1	14-(3,4-dimethylphenyl)-17-[(2-methoxyphenyl)methyl]-4,7-dioxo-12,13,17-triazatetracyclo[8.7.0.0 ² .?0 ¹¹ .?]heptadeca-1,3(8),9,11,13,15-h	5	Powder
77.	399.88	C24H18ClN3O	COc1cccc1Cn1cc2c(nnc2c2cccc12)-c1ccc(C)cc1	3-(4-chlorophenyl)-5-[(2-methoxyphenyl)methyl]-5H-pyrazolo[4,3-c]quinoline	5	Powder
78.	451.526	C28H25N3O3	COc1ccc(Cn2cc3c(nnc3c3cc4OCCO4c4c23)-c2cccc(C)c(C)c2)cc1	14-(3,4-dimethylphenyl)-17-[(4-methoxyphenyl)methyl]-4,7-dioxo-12,13,17-triazatetracyclo[8.7.0.0 ² .?0 ¹¹ .?]heptadeca-1,3(8),9,11,13,15-h	5	Powder
79.	349.4	C20H15NO3S	COc1ccc(cc1)-c1csc2nc(oc(=O)c12)-c1ccc(C)cc1	5-(4-methoxyphenyl)-2-(4-methylphenyl)-4H-thieno[2,3-d][1,3]oxazin-4-one	5	Powder
80.	384.25	C18H10BrN2O2S	BrC1ccc(c1)-c1nc2sc(c-c3cccc3)c2c(=O)o1	2-(3-bromophenyl)-5-phenyl-4H-thieno[2,3-d][1,3]oxazin-4-one	5	Powder
81.	340.73	C13H9ClN2O5S	COc1cc-2c(NS(=O)=O)c3ccc(Cl)cc-23(c1)[N+]([O-])=O	4-chloro-13-methoxy-11-nitro-8,7,7-thia-9-azatricyclo[8.4.0.0 ² .?]tetradeca-(14),2(7),3,5,10,12-hexaene-8,8-dione	5	Powder
82.	392.52	C23H24N2O2S	COc1ccc(cc1)-n1c2CCCCc2c(=S)nc1-c1ccc(OC)cc1	1-(4-ethoxyphenyl)-2-(4-methoxyphenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
83.	299.39	C16H17N3OS	COc1ccc(cc1)N1CNC(=S)N(C1)c1cccc1	5-(4-methoxyphenyl)-1-phenyl-1,3,5-triazinane-2-thione	5	Powder
84.	366.421	C20H22N4O3	CCOC1=NC2Nc3cccc3N(CC)C2C1c1ccc(cc1)[N+]([O-])=O [t:3]	2-ethoxy-4-ethyl-3-(4-nitrophenyl)-3H,3aH,4H,9H,9aH-pyrrolo[2,3-b]quinoxaline	5	Powder
85.	386.84	C19H19ClN4O3	CCOC1=NC2Nc3ccc(Cl)cc3N(C)C2C1c1ccc(cc1)[N+]([O-])=O [t:3]	6-chloro-2-ethoxy-4-methyl-3-(4-nitrophenyl)-3H,3aH,4H,9H,9aH-pyrrolo[2,3-b]quinoxaline	5	Powder
86.	258.36	C13H10N2S2	Cc1sc2n[nH](c=S)c2c1-c1cccc1	6-methyl-5-phenyl-3H,4H-thieno[2,3-d]pyrimidine-4-thione	5	Powder
87.	323.34	C18H10FN2O2S	Fc1cccc1-c1nc2sc(c-c3cccc3)c2c(=O)o1	2-(2-fluorophenyl)-5-phenyl-4H-thieno[2,3-d][1,3]oxazin-4-one	5	Powder
88.	379.43	C21H17NO4S	COc1ccc(cc1)-c1csc2nc(oc(=O)c12)-c1cccc1OC	5-(4-ethoxyphenyl)-2-(2-methoxyphenyl)-4H-thieno[2,3-d][1,3]oxazin-4-one	5	Powder
89.	278.77	C12H7ClN2S2	Clc1ccc(cc1)-c1csc2n[nH](c=S)c12	5-(4-chlorophenyl)-3H,4H-thieno[2,3-d]pyrimidine-4-thione	5	Powder
90.	301.41	C16H19N3OS	Cc1ccc(N2CN(Cc3ccc3)CNC2=S)(C)c1	1-(2,4-dimethylphenyl)-5-(furan-2-ylmethyl)-1,3,5-triazinane-2-thione	5	Powder
91.	235.35	C21H17N3S	CCCN1CNC(=S)N(C1)c1cccc1	1-phenyl-5-propyl-1,3,5-triazinane-2-thione	5	Powder
92.	393.46	C21H19N3O3S	COc1ccc(cc1)-n1c2CCCCc2c(=S)nc1-c1ccc(cc1)[N+]([O-])=O	1-(4-methoxyphenyl)-2-(3-nitrophenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
93.	377.46	C21H19N3O2S	Cc1cccc1-n1c2CCCCc2c(=S)nc1-c1ccc(cc1)[N+]([O-])=O	1-(2-methylphenyl)-2-(3-nitrophenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
94.	391.5	C19H21NO4S2	Cc1cc(cc1C)S(=O)(=O)Nc1ccc2oc(=O)sc2c1)C(C)C(C)C	5-tert-butyl-2,3-dimethyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)benzene-1-sulfonamide	5	Powder
95.	321.37	C14H11NO4S2	Cc1ccc(cc1)S(=O)(=O)Nc1ccc2oc(=O)sc2c1	4-methyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)benzene-1-sulfonamide	5	Powder
96.	367.35	C14H9NO7S2	OC(=O)c1ccc(cc1O)S(=O)(=O)Nc1ccc2oc(=O)sc2c1	2-hydroxy-5-(2-oxo-2H-1,3-benzoxathiol-5-yl)sulfamoylbenzoic acid	5	Powder
97.	397.89	C17H16ClNO4S2	Cc1cc(C)c(C)c(C)c1S(=O)(=O)Nc1cc(Cl)c2oc(=O)sc2c1	N-(7-chloro-2-oxo-2H-1,3-benzoxathiol-5-yl)-2,3,5,6-tetramethylbenzene-1-sulfonamide	5	Powder
98.	383.45	C15H13NO5S3	CCCC(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1cccc1	N-(2-oxo-2H-1,3-benzoxathiol-5-yl)-N-(thiophene-2-sulfonyl)butanamide	5	Powder
99.	367.39	C15H13NO6S2	COc1ccc(OC)c(c1)S(=O)(=O)Nc1ccc2oc(=O)sc2c1	2,5-dimethoxy-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)benzene-1-sulfonamide	5	Powder
100.	511.52	C24H17NO8S2	COc1ccc(OC)c(c1)S(=O)(=O)N(C(=O)c1cccc1)c1cc2sc(=O)oc2c2cccc12	N-(2,5-dimethoxybenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
101.	465.49	C23H15NO6S2	Cc1ccc(cc1)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(4-methylbenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
102.	479.52	C24H17NO6S2	CCc1ccc(cc1)S(=O)(=O)N(C(=O)c1cccc1)c1cc2sc(=O)oc2c2cccc12	N-(4-ethylbenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
103.	485.91	C22H12ClNO6S2	C1c1ccc(cc1)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(4-chlorobenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
104.	479.52	C24H17NO6S2	Cc1ccc(C)c(c1)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(2,5-dimethylbenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
105.	507.58	C26H21NO6S2	Cc1cc(C)c(C)c(c1C)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)-N-(2,3,5,6-tetramethylbenzenesulfonyl)furan-2-carboxamide	5	Powder
106.	493.55	C25H19NO6S2	Cc1cc(C)c(C)c(c1C)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)-N-(2,4,5-trimethylbenzenesulfonyl)furan-2-carboxamide	5	Powder
107.	493.55	C25H19NO6S2	CC(C)c1ccc(cc1)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)-N-[4-(propan-2-yl)benzenesulfonyl]furan-2-carboxamide	5	Powder
108.	507.58	C26H21NO6S2	CC(C)C(C)c1ccc(cc1)S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(4-tert-butylbenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
109.	483.48	C23H14FNO6S2	Cc1cc(F)ccc1S(=O)(=O)N(C(=O)c1ccc1)c1cc2sc(=O)oc2c2cccc12	N-(4-fluoro-2-methylbenzenesulfonyl)-N-(2-oxo-2H-naphtho[2,1-d][1,3]oxathiol-5-yl)furan-2-carboxamide	5	Powder
110.	377.43	C17H15NO5S2	CC(C)C(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1cccc1	N-(benzenesulfonyl)-2-methyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)propanamide	5	Powder
111.	395.42	C17H14FNO5S2	CC(C)C(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1ccc(F)cc1	N-(4-fluorobenzenesulfonyl)-2-methyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)propanamide	5	Powder
112.	383.45	C15H13NO5S3	CC(C)C(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1cccc1	2-methyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)-N-(thiophene-2-sulfonyl)propanamide	5	Powder
113.	395.42	C17H14FNO5S2	CCCC(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1ccc(F)cc1	N-(4-fluorobenzenesulfonyl)-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)butanamide	5	Powder
114.	391.46	C18H17NO5S2	CCCCC(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1cccc1	N-(benzenesulfonyl)-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)pentanamide	5	Powder
115.	397.48	C16H15NO5S3	CCCCC(=O)N(c1ccc2oc(=O)sc2c1)S(=O)(=O)c1cccc1	N-(2-oxo-2H-1,3-benzoxathiol-5-yl)-N-(thiophene-2-sulfonyl)pentanamide	5	Powder
116.	461.53	C18H15NO5S4S3	COc1ccc(NC(=O)CSc2nnc(NC3=NS(=O)=O)c4cccc34)s2)cc1 [t:16]	2-[(5-[(1,1-dioxo-1,7,2-benzothiazol-3-yl)amino]-1,3,4-thiadiazol-2-yl)sulfanyl]-N-(4-methoxyphenyl)acetamide	5	Powder
117.	327.36	C16H13N3O3S	COCC(=O)c1ccc(Nc2nc(=O)c3cccc3c2)cc1	ethyl 4-[(4-oxo-4H-pyrido[3,2-e][1,3]thiazin-2-yl)amino]benzoate	5	Powder
118.	396.51	C22H24N2O3S	CC(=O)Oc1ccc2c(OC)CC22C(C)(C)C(NC(=S)N)2c2cccc2)c1	4',4'-dimethyl-2-phenyl-6'-sulfanylidene-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-7-yl acetate	5	Powder
119.	388.91	C20H21ClN2O2S	CC1(C)CC2(CC(Oc3cc(O)c(C)cc23)C(C)C)C2c2cccc2)NC(=S)N1	6-chloro-7-hydroxy-4',4'-dimethyl-2-phenyl-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-6'-thione	5	Powder
120.	430.95	C22H23ClN2O3S	CC(=O)Oc1cc2OC(Cc3CC(C)C)C(NC(=S)N)3)cc2c1)C1c1cccc1	6-chloro-4',4'-dimethyl-2-phenyl-6'-sulfanylidene-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-7-yl acetate	5	Powder
121.	388.91	C20H21ClN2O2S	CC1(C)CC2(CC(Oc3cc(O)c(C)cc23)C(C)C)C2c2cccc2)NC(=S)N1	2-(2-chlorophenyl)-7-hydroxy-4',4'-dimethyl-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-6'-thione	5	Powder
122.	295.74	C13H10ClNO3S	COc1ccc2NS(=O)(=O)c3ccc(Cl)cc3-c2c1	4-chloro-13-methoxy-8,7,7-thia-9-azatricyclo[8.4.0.0 ² .?]tetradeca-(14),2(7),3,5,10,12-hexaene-8,8-dione	5	Powder
123.	283.35	C15H13N3OS	CCN(c1cccc1)c1nc(=O)c2cccc2s1	2-[ethyl(phenyl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
124.	357.74	C14H7ClF3N3O3S	FC(F)F)c1ccc(Cl)c(Nc2nc(=O)c3cccc3s2)c1	2-[(2-chloro-5-(trifluoromethyl)phenyl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
125.	381.42	C18H18F3N3O3S	COc1cccc1CN1CNC(=S)N(C1)c1cccc1)C(F)F(F)	5-[(2-methoxyphenyl)methyl]-1-[3-(trifluoromethyl)phenyl]-1,3,5-triazinane-2-thione	5	Powder
126.	380.47	C20H20N4O2S	COc1cccc1NC(=O)CSc1nc2C3CCN(CC3)c2cc1CN	2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfanyl]-N-(2-methoxyphenyl)acetamide	5	Powder
127.	434.44	C20H17F3N4O2S	FC(F)F)Oc1ccc(NC(=O)CSc2nc3C4CCN(CC4)c3cc2#N)cc1	2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfanyl]-N-[4-(trifluoromethoxy)phenyl]acetamide	5	Powder
128.	414.91	C20H19ClN4O2S	COc1ccc(Cl)ccc1NC(=O)CSc1nc2C3CCN(CC3)c2cc1CN	N-(5-chloro-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfanyl]acetamide	5	Powder
129.	394.49	C21H22N4O2S	COc1cccc1NC(=O)CSc2nc3C4CCN(CC4)c3cc2CN)C1	2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfanyl]-N-(3-ethoxyphenyl)acetamide	5	Powder
130.	372.41	C17H12N2O4S2	COc1cccc1-c1nnc(SC2=CS(=O)(=O)c3cccc23)o1 [t:14]	3-[(5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl)sulfanyl]-1,7,2-benzothiophene-1,1-dione	5	Powder
131.	387.38	C16H9N3O5S2	[O-][N+](=O)c1cccc1-c1nnc(SC2=CS(=O)(=O)c3cccc23)o1 [t:15]	3-[(5-(2-nitrophenyl)-1,3,4-oxadiazol-2-yl)sulfanyl]-1,7,2-benzothiophene-1,1-dione	5	Powder
132.	432.47	C19H16N2O6S2	COc1ccc(cc1OC)-c1nnc(SC2=CS(=O)(=O)c3cccc23)o1 [t:18]	3-[(5-(3,4,5-trimethoxyphenyl)-1,3,4-oxadiazol-2-yl)sulfanyl]-1,7,2-benzothiophene-1,1-dione	5	Powder
133.	472.42	C18H22BrN3O3S2	Cc1ccc(NC(=O)CN2CCCN(CC2)S(=O)(=O)c2ccc(Br)s2)cc1	2-[4-[(5-bromothiophen-2-yl)sulfanyl]-1,4-diazepan-1-yl]-N-(4-methylphenyl)acetamide	5	Powder
134.	486.44	C19H24BrN3O3S2	Cc1cc(C)ccc(NC(=O)CN2CCCN(CC2)S(=O)(=O)c2ccc(Br)s2)cc1	2-[4-[(5-bromothiophen-2-yl)sulfanyl]-1,4-diazepan-1-yl]-N-(3,5-dimethylphenyl)acetamide	5	Powder
135.	594.39	C19H18BrF6N3O3S2	FC(F)F)F)c1ccc(NC(=O)CN2CCCN(CC2)S(=O)(=O)c2ccc(Br)s2)cc1)C(F)F(F)	N-[3,5-bis(trifluoromethyl)phenyl]-2-[4-[(5-bromothiophen-2-yl)sulfanyl]-1,4-diazepan-1-yl]acetamide	5	Powder
136.	492.83	C17H19BrClN3O3S2	Clc1ccc(NC(=O)CN2CCCN(CC2)S(=O)(=O)c2ccc(Br)s2)cc1	2-[4-[(5-bromothiophen-2-yl)sulfanyl]-1,4-diazepan-1-yl]-N-(4-chlorophenyl)acetamide	5	Powder
137.	508.45	C21H22BrN3O3S2	BrC1ccc(s1)S(=O)(=O)N1C(CCN(CCT(=O)Nc2cccc3cccc23)CC1	2-[4-[(5-bromothiophen-2-yl)sulfanyl]-1,4-diazepan-1-yl]-N-(naphthalen-1-yl)acetamide	5	Powder

207.	316.33	C15H12N2O4S	Cc1c(NC2=NS(=O)=O)c3ccccc23)cccc1C(O)=O [t:4]	3-[(1,1-dioxo-1,2-benzothiazol-3-yl)amino]-2-methylbenzoic acid	5	Powder
208.	344.4	C16H12N2O3S2	Cc1ccc2[nH]c(SC3=CS(=O)=O)c4ccccc34)nc21 [t:9]	3-[(6-methoxy-1H-1,3-benzodiazol-2-yl)sulfonyl]-1,2-benzothioephene-1,1-dione	5	Powder
209.	357.57	C21H27NS2	CCN(CC)c1ccc(cc1)C1SCc2cc(C)c(C)ccc2C1	4-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)-N,N-diethylaniline	5	Powder
210.	311.385	C18H21N3O2	COc1ccc(cc1)n1nc(C)c2c1[nH]c1ccc2=O(C)(C)(C)	6-tert-butyl-1-(4-methoxyphenyl)-3-methyl-1H,4H,7H-pyrazolo[3,4-b]pyridin-4-one	5	Powder
211.	348.46	C21H20N2OS	COc1ccc(cc1)n1c2CCCCc2c(S)nc1-c1cccc1	1-(3-methoxyphenyl)-2-phenyl-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
212.	327.34	C17H17N3O4	CC(=O)C(C)cc(=O)c2c(C)nn(-c3ccc(OC)cc3)c2[nH]1	methyl 2-[1-(4-methoxyphenyl)-3-methyl-4-oxo-1H,4H,7H-pyrazolo[3,4-b]pyridin-6-yl]acetate	5	Powder
213.	437.32	C21H22Cl2N2O4	Clc1ccc(OCc(=O)N2CCCN(C)C2(C)=O)COCc2ccc(Cl)cc2cc1	2-(4-chlorophenoxy)-1-[4-(2-(4-chlorophenoxy)acetyl)-1,4-diazepan-1-yl]ethan-1-one	5	Powder
214.	493.43	C25H43OCl2N2O4	CC(OC)c1cc(C)cc(C)C(=O)N1CCCN(C)C1(C)=O(C)(C)C1ccc(Cl)cc1C	2-(4-chloro-2-methylphenoxy)-1-[4-(2-(4-chloro-2-methylphenoxy)propanoyl)-1,4-diazepan-1-yl]propan-1-one	5	Powder
215.	423.35	C20H20Cl2N2O2S	CC1(C)CC2(CC)OC3cc(O)c(C)cc23)c2ccccc2(C)N(C)=S)N1	6-chloro-2-(2-chlorophenyl)-7-hydroxy-4',4'-dimethyl-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-6'-thione	5	Powder
216.	539.62	C26H25N3O6S2	CC1(C)CC2(CC)OC3cc(OS(=O)=O)c4cccc4[NH]([O])=O)ccc23)c2ccccc2)NC(=S)N1	4',4'-dimethyl-2-phenyl-6'-sulfanylidene-2,3-dihydrospiro[1-benzopyran-4,2'-[1,5]diazinane]-7-yl 2-nitrobenzene-1-sulfonate	5	Powder
217.	272.38	C14H12N2S2	Cc1ccc(cc1C)-c1csc2nc[nH]c1(=S)c1c2	5-(3,4-dimethylphenyl)-3H,4H-thieno[2,3-d]pyrimidine-4-thione	5	Powder
218.	329.51	C19H27N3S	Cc1ccc(C)c(c1)N1CN(C)CC2=CC(C)C2)CNC1=S [t:14]	5-[2-(cyclohex-1-en-1-yl)ethyl]-1-(2,5-dimethylphenyl)-1,3,5-triazinane-2-thione	5	Powder
219.	288.31	C17H12N4O	N(c1cccc1)c1ncnc2Oc3ccccc3c=Nc12 [c:21]	N-phenyl-2-oxa-4,6,9-triazatricyclo[9.4.0.0 ² .?]pentadeca-(15),3(8),4,6,9,11,13-heptaen-7-amine	5	Powder
220.	398.45	C19H14N2O4S2	O=C(Cc1ccccc1)Oc1ccccc1NC1=NS(=O)=O)c2ccccc12 [t:18]	2-[(1,1-dioxo-1,2-benzothiazol-3-yl)amino]phenyl 2-(thiophen-2-yl)acetate	5	Powder
221.	342.41	C18H18N2O3S	O=C(CN1c2ccccc2-c2ccccc2S1(=O)=O)N1CCCC1	9-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-8??-thia-9-azatricyclo[6.4.0.0 ² .?]tetradeca-(14),2(7),3,5,10,12-hexaene-8,8-dione	5	Powder
222.	368.433	C21H24N2O4	O=C(COC1ccccc1)N1CCCN(C)C1(C)=O)COC1ccccc1	2-phenoxy-1-[4-(2-phenoxyacetyl)-1,4-diazepan-1-yl]ethan-1-one	5	Powder
223.	396.487	C23H28N2O4	Cc1ccccc1OCC(=O)N1CCCN(C)C1(C)=O)COC1ccccc1C	2-(2-methylphenoxy)-1-[4-(2-(2-methylphenoxy)acetyl)-1,4-diazepan-1-yl]ethan-1-one	5	Powder
224.	322.4	C13H14N4O2S2	CC(C)(C)C1nnc(NC2=NS(=O)=O)c3ccccc23)S1 [t:9]	3-[(5-tert-butyl-1,3,4-thiadiazol-2-yl)amino]-1,2-benzothiazole-1,1-dione	5	Powder
225.	418.51	C24H22N2O3S	CCc1ccc(cc1)N1C(=S)N(C)C2C(C)(C)Oc1ccccc21(C)=O)c1cccc1	10-(4-ethylphenyl)-12-(furan-2-carbonyl)-9-methyl-8-oxa-10,12-diazatricyclo[7.3.1.0 ² .?]trideca-(2(7),3,5-triene-11-thione	5	Powder
226.	347.48	C18H25N3O2S	CCOC(=O)C1cnc(C)C1N1CN(C)C1(S)C1CCCC1	ethyl 4-(5-cyclohexyl-2-sulfanylidene-1,3,5-triazinan-1-yl)benzoate	5	Powder
227.	418.44	C20H17F3N4OS	FC(F)(F)c1ccc(NC(=O)C)Sc2nc3C4CCN(C)C4c3cc2C#N)c1	2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfonyl]-N-[3-(trifluoromethyl)phenyl]acetamide	5	Powder
228.	422.5	C22H22N4O3S	CCOC(=O)c1ccc(NC(=O)C)Sc2nc3C4CCN(C)C4c3cc2C#N)nc1	ethyl 4-[2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfonyl]acetamido]benzoate	5	Powder
229.	295.83	C14H18ClN3S	Clc1ccc(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	4-(chlorophenyl)-1-[[1(E)-cycloheptylidene]amino]thiourea	5	Powder
230.	279.38	C14H18FN3S	Fc1ccc(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	1-[[1(Z)-cycloheptylidene]amino]-3-(4-fluorophenyl)thiourea	5	Powder
231.	315.35	C15H13N3O3S	COc1ccc(OC)c(Nc2nc(=O)c3ccccc3s2)c1	2-[(2,5-dimethoxyphenyl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
232.	269.42	C13H19NO2S	CC1CCC2C(C1)c1sc(=O)[nH]c1SC2(C)C	5,5,8-trimethyl-2H,3H,5H,5aH,6H,7H,8H,9H,9aH-isothiochromeno[3,4-d][1,3]thiazol-2-one	5	Powder
233.	335.38	C19H13NO3S	O=C(N1c2ccccc2-c2ccccc2S1(=O)=O)c1ccccc1	9-benzoyl-8??-thia-9-azatricyclo[8.4.0.0 ² .?]tetradeca-(14),2(7),3,5,10,12-hexaene-8,8-dione	5	Powder
234.	313.33	C15H11N3O3S	O=c1nc(Nc2ccc3OCC3c2)sc2ncccc12	2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
235.	419.32	C19H16Cl2N4OS	Clc1ccc(C)c1NC(=O)C)Sc1nc2C3CCN(C)C3c2cc1C#N	2-[(4-cyano-1,6-diazatricyclo[6.2.2.0 ² .?]dodeca-2,4,6-trien-5-yl)sulfonyl]-N-(2,6-dichlorophenyl)acetamide	5	Powder
236.	387.38	C16H9N3O5S2	[O][N+](=O)c1ccc(cc1)-c1nnc(SC2=CS(=O)=O)c3ccccc23)O1 [t:15]	3-[(5-(4-nitrophenyl)-1,3,4-oxadiazol-2-yl)sulfonyl]-1,2-benzothioephene-1,1-dione	5	Powder
237.	402.42	C22H14N2O4S	O=C1CCC(=O)N1c1ccc(cc1)-c1nc2sc(-c3ccccc3)c2c(=O)O1	1-(4-(4-oxo-5-phenyl-4H-thieno[2,3-d][1,3]oxazin-2-yl)phenyl)pyrrolidine-2,5-dione	5	Powder
238.	352.38	C15H12N8OS	COc1ccccc1-n1nnc1Sc1nmm1-c1ccccc1	1-(2-methoxyphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
239.	352.38	C15H12N8OS	COc1ccc(cc1)n1nnc1Sc1nmm1-c1ccccc1	1-(4-methoxyphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
240.	350.4	C16H14N8S	Cc1ccc(C)c(c1)n1nnc1Sc1nmm1-c1ccccc1	1-(2,5-dimethylphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
241.	336.38	C15H12N8S	Cc1ccccc1-n1nnc1Sc1nmm1-c1ccccc1	1-(2-methylphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
242.	350.4	C16H14N8S	Cc1ccc(C)c(c1)n1nnc1Sc1nmm1-c1ccccc1	1-(2,4-dimethylphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
243.	322.35	C14H10N8S	S(c1nmm1-c1ccccc1)n1nmm1-c1ccccc1	1-phenyl-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
244.	366.4	C16H14N8OS	COc1ccc(C)cc1-n1nnc1Sc1nmm1-c1ccccc1	1-(2-methoxy-5-methylphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
245.	408.458	C22H24N4O4	CCOC(=O)C1=C(C)Nc2ccccc2N=C1NC(=O)Nc1ccccc1OC [c:5,17]	ethyl 2-ethyl-4-[[2-(methoxyphenyl)carbamoyl]amino]-1H-1,5-benzodiazepine-3-carboxylate	5	Powder
246.	447.32	C21H24OCl2N4O3	CCOC(=O)C1=C(C)Nc2ccccc2N=C1NC(=O)Nc1ccc(Cl)c(C)1 [c:5,17]	ethyl 4-[[3-(4-dichlorophenyl)carbamoyl]amino]-2-ethyl-1H-1,5-benzodiazepine-3-carboxylate	5	Powder
247.	337.302	C16H14F3N3O2	COc1cc(=O)c2c(C)nn(-c3ccccc3C(F)(F)F)c2[nH]1	6-(methoxy-1-phenyl)-3-methyl-1-[2-(trifluoromethyl)phenyl]-1H,4H,7H-pyrazolo[3,4-b]pyridin-4-one	5	Powder
248.	302.337	C18H14N4O	Cc1nn(-c2ccccc2)c2[nH]c(cc(=O)c12)-c1ccccc1	3-methyl-1-phenyl-6-(pyridin-3-yl)-1H,4H,7H-pyrazolo[3,4-b]pyridin-4-one	5	Powder
249.	315.376	C20H17N3O	CCc1cc(=O)c2c(C)nn(-c3ccccc3)c2[nH]1-c1ccccc1	6-ethyl-1,3-diphenyl-1H,4H,7H-pyrazolo[3,4-b]pyridin-4-one	5	Powder
250.	350.4	C16H14N8S	Cc1ccc(cc1C)-n1nnc1Sc1nmm1-c1ccccc1	1-(2,3-dimethylphenyl)-5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1H-1,2,3,4-tetrazole	5	Powder
251.	330.46	C18H18O2S2	Cc1cc2CSC(SCc2cc1C)c1ccc2OCc2e1	5-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)-2H-1,3-benzodioxole	5	Powder
252.	345.48	C18H19NO2S2	Cc1cc2CSC(C)(SCc2cc1C)c1ccc(cc1)[N+][O-]=O	3,7,8-trimethyl-3-(4-nitrophenyl)-3,5-dihydro-1H-2,4-benzodithiepine	5	Powder
253.	275.311	C17H13N3O	Cc1nn(-c2ccccc2)c2[nH]c3ccccc3c(=O)c1c2	3-methyl-1-phenyl-1H,4H,9H-pyrazolo[3,4-b]quinolin-4-one	5	Powder
254.	320.308	C17H12N4O3	Cc1nn(-c2ccc(cc2)[N+][O-])=O)c2[nH]c3ccccc3c(=O)c1c2	3-methyl-1-(4-nitrophenyl)-1H,4H,9H-pyrazolo[3,4-b]quinolin-4-one	5	Powder
255.	329.39	C15H18F3N3S	FC(F)(F)c1ccccc1-#[7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	1-[[1(E)-cycloheptylidene]amino]-3-[3-(trifluoromethyl)phenyl]thiourea	5	Powder
256.	363.83	C15H17ClF3N3S	FC(F)(F)c1ccc(Cl)c(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	3-[2-chloro-5-(trifluoromethyl)phenyl]-1-[[1(Z)-cycloheptylidene]amino]thiourea	5	Powder
257.	289.44	C16H23N3S	[#6]-c1ccc(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	1-[[1(E)-cycloheptylidene]amino]-3-(2,4-dimethylphenyl)thiourea	5	Powder
258.	295.83	C14H18ClN3S	Clc1ccc(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	3-(3-chlorophenyl)-1-[[1(Z)-cycloheptylidene]amino]thiourea	5	Powder
259.	279.38	C14H18FN3S	Fc1ccc(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	1-[[1(E)-cycloheptylidene]amino]-3-(3-fluorophenyl)thiourea	5	Powder
260.	345.48	C18H19NO2S2	Cc1cc2CSC(C)(SCc2cc1C)c1ccc(cc1)[N+][O-]=O	3,7,8-trimethyl-3-(3-nitrophenyl)-3,5-dihydro-1H-2,4-benzodithiepine	5	Powder
261.	314.51	C19H22S2	Cc1ccc(cc1)C1(C)SCc2cc(C)c(C)cc2C1	3,7,8-trimethyl-3-(4-methylphenyl)-3,5-dihydro-1H-2,4-benzodithiepine	5	Powder
262.	309.39	C17H15N3OS	Cc1ccc(cc1)N(C)C)C1nc(=O)c2ccccc2s1	2-[(4-methylphenyl)(prop-2-en-1-yl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
263.	311.4	C17H17N3OS	CCCN(c1ccc(C)cc1)c1nc(=O)c2ccccc2s1	2-[(4-methylphenyl)(propyl)amino]-4H-pyrido[3,2-e][1,3]thiazin-4-one	5	Powder
264.	376.81	C17H13ClN2O4S	COc1cc2nc(NC(=O)C)ccc(C)cc3sc(=O)c2cc1OC	4-chloro-N-(6,7-dimethoxy-4-oxo-4H-3,1-benzothiazin-2-yl)benzamide	5	Powder
265.	338.43	C19H18N2O2S	CC(C)(C)c1ccc(cc1)C(=O)Nc1nc2ccccc2c(=O)S1	4-tert-butyl-N-(4-oxo-4H-3,1-benzothiazin-2-yl)benzamide	5	Powder
266.	398.48	C21H22N2O4S	COc1cc2nc(NC(=O)C)ccc(C)C(C)(C)sc1=O)c2cc1OC	4-tert-butyl-N-(6,7-dimethoxy-4-oxo-4H-3,1-benzothiazin-2-yl)benzamide	5	Powder
267.	394.8	C17H12ClFN2O4S	COc1cc2nc(NC(=O)C)ccc(F)cc3sc(=O)c2cc1OC	2-chloro-N-(6,7-dimethoxy-4-oxo-4H-3,1-benzothiazin-2-yl)-4-fluorobenzamide	5	Powder
268.	510.24	C20H18Br2N2O2S	CCCCc1ccc(cc1)C(=O)Nc1nc2c(Br)cc(Br)cc2c(=O)S1	N-(6,8-dibromo-4-oxo-4H-3,1-benzothiazin-2-yl)-4-pentylbenzamide	5	Powder
269.	454.14	C16H10Br2N2O2S	Cc1ccccc1C(=O)Nc1nc2c(Br)cc(Br)cc2c(=O)S1	N-(6,8-dibromo-4-oxo-4H-3,1-benzothiazin-2-yl)-2-methylbenzamide	5	Powder
270.	303.47	C17H25N3S	[#6]-c1cc(-[#6]c(-[#7]-[#6](=S)-[#7][#7]-[#6]-2[#6]-[#6]-[#6]-[#6]-2)c1	1-[[1(E)-cycloheptylidene]amino]-3-(2,4,6-trimethylphenyl)thiourea	5	Powder
271.	368.56	C21H24N2S2	CN(CCC#N)c1ccc(cc1)C1SCc2cc(C)c(C)cc2C1	3-[(4-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)phenyl)(methyl)amino]propanenitrile	5	Powder
272.	426.37	C18H13F3N2O5S	COc1cc2nc(NC(=O)C)ccc(OC(F)(F)F)cc3sc(=O)c2cc1OC	N-(6,7-dimethoxy-4-oxo-4H-3,1-benzothiazin-2-yl)-4-(trifluoromethoxy)benzamide	5	Powder
273.	243.32	C12H7N2S2	S=c1nnc2sc(-c3ccccc3)c1c2	5-phenylthieno[2,3-d]pyrimidine-4-thione	5	Powder
274.	454.55	C26H22N4O2S	O=N(=O)c1ccc(cc1)-c1nc(=S)c2CCCCc2n1-c1ccc(Cc2ccccc2)cc1	2-(3-nitrophenyl)-1-[4-(pyridin-4-yl)methyl]phenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
275.	393.46	C21H19N3O3S	COc1ccccc1-n1c2CCCCc2c(S)nc1-c1ccccc1)N(=O)=O	1-(3-methoxyphenyl)-2-(3-nitrophenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder

276.	377.46	C21H19N3O2S	Cc1cccc1-n1c2CCCCc2c(=S)nc1-c1cccc(c1)N(=O)=O	1-(2-methylphenyl)-2-(3-nitrophenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
277.	275.34	C13H8FN2S2	Cc1sc2ncnc(=S)c2c1-c1ccc(F)cc1	5-(4-fluorophenyl)-6-methylthieno[2,3-d]pyrimidine-4-thione	5	Powder
278.	291.79	C13H8ClN2S2	Cc1sc2ncnc(=S)c2c1-c1ccc(Cl)cc1	5-(4-chlorophenyl)-6-methylthieno[2,3-d]pyrimidine-4-thione	5	Powder
279.	441.418	C25H16FN3O4	Fe1ccc(Cn2cc3c(nnc3cc4OCOC4cc23)-c2ccc3OCOC3c2)cc1	5-(2H-1,3-benzodioxol-5-yl)-8-[(4-fluorophenyl)methyl]-12,14-dioxo-3,4,8-triazatetracyclo[7.7.0.0 ^{5,6} .0 ^{11,13}]hexadeca-1(16),2,4,6,9,11(15)-hexaene	5	Powder
280.	379.419	C24H17N3O2	C(c1cccc1)n1cc2c(nnc2c2c3OCOC3cc12)-c1cccc1	8-benzyl-5-phenyl-12,14-dioxo-3,4,8-triazatetracyclo[7.7.0.0 ^{5,6} .0 ^{11,13}]hexadeca-1(16),2,4,6,9,11(15)-hexaene	5	Powder
281.	389.48	C19H19NO4S2	O=c1oc2ccc(NS(=O)(=O)c3ccc(cc3)C3CCCC3)cc2s1	4-cyclohexyl-N-(2-oxo-2H-1,3-benzoxathiol-5-yl)benzene-1-sulfonamide	5	Powder
282.	422.452	C23H18N8O	COc1cccc1C=Cc1n1nn1-c1cccc1)c1n1nn1-c1cccc1	5-[2-(2-methoxyphenyl)-1-(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)ethenyl]-1-phenyl-1H-1,2,3,4-tetrazole	5	Powder
283.	268.252	C14H10N3O3	Cc1nn(-c2cccc2)c2ncc(C(O)=O)c(-O)c12	3-methyl-4-oxo-1-phenylpyrazolo[3,4-b]pyridine-5-carboxylic acid	5	Powder
284.	380.48	C22H21FN2OS	CCOc1ccc(cc1)-n1c2CCCCc2c(=S)nc1-c1ccc(F)cc1	1-(4-ethoxyphenyl)-2-(4-fluorophenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
285.	350.46	C21H19FN2S	Cc1ccc(cc1)-n1c2CCCCc2c(=S)nc1-c1ccc(F)cc1	2-(4-fluorophenyl)-1-(4-methylphenyl)-1,4,5,6,7,8-hexahydroquinazoline-4-thione	5	Powder
286.	424.541	C25H32N2O4	CCC(Oc1cccc1)C(=O)N1CCCN(CC1)C(=O)C(CC)Oc1cccc1	2-phenoxy-1-(4-(2-phenoxybutanoyl)-1,4-diazepan-1-yl)butan-1-one	5	Powder
287.	465.37	C23H26Cl2N2O4	CC(Oc1cccc(Cl)c1)C(=O)N1CCCN(CC1)C(=O)C(Oc1cccc(Cl)c1)c1	2-(3-chlorophenoxy)-1-(4-(2-(3-chlorophenoxy)propanoyl)-1,4-diazepan-1-yl)propan-1-one	5	Powder
288.	329.39	C15H18F3N3S	FC(F)(F)c1cccc1-[#7]-[#6](=S)-[#7][#7]-[#6]-1[#6]-[#6]-[#6]-[#6]-1	1-(cycloheptylideneamino)-3-[2-(trifluoromethyl)phenyl]thiourea	5	Powder
289.	532.45	C24H21O2S2	Cc1cc2CSC(SCc2cc1C)c1cccc1OC(=O)c1ccc(l)cc1	2-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)phenyl 4-iodobenzoate	5	Powder
290.	307.397	C19H21N3O	CCOC1=NC2Nc3cccc3N(C)C2C1c1cccc1 [t:3]	2-ethoxy-4-methyl-3-phenyl-3H,3aH,4H,9H,9aH-pyrrolo[2,3-b]quinoxaline	5	Powder
291.	266.29	C9H6N4O2S2	O=S1(=O)N=C(Nc2nncs2)c2cccc12 [t:3]	3-[(1,3,4-thiadiazol-2-yl)amino]-1,2,4-benzothiazole-1,1-dione	5	Powder
292.	291.41	C15H21N3OS	COc1cccc(NC(=S)NN=C2CCCCC2)c1	1-(cycloheptylideneamino)-3-(3-methoxyphenyl)thiourea	5	Powder
293.	456.62	C28H24O2S2	Cc1cc2CSC(SCc2cc1C)c1cccc1OC(=O)c1cccc2cccc12	2-(7,8-dimethyl-3,5-dihydro-1H-2,4-benzodithiepin-3-yl)phenyl naphthalene-1-carboxylate	5	Powder
294.	364.43	C17H16N8S	CC(C)c1ccc(cc1)-n1nnc1Sc1n1nn1-c1cccc1	5-[(1-phenyl-1H-1,2,3,4-tetrazol-5-yl)sulfonyl]-1-[4-(propan-2-yl)phenyl]-1H-1,2,3,4-tetrazole	5	Powder