**SUPPLEMENTARY INFORMATION**

**Identification of new GLUT2-selective inhibitors through *in silico* ligand screening and validation in eukaryotic expression systems**

Sina Schmidl1,#, Oleg Ursu2,3,#, Cristina V. Iancu4, Mislav Oreb1,

Tudor Oprea2,\*and Jun-yong Choe4,5,\*

1 Institute of Molecular Biosciences, Faculty of Biological Sciences, Goethe University Frankfurt, Frankfurt am Main, Germany.

2 Translational Informatics Division, Department of Internal Medicine, The University of New Mexico School of Medicine, Albuquerque, NM 87131, USA.

3 Present address: Computational and Structural Chemistry, Merck & Co., Inc., 2000 Galloping Hill Road, Kenilworth, NJ 07033, USA.

4 Department of Chemistry, East Carolina Diabetes and Obesity Institute, East Carolina University, Greenville, NC 27834 USA.

5 Department of Biochemistry and Molecular Biology, The Chicago Medical School, Rosalind Franklin University of Medicine and Science, North Chicago, IL 60064 USA.

# These authors contributed equally.

\*Corresponding authors:Jun-yong Choe, E-mail: choej18@ecu.edu

Tudor Oprea, E-mail: toprea@salud.unm.edu

Supplementary Figure S1

Supplementary Figure S2

Supplementary Table S1

 



**Figure S1. GLUT homology for GLUT1-5.** (A, B)The homology models were generated in MOE (https://www.chemcomp.com) based on the crystal structure of GLUT1 (PDB ID: 4PYP), with the sequence alignment color-coded; blue regions show sequence conservation, red ones show the highest sequence variation. GLUT2 is more closely related to GLUT1, 3 and 4 (52-65% sequence identity) as compared with GLUT5 (40% sequence identity); however, the loop between the two halves of the transporter (highlighted by a red dotted ellipse) shows a higher variation (the sequence identity among GLUT1, 2, 3, and 4 is 33-61%, and that between GLUT2 and 5 is 35%). The yellow ellipse labeled G2i shows the approximate location of GLUT2 inhibitors. (A) Homology model showing the sequence conservation (blue) for GLUT1, 2, 3 and 4. (B) Homology model showing the sequence conservation (blue) between GLUT2 and 5. (C) Amino acid sequence alignment (https://www.ibi.vu.nl/programs/pralinewww/) of GLUT1-5 shows three unconserved areas: 1) between TM helices 1 and 2 in which GLUT2 has extra ~35 amino acid residues compared with the other GLUTs; 2) between TM helices 6 and 7 (the large cytoplasmic loop highlighted by the red ellipse in A-B); and 3) after TM helix 12.

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**Figure S2. Michaelis-Menten curves for glucose and fructose transport in GLUT2-expressing *hxt*0 yeast system.** Glucose (A) and fructose (B) transport activity by GLUT2∆loopS\_Q455R in EBY.S7 yeast cells. Transport activity was initiated by the addition of C14-hexose (glucose or fructose) to cells in the PBS buffer. After 10 mins, transport activity was stopped, and the radioactivity accumulated in cells was measured. See Materials and Methods for details. Data analysis for calculating KM values and the graphs were generated with GraphPad Prism (https://www.graphpad.com).

**Table S1. *In silico* ligand screening candidates tested for GLUT2 transport inhibition.** The structure identifier (STRUCT\_ID), commercial information (SUPPLIER and CATALOG #), chemical name (CHEM\_NAME), SMILES code (SMILES), and the molecular formula (MF) are indicated for each compound (except for some unavailable chemicals’ names). Identified potent GLUT2 inhibitors (G2iA-K) are in bold, red font.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| STRUCTURE\_ID | SUPPLIER | SUPPLIER\_CATALOG # | CHEM\_NAME | SMILES | MF |
| 448434472 | Ark Pharm | AK242035 |  | N1(CCN(CC1)c2ncc(cc2)c3cc4[n](cc(c4c(c3)C(=O)NCc5c(nc(cc5C)C)O)C)C(C)C)C | C31H38O2N6 |
| 403941836 | Ark Pharm | AK317596  | 5-(ethyl(tetrahydro-2H-pyran-4-yl)amino)-N-((2-hydroxy-4,6-dimethylpyridin-3-yl)methyl)-4-methyl-4'-(morpholinomethyl)-[1,1'-biphenyl]-3-carboxamide | N5(CCOCC5)Cc1ccc(cc1)c2cc(c(c(c2)C(=O)NCc4c(nc(cc4C)C)O)C)N(C3CCOCC3)CC | C34H44O4N4 |
| 407639426 | Target Molecule Corp. | T1905 | 1-cyclopentyl-N-((2-hydroxy-4,6-dimethylpyridin-3-yl)methyl)-6-(4-(morpholinomethyl)phenyl)-1H-indazole-4-carboxamide | N6(CCOCC6)Cc1ccc(cc1)c2cc3[n](ncc3c(c2)C(=O)NCc5c(nc(cc5C)C)O)C4CCCC4 | C32H37O3N5 |
| 27829088 | ChemBridge Corporation | 5340763 | 2-(3,5-diphenyl-4,5-dihydro-1H-pyrazol-1-yl)-4-(4-fluorophenyl)-6-phenylpyrimidine | Fc1ccc(cc1)c2nc(nc(c2)c6ccccc6)N3NC(=CC3c5ccccc5)c4ccccc4 | C31H23N4F1 |
| 30023243 | ChemBridge Corporation | 5720478 | 4-(4-benzhydryl-1-piperazinyl)-1-phenyl-6-(1-piperidinyl)-1H-pyrazolo[3,4-d]pyrimidine | N3(CCN(CC3)c4nc(nc6[n](ncc64)c7ccccc7)N5CCCCC5)C(c2ccccc2)c1ccccc1 | C33H35N7 |
| 466119877 | **ChemBridge Corporation** | **77390155** | **2-{5-(methoxymethyl)-4-[(4-phenyl-1-piperazinyl)carbonyl]-1H-pyrazol-1-yl}-6,7-dihydro-5H-benzo[6,7]cyclohepta[1,2-d]pyrimidine (G2iD)** | **[n]4(ncc(c4COC)C(=O)N5CCN(CC5)c6ccccc6)c1nc2c(cn1)CCCc3c2cccc3** | **C29H30O2N6** |
| 549939793 | ChemBridge Corporation | 94887258 |  | FC(F)(F)c1cc(ccc1)OC[C@@H]2CN(C[C@@H](C2)C(=O)NCCc4c5c([nH]c4)cccc5)CCc3ccccc3 | C32H34O2N3F3 |
| 549930126 | ChemBridge Corporation | 26385775 |  | N2(C[C@H](C[C@H](C2)C(=O)NCCc5c6c([nH]c5)cccc6)COc3cc4c(cc3)CCC4)Cc1cc(c(cc1)OC)OC | C35H41O4N3 |
| 347006762 | ChemBridge Corporation | 40266327 | (3R,5S)-5-[(2,3-dihydro-1H-inden-5-yloxy)methyl]-1-(2-naphthylmethyl)-N-(2-phenylethyl)-3-piperidinecarboxamide | N3(C[C@H](C[C@H](C3)C(=O)NCCc6ccccc6)COc4cc5c(cc4)CCC5)Cc1cc2c(cc1)cccc2 | C35H38O2N2 |
| 181925102 | ChemBridge Corporation | 18817511 | 3-(1-benzothien-7-yl)-1-(cyclopropylmethyl)-6-[(4,6-dimethyl-2-oxo-1,2-dihydro-3-pyridinyl)carbonyl]-5,6,7,8-tetrahydro[1,6]naphthyridin-2(1H)-one | [s]1c2c(cc1)cccc2C3=CC4=C(N(C3=O)CC6CC6)CCN(C4)C(=O)c5c(nc(cc5C)C)O | C28H27O3N3S1 |
| 181950723 | ChemBridge Corporation | 42621764 | N-benzyl-N,1-dimethyl-5-(spiro[indene-1,4'-piperidin]-1'-yl)-4,5,6,7-tetrahydro-1H-indazole-3-carboxamide | [n]1(nc(c3c1CCC(C3)N4CCC5(CC4)c6c(cccc6)C=C5)C(=O)N(Cc2ccccc2)C)C | C30H34O1N4 |
| 181921786 | ChemBridge Corporation | 16753878 | 1,8-bis(2-phenylethyl)-3-(3-pyridinylmethyl)-1,3,8-triazaspiro[4.5]decane-2,4-dione | N2(C4(CCN(CC4)CCc5ccccc5)C(=O)N(C2=O)Cc3cnccc3)CCc1ccccc1 | C29H32O2N4 |
| 181940757 | ChemBridge Corporation | 32425739 | 8-(2,6-dimethyl-5-heptenyl)-1-(2-phenylethyl)-3-(3-pyridinylmethyl)-1,3,8-triazaspiro[4.5]decane-2,4-dione | N2(C4(CCN(CC4)CC(CCC=C(C)C)C)C(=O)N(C2=O)Cc3cnccc3)CCc1ccccc1 | C30H40O2N4 |
| 181915466 | ChemBridge Corporation | 12052429 | 1-(4-methoxybenzyl)-4-{[(1R,2R)-2-phenylcyclopropyl]carbonyl}-6-(3-pyridinylmethoxy)-1,4-diazepan-2-one | N3(CC(CN(C(=O)C3)Cc5ccc(cc5)OC)OCc4cnccc4)C(=O)[C@H]1[C@@H](C1)c2ccccc2 | C29H31O4N3 |
| 182070366 | ChemBridge Corporation | 94419756 | 8-(1H-indol-3-ylmethyl)-3-isobutyl-1-[2-(4-methoxyphenyl)ethyl]-1,3,8-triazaspiro[4.5]decane-2,4-dione | [nH]1c2c(c(c1)CN3CCC4(N(C(=O)N(C4=O)CC(C)C)CCc5ccc(cc5)OC)CC3)cccc2 | C29H36O3N4 |
| 181349814 | **ChemBridge Corporation** | **57791277** | **2-(4-(1-benzothien-3-yl)-2-{[4-(2-pyridinyl)-1-piperazinyl]methyl}phenoxy)-N-(1,3-thiazol-2-ylmethyl)acetamide (G2iE)** | **[s]1c(ncc1)CNC(=O)COc2c(cc(cc2)c5c6c([s]c5)cccc6)CN3CCN(CC3)c4ncccc4** | **C30H29O2N5S2** |
| 466125339 | ChemBridge Corporation | 87775506 |  | [s]1c(c(cc1C)c2nc(ncc2)[n]3ncc(c3C5CC5)C(=O)N(Cc4cc(ccc4)OC)C)C | C26H27O2N5S1 |
| 181305778 | **ChemBridge Corporation** | **26258872** | **2-(5-cyclopropyl-4-{[4-(2-ethoxyphenyl)-1-piperazinyl]carbonyl}-1H-pyrazol-1-yl)-4-(5-methyl-2-furyl)pyrimidine (G2iJ)** | **[n]3(ncc(c3C6CC6)C(=O)N4CCN(CC4)c5c(cccc5)OCC)c1nc(ccn1)c2[o]c(cc2)C** | **C28H30O3N6** |
| 181336555 | ChemBridge Corporation | 47200727 | methyl 3-[4-{1-[(2-methyl-1H-indol-3-yl)methyl]-4-piperidinyl}-2-(4-pyridinyl)-5-pyrimidinyl]phenyl ether | N3(CCC(CC3)c4nc(ncc4c6cc(ccc6)OC)c5ccncc5)Cc1c2c([nH]c1C)cccc2 | C31H31O1N5 |
| 181267787 | ChemBridge Corporation | 11197728 | 2-[2,5-dioxo-3-phenyl-1-(3-pyridinylmethyl)-3-pyrrolidinyl]-N-methyl-N-[2-(trifluoromethyl)benzyl]acetamide | FC(F)(F)c1c(cccc1)CN(C)C(=O)CC3(CC(=O)N(C3=O)Cc4cnccc4)c2ccccc2 | C27H24O3N3F3 |
| 181971369 | ChemBridge Corporation | 68833669 | {4-{[4-(2,5-dimethylphenyl)-1-piperazinyl]carbonyl}-1-[4-(2-thienyl)-2-pyrimidinyl]-1H-pyrazol-5-yl}methyl methyl ether | [s]1c(ccc1)c2nc(ncc2)[n]3ncc(c3COC)C(=O)N4CCN(CC4)c5c(ccc(c5)C)C | C26H28O2N6S1 |
| 181931148 | ChemBridge Corporation | 23777777 | 3-({3-[4-(2-methoxyphenyl)-1-piperazinyl]-1-piperidinyl}carbonyl)-4,6-dimethyl-2(1H)-pyridinone | N3(CCN(CC3)c4c(cccc4)OC)C1CN(CCC1)C(=O)c2c(nc(cc2C)C)O | C24H32O3N4 |
| 181278705 | **ChemBridge Corporation** | **15094108** | **2-(5-cyclopropyl-4-{[4-(2-methoxyphenyl)-1-piperazinyl]carbonyl}-1H-pyrazol-1-yl)-4-(2-thienyl)pyrimidine (G2iC)** | **[s]1c(ccc1)c2nc(ncc2)[n]3ncc(c3C6CC6)C(=O)N4CCN(CC4)c5c(cccc5)OC** | **C26H26O2N6S1** |
| 181284072 | ChemBridge Corporation | 16803568 | 6-[(4'-methyl[1,1'-biphenyl]-4-yl)carbonyl]-1-{[4-(2-pyridinyl)-1-piperazinyl]carbonyl}-6-azaspiro[2.5]octane | N2(CCN(CC2)C(=O)C3C4(CCN(CC4)C(=O)c5ccc(cc5)c6ccc(cc6)C)C3)c1ncccc1 | C31H34O2N4 |
| 181268085 | ChemBridge Corporation | 11381046 | 2-{5-cyclopropyl-4-[(4-phenyl-1-piperazinyl)carbonyl]-1H-pyrazol-1-yl}-4-(3-methoxyphenyl)pyrimidine | [n]3(ncc(c3C6CC6)C(=O)N4CCN(CC4)c5ccccc5)c1nc(ccn1)c2cc(ccc2)OC | C28H28O2N6 |
| 181962616 | ChemBridge Corporation | 56596371 | 2-[4-[(4-cyclopentyl-1-piperazinyl)carbonyl]-5-(methoxymethyl)-1H-pyrazol-1-yl]-4-(2,5-dimethyl-3-thienyl)pyrimidine | [s]1c(c(cc1C)c2nc(ncc2)[n]3ncc(c3COC)C(=O)N4CCN(CC4)C5CCCC5)C | C25H32O2N6S1 |
| 182001206 | **ChemBridge Corporation** | **88168217** | **5-cyclopropyl-1-(5,6-dihydrobenzo[h]quinazolin-2-yl)-N-methyl-N-(5-quinolinylmethyl)-1H-pyrazole-4-carboxamide (G2iF)** | **[n]4(ncc(c4C7CC7)C(=O)N(Cc5c6c(nccc6)ccc5)C)c1nc2c(cn1)CCc3c2cccc3** | **C30H26O1N6** |
| 181149526 | ChemBridge Corporation | 35941485 | N-{[3-(1-benzofuran-2-yl)-1-benzyl-1H-pyrazol-4-yl]methyl}-2-(3,5-dimethyl-1H-pyrazol-4-yl)-N-methylethanamine | [n]2(nc(c(c2)CN(CCc5c([nH]nc5C)C)C)c3[o]c4c(c3)cccc4)Cc1ccccc1 | C27H29O1N5 |
| 181121814 | ChemBridge Corporation | 24355885 | 3-[(3-{3-oxo-3-[4-(2-pyridinyl)-1-piperazinyl]propyl}-1-piperidinyl)carbonyl]-1H-indazole | N2(CCN(CC2)C(=O)CCC3CN(CCC3)C(=O)c4n[nH]c5c4cccc5)c1ncccc1 | C25H30O2N6 |
| 947315724 | ChemBridge Corporation | 78029423 |  | [s]1c2c(c(c1)C(=O)N3CCNC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)C3)Cc5c6c([nH]c5)cccc6)C)C)Cc4ccccc4)CCCC2 | C37H42O5N6S1 |
| 258707156 | Princeton BioMolecular Research, Inc. | OSSL\_325802 | 5-(4-methylphenyl)-2-phenyl-7-{4-[2-(4-pyridinyl)ethyl]-1,4-diazepan-1-yl}[1,3]oxazolo[4,5-d]pyrimidine | N2(CCN(CCC2)c3nc(nc5nc([o]c53)c6ccccc6)c4ccc(cc4)C)CCc1ccncc1 | C30H30O1N6 |
| 34977075 | Princeton BioMolecular Research, Inc. | OSSL\_392390 | 7-[3-(1,3-benzothiazol-2-ylsulfanyl)propyl]-3-methyl-8-(4-phenyl-1-piperazinyl)-3,7-dihydro-1H-purine-2,6-dione | [s]1c2c(nc1SCCC[n]3c4c(nc3N5CCN(CC5)c6ccccc6)N(C(=O)NC4=O)C)cccc2 | C26H27O2N7S2 |
| 35943973 | Princeton BioMolecular Research, Inc. | OSSL\_575565 | 2-(3-[1,1'-biphenyl]-4-yl-1-{[5-(5-chloro-2-thienyl)-7-(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-2-yl]carbonyl}-4,5-dihydro-1H-pyrazol-5-yl)phenol | FC(F)(F)C1=CC(=Nc3[n]1nc(c3)C(=O)N4NC(=CC4c7c(cccc7)O)c5ccc(cc5)c6ccccc6)c2[s]c(cc2)Cl | C33H21O2N5Cl1S1F3 |
| 63176616 | Princeton BioMolecular Research, Inc. | OSSL\_586205 | 2-[3,5-bis(2,4-dimethoxyphenyl)-1H-pyrazol-1-yl]-4-(4-fluorophenyl)-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5ccc(cc5)F)[n]2nc(cc2c4c(cc(cc4)OC)OC)c3c(cc(cc3)OC)OC | C30H24O4N4F4 |
| 63178386 | Princeton BioMolecular Research, Inc. | OSSL\_587015 | 2-[3,5-bis(3,4-dimethoxyphenyl)-1H-pyrazol-1-yl]-4-(4-fluorophenyl)-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5ccc(cc5)F)[n]2nc(cc2c4cc(c(cc4)OC)OC)c3cc(c(cc3)OC)OC | C30H24O4N4F4 |
| 63178397 | Princeton BioMolecular Research, Inc. | OSSL\_589046 | 2-{3,5-bis[4-(difluoromethoxy)phenyl]-1H-pyrazol-1-yl}-4-phenyl-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5ccccc5)[n]2nc(cc2c4ccc(cc4)OC(F)F)c3ccc(cc3)OC(F)F | C28H17O2N4F7 |
| 40904376 | Princeton BioMolecular Research, Inc. | OSSL\_768205 | N-benzyl-1-(1H-indol-3-ylmethyl)-N-(2-phenylethyl)-4-piperidinamine oxalate | N3(CCC(CC3)N(CCc5ccccc5)Cc4ccccc4)Cc1c2c([nH]c1)cccc2.OC(=O)C(=O)O | C31H35O4N3 |
| 35085263 | Scientific Exchange, Inc. | M-033644 | 6-amino-3-(1-naphthyl)-4-[4-(1-naphthylmethoxy)phenyl]-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile | [nH]1nc(c4c1OC(=C(C4c5ccc(cc5)OCc6c7c(ccc6)cccc7)C#N)N)c2c3c(ccc2)cccc3 | C34H24O2N4 |
| 27659180 | Specs | AG-205/11132108 | 2-(3-{2-[3-(4-fluorophenyl)-5-(4-isopropylphenyl)-2,5-dihydro-1H-pyrazol-1-yl]-1,3-thiazol-4-yl}phenyl)-1H-isoindole-1,3(2H)-dione | Fc1ccc(cc1)C2=CC(N(N2)c4[s]cc(n4)c5cc(ccc5)N6C(=O)c7c(cccc7)C6=O)c3ccc(cc3)C(C)C | C35H27O2N4S1F1 |
| 27916761 | Specs | AG-690/13508135 | 4-(4-tert-butylphenyl)-2-{[2-oxo-2-(10H-phenothiazin-10-yl)ethyl]sulfanyl}-6-phenylnicotinonitrile | S1c2c(cccc2)N(c6c1cccc6)C(=O)CSc3nc(cc(c3C#N)c5ccc(cc5)C(C)(C)C)c4ccccc4 | C36H29O1N3S2 |
| 27824288 | Specs | AG-690/40750941 | N-(4-chlorobenzyl)-N-(1-naphthyl)-2-[(2-phenyl-4-quinazolinyl)sulfanyl]acetamide | S(CC(=O)N(Cc6ccc(cc6)Cl)c4c5c(ccc4)cccc5)c1nc(nc3c1cccc3)c2ccccc2 | C33H24O1N3Cl1S1 |
| 27883605 | Specs | AG-690/40753767 | 2-phenoxyethyl 4-[2-(benzyloxy)phenyl]-7-(3,4-dimethoxyphenyl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydro-3-quinolinecarboxylate | N1C2=C(C(C(=C1C)C(=O)OCCOc6ccccc6)c4c(cccc4)OCc5ccccc5)C(=O)CC(C2)c3cc(c(cc3)OC)OC | C40H39O7N1 |
| 27659184 | Specs | AG-205/11132170 | N-(4-{2-[3-(4-fluorophenyl)-5-(4-isopropylphenyl)-2,5-dihydro-1H-pyrazol-1-yl]-1,3-thiazol-4-yl}phenyl)-4-methylbenzenesulfonamide | Fc1ccc(cc1)C2=CC(N(N2)c4[s]cc(n4)c5ccc(cc5)N[S](=O)(=O)c6ccc(cc6)C)c3ccc(cc3)C(C)C | C34H31O2N4S2F1 |
| 27644832 | Specs | AN-919/14712055 | 4-(4-methoxyphenyl)-2-(10H-phenothiazin-10-ylcarbonyl)-6-phenylthieno[2,3-b]pyridin-3-amine | [s]1c2nc(cc(c2c(c1C(=O)N5c6c(cccc6)Sc7c5cccc7)N)c4ccc(cc4)OC)c3ccccc3 | C33H23O2N3S2 |
| 35975457 | InterBioScreen Ltd. | STOCK7S-69659 | (8S,8aR,11aS)-10-(2-naphthyl)-9,11-dioxo-N-[3-(trifluoromethyl)phenyl]-8a,9,10,11,11a,11b-hexahydro-8H-pyrrolo[3',4':3,4]pyrrolo[2,1-a]isoquinoline-8-carboxamide | FC(F)(F)c1cc(ccc1)NC(=O)[C@H]2N3C([C@@H]5[C@H]2C(=O)N(C5=O)c6cc7c(cc6)cccc7)c4c(cccc4)C=C3 | C32H22O3N3F3 |
| 29332280 | InterBioScreen Ltd. | STOCK7S-68264 | 3-benzhydryl 1-methyl (1S,2R,3R)-1-cyano-2-[4-(dimethylamino)phenyl]-1,2,3,10b-tetrahydropyrrolo[2,1-a]isoquinoline-1,3-dicarboxylate | N21[C@H]([C@@H]([C@@](C2c6c(cccc6)C=C1)(C(=O)OC)C#N)c5ccc(cc5)N(C)C)C(=O)OC(c4ccccc4)c3ccccc3 | C37H33O4N3 |
| 29351964 | InterBioScreen Ltd. | STOCK7S-65756 | benzhydryl (8S,8aR,11aS)-10-(4-methoxyphenyl)-9,11-dioxo-8a,9,10,11,11a,11b-hexahydro-8H-pyrrolo[3',4':3,4]pyrrolo[2,1-a]isoquinoline-8-carboxylate | N21[C@@H]([C@H]5[C@@H](C2c7c(cccc7)C=C1)C(=O)N(C5=O)c6ccc(cc6)OC)C(=O)OC(c4ccccc4)c3ccccc3 | C35H28O5N2 |
| 29728600 | Life Chemicals Inc. | F0417-2422 | ethyl 5-({2-[(4-benzoylbenzoyl)amino]benzoyl}oxy)-2-methyl-1-phenyl-1H-indole-3-carboxylate | [n]2(c3c(c(c2C)C(=O)OCC)cc(cc3)OC(=O)c4c(cccc4)NC(=O)c5ccc(cc5)C(=O)c6ccccc6)c1ccccc1 | C39H30O6N2 |
| 30865539 | **Life Chemicals Inc.** | **F0575-0046** | **4-(5-(4-fluorophenyl)-1-{[(2-methyl-1H-indol-3-yl)sulfanyl]acetyl}-4,5-dihydro-1H-pyrazol-3-yl)phenyl methyl ether (G2iA)** | **Fc1ccc(cc1)C2N(NC(=C2)c5ccc(cc5)OC)C(=O)CSc3c4c([nH]c3C)cccc4** | **C27H24O2N3S1F1** |
| 29791344 | Life Chemicals Inc. | F0721-0768 | N-{[5-{[2-(3,4-dihydro-1(2H)-quinolinyl)-2-oxoethyl]sulfanyl}-4-(2-methoxyphenyl)-4H-1,2,4-triazol-3-yl]methyl}-4-[(dimethylamino)sulfonyl]benzamide | [S](=O)(=O)(N(C)C)c1ccc(cc1)C(=O)NCc2[n](c(nn2)SCC(=O)N4CCCc5c4cccc5)c3c(cccc3)OC | C30H32O5N6S2 |
| 30335515 | Life Chemicals Inc. | F0913-4612 | 3-{[4-(2,5-dimethylphenyl)-1-piperazinyl]carbonyl}-6-{[4-(4-fluorophenyl)-1-piperazinyl]sulfonyl}-4(1H)-quinolinone | Fc1ccc(cc1)N2CCN(CC2)[S](=O)(=O)c3cc4c(ncc(c4O)C(=O)N5CCN(CC5)c6c(ccc(c6)C)C)cc3 | C32H34O4N5S1F1 |
| 29793191 | Life Chemicals Inc. | F0737-0110 | N-[3-(1,3-benzothiazol-2-yl)-6-methyl-4,5,6,7-tetrahydro-1-benzothien-2-yl]-4-(2,3-dihydro-1H-indol-1-ylsulfonyl)benzamide | [S](=O)(=O)(N6CCc7c6cccc7)c1ccc(cc1)C(=O)Nc2[s]c3c(c2c4[s]c5c(n4)cccc5)CCC(C3)C | C31H27O3N3S3 |
| 29606176 | Labotest | LT01321967 | N-(2-benzoyl-4-bromophenyl)-4-[(6-chloro-4-phenyl-2-quinazolinyl)amino]benzamide | Brc1cc(c(cc1)NC(=O)c3ccc(cc3)Nc4nc5c(c(n4)c6ccccc6)cc(cc5)Cl)C(=O)c2ccccc2 | C34H22O2N4Cl1Br1 |
| 65382808 | Otava | 7006549 | 4-[4-(benzyloxy)phenyl]-3-(2-hydroxyphenyl)-5-(3-pyridinylmethyl)-4,5-dihydropyrrolo[3,4-c]pyrazol-6(1H)-one | [nH]1nc(c3c1C(=O)N(C3c5ccc(cc5)OCc6ccccc6)Cc4cnccc4)c2c(cccc2)O | C30H24O3N4 |
| 77016607 | Pharmeks LTD. | PHAR335882 | 4-(bis(3-hydroxy-5-methyl-1H-pyrazol-4-yl)methyl)phenyl 4-fluorobenzoate | Fc1ccc(cc1)C(=O)Oc2ccc(cc2)C(c4c([nH]nc4O)C)c3c([nH]nc3O)C | C22H19O4N4F1 |
| 458452454 | Pharmeks LTD. | PHAR363782 |  | N3(C(=CC(=O)C(C3=O)C(CC(=O)OC)c4[o]c(cc4)c5c(cccc5)C(=O)O)C)CCc1c2c([nH]c1)cccc2 | C31H28O7N2 |
| 34979766 | Pharmeks LTD. | PHAR083314 | 8-benzoyl-4-(4-bromobenzoyl)-2-(3,5-dichlorophenyl)-3a,4,9a,9b-tetrahydro-1H-pyrrolo[3,4-a]indolizine-1,3(2H)-dione | Brc1ccc(cc1)C(=O)C2N3C(C5C2C(=O)N(C5=O)c6cc(cc(c6)Cl)Cl)C=C(C=C3)C(=O)c4ccccc4 | C30H19O4N2Cl2Br1 |
| 29363082 | Pharmeks LTD. | PHAR089794 | (11beta)-11,17-dihydroxy-3,20-dioxopregna-1,4-dien-21-yl 4-{[2-(2,2-dimethyl-4-phenyltetrahydro-2H-pyran-4-yl)ethyl]amino}-4-oxobutanoate | N(CCC6(CC(OCC6)(C)C)c5ccccc5)C(=O)CCC(=O)OCC(=O)[C@@]1([C@@]2(C(C3C([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@H](C2)O)CC1)C)O | C40H53O8N1 |
| 50759467 | **Enamine** | **Z30131423** | **N-[2-(2-chlorophenyl)-2-(1H-indol-3-yl)ethyl]-2-(1H-indol-3-yl)acetamide (G2iH)** | **Clc1c(cccc1)C(CNC(=O)Cc4c5c([nH]c4)cccc5)c2c3c([nH]c2)cccc3** | **C26H22O1N3Cl1** |
| 95817411 | Enamine | Z109718458 | 5-[1,1'-biphenyl]-4-yl-N-[(4,6-dimethyl-2-oxo-1,2-dihydro-3-pyridinyl)methyl]-2-thiophenecarboxamide | [s]1c(ccc1C(=O)NCc4c(nc(cc4C)C)O)c2ccc(cc2)c3ccccc3 | C25H22O2N2S1 |
| 30206540 | Enamine | T0513-5507 | 2-({2-[2,5-dimethyl-1-(2-phenylethyl)-1H-pyrrol-3-yl]-2-oxoethyl}sulfanyl)-6-methyl-5-(4-methylphenyl)-3-phenylthieno[2,3-d]pyrimidin-4(3H)-one | [s]1c2c(c(c1C)c6ccc(cc6)C)C(=O)N(C(=N2)SCC(=O)c4c([n](c(c4)C)CCc5ccccc5)C)c3ccccc3 | C36H33O2N3S2 |
| 29399326 | Enamine | Z19304338 | N-(9-ethyl-9H-carbazol-3-yl)-2-{[5-(1H-indol-3-yl)-1,3,4-oxadiazol-2-yl]sulfanyl}acetamide | S(CC(=O)Nc4cc5c([n](c6c5cccc6)CC)cc4)c1nnc([o]1)c2c3c([nH]c2)cccc3 | C26H21O2N5S1 |
| 155920809 | Enamine | Z244415796 | 3-(1-{(2E)-3-[2-(4-fluorophenyl)-1,3-thiazol-4-yl]-2-propenoyl}-1,2,3,6-tetrahydro-4-pyridinyl)-1H-pyrrolo[2,3-b]pyridine | Fc1ccc(cc1)c2[s]cc(n2)\C=C\C(=O)N3CCC(=CC3)c4c5c([nH]c4)nccc5 | C24H19O1N4S1F1 |
| 27082796 | Enamine | T5603758 | N-(2-benzoyl-4-methylphenyl)-4-[(6-methyl-4-phenyl-2-quinazolinyl)amino]benzamide | N(c4ccc(cc4)C(=O)Nc5c(cc(cc5)C)C(=O)c6ccccc6)c1nc2c(c(n1)c3ccccc3)cc(cc2)C | C36H28O2N4 |
| 112921324 | Enamine | Z220595048 | N-(1-isoquinolinylmethyl)-4-[5-(4-methoxyphenyl)-3-phenyl-4,5-dihydro-1H-pyrazol-1-yl]-4-oxobutanamide | N3(NC(=CC3c5ccc(cc5)OC)c4ccccc4)C(=O)CCC(=O)NCc1nccc2c1cccc2 | C30H28O3N4 |
| 371582429 | Enamine | Z1446647643 | 3-[1-(3-fluorobenzoyl)-5-(4-fluorophenyl)-2,5-dihydro-1H-pyrazol-3-yl]-6-methyl-4-phenyl-2-quinolinol | Fc1cc(ccc1)C(=O)N2NC(=CC2c6ccc(cc6)F)c3c(nc4c(c3c5ccccc5)cc(cc4)C)O | C32H23O2N3F2 |
| 947324579 | Enamine | Z2858952890 |  | [s]1c(ccc1C(=O)O)CN(C5CC6(N(CC5)C(=O)OC(C)(C)C)CCCCC6)C(=O)OCC2c3c(cccc3)c4c2cccc4 | C36H42O6N2S1 |
| 113915710 | Enamine | Z234513220 | 3-{1-[(1,3-diphenyl-1H-pyrazol-5-yl)carbonyl]-1,2,3,6-tetrahydro-4-pyridinyl}-1H-pyrrolo[2,3-b]pyridine | [n]2(nc(cc2C(=O)N4CCC(=CC4)c5c6c([nH]c5)nccc6)c3ccccc3)c1ccccc1 | C28H23O1N5 |
| 388606908 | Enamine | Z1558581164 | N-(2-(1-(6-chloro-4-phenylquinazolin-2-yl)-5-(4-(dimethylamino)phenyl)-2,5-dihydro-1H-pyrazol-3-yl)phenyl)methanesulfonamide | [S](=O)(=O)(Nc1c(cccc1)C2=CC(N(N2)c4nc5c(c(n4)c6ccccc6)cc(cc5)Cl)c3ccc(cc3)N(C)C)C | C32H29O2N6Cl1S1 |
| 33510957 | Enamine | Z18699620 | 2-(1H-indol-3-yl)-2-oxoethyl 3-[(2-methyl-2,3-dihydro-1H-indol-1-yl)sulfonyl]benzoate | [S](=O)(=O)(N4C(Cc5c4cccc5)C)c1cc(ccc1)C(=O)OCC(=O)c2c3c([nH]c2)cccc3 | C26H22O5N2S1 |
| 118879125 | Enamine | Z243366928 | 2-[hexyl(4-phenyl-1,3-thiazol-2-yl)amino]-2-oxoethyl 6-(1H-1,2,4-triazol-1-yl)nicotinate | [s]1c(nc(c1)c4ccccc4)N(CCCCCC)C(=O)COC(=O)c2cnc(cc2)[n]3ncnc3 | C25H26O3N6S1 |
| 428762224 | Enamine | Z1891749033 |  | Clc1cc(ccc1)N2CCN(CC2)C(=O)c3ccc(cc3)Nc4nc5c(c(n4)c6ccc(cc6)Cl)cccc5 | C31H25O1N5Cl2 |
| 30846314 | Enamine | Z19316401 | methyl 4-{3-phenyl-1-[(4-quinazolinylsulfanyl)acetyl]-4,5-dihydro-1H-pyrazol-5-yl}phenyl ether | S(CC(=O)N3NC(=CC3c5ccc(cc5)OC)c4ccccc4)c1ncnc2c1cccc2 | C26H22O2N4S1 |
| 37807463 | Enamine | Z25492200 | 2-{[4-(3,4-dimethylphenyl)-1-phenyl-1H-imidazol-2-yl]sulfanyl}-1-(2-methyl-1H-indol-3-yl)ethanone | S(CC(=O)c4c5c([nH]c4C)cccc5)c1[n](cc(n1)c3cc(c(cc3)C)C)c2ccccc2 | C28H25O1N3S1 |
| 29606134 | Enamine | T5605033 | N-(2-benzoyl-4-bromophenyl)-3-[(6-bromo-4-phenyl-2-quinazolinyl)amino]benzamide | Brc1cc(c(cc1)NC(=O)c3cc(ccc3)Nc4nc5c(c(n4)c6ccccc6)cc(cc5)Br)C(=O)c2ccccc2 | C34H22O2N4Br2 |
| 29116573 | Enamine | T0513-8000 | 2-({2-[2,5-dimethyl-1-(2-phenylethyl)-1H-pyrrol-3-yl]-2-oxoethyl}sulfanyl)-3,6-diphenylthieno[2,3-d]pyrimidin-4(3H)-one | [s]1c2c(cc1c6ccccc6)C(=O)N(C(=N2)SCC(=O)c4c([n](c(c4)C)CCc5ccccc5)C)c3ccccc3 | C34H29O2N3S2 |
| 388606909 | Enamine | Z1558581147 | 6-chloro-2-(5-(4-ethoxyphenyl)-3-(m-tolyl)-2,5-dihydro-1H-pyrazol-1-yl)-4-phenylquinazoline | Clc1cc2c(nc(nc2c6ccccc6)N3NC(=CC3c5ccc(cc5)OCC)c4cc(ccc4)C)cc1 | C32H27O1N4Cl1 |
| 406070290 | Enamine | EN300-117175 | 4-(N-(4-cyclohexylbenzyl)-2-((2,3,4,5,6-pentafluoro-N-methylphenyl)sulfonamido)acetamido)-2-hydroxybenzoic acid | Fc1c(c(c(c(c1F)F)[S](=O)(=O)N(CC(=O)N(Cc3ccc(cc3)C4CCCCC4)c2cc(c(cc2)C(=O)O)O)C)F)F | C29H27O6N2S1F5 |
| 28678113 | Vitas-M Laboratory, Ltd. | STK269113 | 2-[1,1'-biphenyl]-4-yl-2-oxoethyl 2-[1,1'-biphenyl]-4-yl-6-methyl-4-quinolinecarboxylate | n1c2c(c(cc1c5ccc(cc5)c6ccccc6)C(=O)OCC(=O)c3ccc(cc3)c4ccccc4)cc(cc2)C | C37H27O3N1 |
| 34885276 | Vitas-M Laboratory, Ltd. | STK296037 | 1,3-dioxo-2-{3-[(3-phenoxyanilino)carbonyl]phenyl}-N-(3-phenoxyphenyl)-5-isoindolinecarboxamide | N4(C(=O)c5c(ccc(c5)C(=O)Nc6cc(ccc6)Oc7ccccc7)C4=O)c1cc(ccc1)C(=O)Nc2cc(ccc2)Oc3ccccc3 | C40H27O6N3 |
| 36012691 | Vitas-M Laboratory, Ltd. | STK279195 | 4,4'-((3-bromo-4-(naphthalen-1-ylmethoxy)phenyl)methylene)bis(3-methyl-1H-pyrazol-5-ol) | Brc1c(ccc(c1)C(c5c([nH]nc5C)O)c4c([nH]nc4C)O)OCc2c3c(ccc2)cccc3 | C26H23O3N4Br1 |
| 63176574 | Vitas-M Laboratory, Ltd. | STK313895 | 2-[3,5-bis(3,4-dimethoxyphenyl)-1H-pyrazol-1-yl]-4-(2-thienyl)-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5[s]ccc5)[n]2nc(cc2c4cc(c(cc4)OC)OC)c3cc(c(cc3)OC)OC | C28H23O4N4S1F3 |
| 63176613 | Vitas-M Laboratory, Ltd. | STK313915 | 2-[3,5-bis(3,4-dimethoxyphenyl)-4-ethyl-1H-pyrazol-1-yl]-4-(4-fluorophenyl)-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5ccc(cc5)F)[n]2nc(c(c2c4cc(c(cc4)OC)OC)CC)c3cc(c(cc3)OC)OC | C32H28O4N4F4 |
| 63176630 | Vitas-M Laboratory, Ltd. | STK313922 | 2-[3,5-bis(3,4-dimethoxyphenyl)-4-ethyl-1H-pyrazol-1-yl]-4-phenyl-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5ccccc5)[n]2nc(c(c2c4cc(c(cc4)OC)OC)CC)c3cc(c(cc3)OC)OC | C32H29O4N4F3 |
| 63178383 | Vitas-M Laboratory, Ltd. | STK314253 | 2-[3,5-bis(3,4-dimethoxyphenyl)-4-methyl-1H-pyrazol-1-yl]-4-(3-methoxyphenyl)-6-(trifluoromethyl)pyrimidine | FC(F)(F)c1nc(nc(c1)c5cc(ccc5)OC)[n]2nc(c(c2c4cc(c(cc4)OC)OC)C)c3cc(c(cc3)OC)OC | C32H29O5N4F3 |
| 28394210 | Vitas-M Laboratory, Ltd. | STK038146 | N-benzyl-N-(4,5-diphenyl-1,3-thiazol-2-yl)-2-[(4-hydroxy-6-phenyl-2-pyrimidinyl)sulfanyl]acetamide | [s]1c(nc(c1c6ccccc6)c5ccccc5)N(Cc4ccccc4)C(=O)CSc2nc(cc(n2)c3ccccc3)O | C34H26O2N4S2 |
| 29999180 | Vitas-M Laboratory, Ltd. | STK053875 | 2-(4-tert-butylphenoxy)-N-(2-{[(4-tert-butylphenoxy)acetyl]anilino}ethyl)-N-phenylacetamide | N(CCN(c4ccccc4)C(=O)COc3ccc(cc3)C(C)(C)C)(c2ccccc2)C(=O)COc1ccc(cc1)C(C)(C)C | C38H44O4N2 |
| 28414872 | Vitas-M Laboratory, Ltd. | STK392050 | 1-(9H-fluoren-2-yl)-2-{[5-(2-furyl)-4-phenyl-4H-1,2,4-triazol-3-yl]sulfanyl}ethanone | S(CC(=O)c4cc5c(cc4)c6c(cccc6)C5)c1[n](c(nn1)c3[o]ccc3)c2ccccc2 | C27H19O2N3S1 |
| 27806338 | Vitas-M Laboratory, Ltd. | STK043440 | N-[1-(4-methoxybenzoyl)-2-methyl-1,2,3,4-tetrahydro-4-quinolinyl]-4-pentyl-N-phenylbenzamide | N2(C(CC(c5c2cccc5)N(c4ccccc4)C(=O)c3ccc(cc3)CCCCC)C)C(=O)c1ccc(cc1)OC | C36H38O3N2 |
| 39750226 | Vitas-M Laboratory, Ltd. | STL052698 | 9a-((E)-2-{4-[3-(3-chloro-4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]phenyl}ethenyl)-9,9-dimethyl-9,9a-dihydro-1H-imidazo[1,2-a]indol-2(3H)-one | Clc1c(ccc(c1)c2n[n](cc2c4ccc(cc4)\C=C\C65N(CC(=O)N6)c7c(cccc7)C5(C)C)c3ccccc3)OC | C36H31O2N4Cl1 |
| 158573473 | Vitas-M Laboratory, Ltd. | STK636849 | N-{2-[5-(benzyloxy)-1H-indol-3-yl]ethyl}-3-(4-pyridinyl)-1,2,4-oxadiazole-5-carboxamide | [nH]1c2c(c(c1)CCNC(=O)c4nc(n[o]4)c5ccncc5)cc(cc2)OCc3ccccc3 | C25H21O3N5 |
| 31278512 | Vitas-M Laboratory, Ltd. | STK681999 | 2-{[4-(1-adamantyl)-1-piperazinyl]carbonyl}-5,7-diphenylpyrazolo[1,5-a]pyrimidine | [n]21nc(cc2N=C(C=C1c8ccccc8)c7ccccc7)C(=O)N3CCN(CC3)C54CC6CC(C5)CC(C4)C6 | C33H35O1N5 |
| 47635094 | Vitas-M Laboratory, Ltd. | STK686647 | 4-(4-chlorophenyl)-1-(4-isopropylphenyl)-N-(3-methoxyphenyl)-5,6,7,8-tetrahydro-2a,4a-diazacyclopenta[cd]azulene-2-carboxamide | Clc1ccc(cc1)C2=C[n]3c4c(c(c3C(=O)Nc6cc(ccc6)OC)c5ccc(cc5)C(C)C)CCCCN42 | C33H32O2N3Cl1 |
| 47635071 | Vitas-M Laboratory, Ltd. | STK782131 | 4-(3,4-dimethylphenyl)-N-(4-methoxyphenyl)-1-(4-methylphenyl)-5,6,7,8-tetrahydro-2a,4a-diazacyclopenta[cd]azulene-2-carboxamide | [n]21c3c(c(c2C(=O)Nc6ccc(cc6)OC)c5ccc(cc5)C)CCCCN3C(=C1)c4cc(c(cc4)C)C | C33H33O2N3 |
| 27366974 | Vitas-M Laboratory, Ltd. | STK528173 | ethyl 3-{[(1-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]-3,4-dihydro-2(1H)-isoquinolinyl)acetyl]amino}-5-methoxy-1H-indole-2-carboxylate | [nH]1c2c(c(c1C(=O)OCC)NC(=O)CN3CCc4c(cccc4)C3CN5C(=O)c6c(cccc6)C5=O)cc(cc2)OC | C32H30O6N4 |
| 27546167 | Vitas-M Laboratory, Ltd. | STK717513 | 4-ethyl-2-[4-(4-methyl-1,3-thiazol-2-yl)-1H-pyrazol-3-yl]-5-(1-naphthylmethoxy)phenol | [s]1c(nc(c1)C)c2c[nH]nc2c3c(cc(c(c3)CC)OCc4c5c(ccc4)cccc5)O | C26H23O2N3S1 |
| 27304178 | Vitas-M Laboratory, Ltd. | STK526378 | ethyl 6-amino-2-({[4-(4-chlorophenyl)-3-cyano-6-(2-thienyl)-2-pyridinyl]sulfanyl}methyl)-5-cyano-4-(3-pyridinyl)-4H-pyran-3-carboxylate | [s]1c(ccc1)c2nc(c(c(c2)c5ccc(cc5)Cl)C#N)SCC3=C(C(C(=C(O3)N)C#N)c4cnccc4)C(=O)OCC | C31H22O3N5Cl1S2 |
| 27348341 | Vitas-M Laboratory, Ltd. | STK528432 | N-(4-fluorobenzyl)-N'-(1-naphthyl)-N-[4-(9H-thioxanthen-9-yl)phenyl]urea | Fc1ccc(cc1)CN(c4ccc(cc4)C5c6c(cccc6)Sc7c5cccc7)C(=O)Nc2c3c(ccc2)cccc3 | C37H27O1N2S1F1 |
| 27558683 | Vitas-M Laboratory, Ltd. | STK532121 | 4-(3-methoxyphenyl)-1-(phenethylthio)-4H-spiro[benzo[h][1,2,4]triazolo[4,3-a]quinazoline-6,1'-cyclohexan]-5(7H)-one | S(CCc7ccccc7)c1[n]2c(nn1)N(C(=O)C4=C2c5c(cccc5)CC64CCCCC6)c3cc(ccc3)OC | C33H32O2N4S1 |
| 48658033 | Vitas-M Laboratory, Ltd. | STK597215 | 4-(3,4-dimethylphenyl)-1-(4-ethylphenyl)-N-(3-methylphenyl)-5,6,7,8-tetrahydro-2a,4a-diazacyclopenta[cd]azulene-2-carboxamide | [n]21c3c(c(c2C(=O)Nc6cc(ccc6)C)c5ccc(cc5)CC)CCCCN3C(=C1)c4cc(c(cc4)C)C | C34H35O1N3 |
| 28869109 | Vitas-M Laboratory, Ltd. | STK065789 | 4-[bis(5-hydroxy-3-methyl-1H-pyrazol-4-yl)methyl]-2-ethoxyphenyl 2-chlorobenzoate | Clc1c(cccc1)C(=O)Oc2c(cc(cc2)C(c4c([nH]nc4C)O)c3c([nH]nc3C)O)OCC | C24H23O5N4Cl1 |
| 27462543 | Vitas-M Laboratory, Ltd. | STK084760 | N-{2-methyl-1-[(2-naphthyloxy)acetyl]-1,2,3,4-tetrahydro-4-quinolinyl}-2-(2-naphthyloxy)-N-phenylacetamide | N3(C(CC(c7c3cccc7)N(c6ccccc6)C(=O)COc4cc5c(cc4)cccc5)C)C(=O)COc1cc2c(cc1)cccc2 | C40H34O4N2 |
| 30738164 | ChemDiv, Inc | 5867-4076 | N-[3-(1,3-benzothiazol-2-yl)phenyl]-3-[(5-phenyl[1,3]thiazolo[2,3-c][1,2,4]triazol-3-yl)sulfanyl]propanamide | S1c2[n](c(nn2)SCCC(=O)Nc4cc(ccc4)c5[s]c6c(n5)cccc6)C(=C1)c3ccccc3 | C26H19O1N5S3 |
| 40756209 | ChemDiv, Inc | C797-0522 | 1-[1-(2,5-dimethylbenzyl)-1H-benzimidazol-2-yl]-N-[2-(1H-indol-3-yl)ethyl]-4-piperidinecarboxamide | N4(CCC(CC4)C(=O)NCCc5c6c([nH]c5)cccc6)c1[n](c3c(n1)cccc3)Cc2c(ccc(c2)C)C | C32H35O1N5 |
| 40768166 | ChemDiv, Inc | C797-0834 | 4-({[3-(4-methoxybenzyl)-3H-imidazo[4,5-c]pyridin-2-yl]sulfanyl}methyl)-N-(4-methylbenzyl)benzamide | S(Cc4ccc(cc4)C(=O)NCc5ccc(cc5)C)c1[n](c3c(n1)ccnc3)Cc2ccc(cc2)OC | C30H28O2N4S1 |
| 61639904 | ChemDiv, Inc | C878-1784 | 3-[4-(2,3-dihydro-1H-indol-1-ylcarbonyl)benzyl]-2-[(4-methylbenzyl)sulfanyl]-3H-imidazo[4,5-c]pyridine | S(Cc6ccc(cc6)C)c1[n](c5c(n1)ccnc5)Cc2ccc(cc2)C(=O)N3CCc4c3cccc4 | C30H26O1N4S1 |
| 61602513 | ChemDiv, Inc | D016-1208 | 1-[5-{3-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-2-hydroxypropoxy}-2-methyl-1-(4-methylphenyl)-1H-indol-3-yl]ethanone | Clc1cc(c(cc1)C)N2CCN(CC2)CC(O)COc3cc4c([n](c(c4C(=O)C)C)c5ccc(cc5)C)cc3 | C32H36O3N3Cl1 |
| 30295813 | ChemDiv, Inc | C096-0092 | 2-(5-{[4-(2-methoxyphenyl)-1-piperazinyl]sulfonyl}-6-methyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)-N-methyl-N-[2-(2-pyridinyl)ethyl]acetamide | [S](=O)(=O)(N4CCN(CC4)c5c(cccc5)OC)c1c2c([s]c1C)N=CN(C2=O)CC(=O)N(CCc3ncccc3)C | C28H32O5N6S2 |
| 64190611 | ChemDiv, Inc | C794-1611 | 1-(5-{2-[(4-ethoxyanilino)methyl]-1H-pyrrol-1-yl}-1,3,4-thiadiazol-2-yl)-N-[2-(1H-indol-3-yl)ethyl]-4-piperidinecarboxamide | [s]1c(nnc1N4CCC(CC4)C(=O)NCCc5c6c([nH]c5)cccc6)[n]2c(ccc2)CNc3ccc(cc3)OCC | C31H35O2N7S1 |
| 111269525 | ChemDiv, Inc | F154-0105 | 4-({2-[(4-chlorobenzyl)sulfanyl]-3H-imidazo[4,5-c]pyridin-3-yl}methyl)-N-cyclooctylbenzamide | S(Cc5ccc(cc5)Cl)c1[n](c4c(n1)ccnc4)Cc2ccc(cc2)C(=O)NC3CCCCCCC3 | C29H31O1N4Cl1S1 |
| 111269527 | ChemDiv, Inc | F154-0109 | 4-({2-[(2-chloro-4-fluorobenzyl)sulfanyl]-3H-imidazo[4,5-c]pyridin-3-yl}methyl)-N-cyclooctylbenzamide | Fc1cc(c(cc1)CSc2[n](c5c(n2)ccnc5)Cc3ccc(cc3)C(=O)NC4CCCCCCC4)Cl | C29H30O1N4Cl1S1F1 |
| 111269549 | ChemDiv, Inc | F154-0183 | 4-chlorobenzyl 3-[4-(2,3-dihydro-1H-indol-1-ylcarbonyl)benzyl]-3H-imidazo[4,5-c]pyridin-2-yl sulfide | S(Cc6ccc(cc6)Cl)c1[n](c5c(n1)ccnc5)Cc2ccc(cc2)C(=O)N3CCc4c3cccc4 | C29H23O1N4Cl1S1 |
| 111269574 | ChemDiv, Inc | F154-0254 | 4-({2-[(3-chlorobenzyl)sulfanyl]-3H-imidazo[4,5-c]pyridin-3-yl}methyl)-N-(2,4-dimethylphenyl)benzamide | S(Cc5cc(ccc5)Cl)c1[n](c4c(n1)ccnc4)Cc2ccc(cc2)C(=O)Nc3c(cc(cc3)C)C | C29H25O1N4Cl1S1 |
| 111269732 | ChemDiv, Inc | F154-0645 | N-(2-methylbenzyl)-4-[(2-{[3-(trifluoromethyl)benzyl]sulfanyl}-3H-imidazo[4,5-c]pyridin-3-yl)methyl]benzamide | FC(F)(F)c1cc(ccc1)CSc2[n](c5c(n2)ccnc5)Cc3ccc(cc3)C(=O)NCc4c(cccc4)C | C30H25O1N4S1F3 |
| 182707700 | ChemDiv, Inc | G430-1653 | (1-(2-(3,4-dimethylphenyl)pyrazolo[1,5-a]pyrazin-4-yl)piperidin-3-yl)(4-phenylpiperazin-1-yl)methanone | [n]21nc(cc2C(=NC=C1)N4CC(CCC4)C(=O)N5CCN(CC5)c6ccccc6)c3cc(c(cc3)C)C | C30H34O1N6 |
| 30335059 | ChemDiv, Inc | K781-0391 | 3-(4-(tert-butyl)benzamido)-N-(3-chlorobenzyl)-4-(8-oxo-1,5,6,8-tetrahydro-2H-1,5-methanopyrido[1,2-a][1,5]diazocin-3(4H)-yl)benzamide | Clc1cc(ccc1)CNC(=O)c2cc(c(cc2)N4CC5CN6C(=CC=CC6=O)C(C4)C5)NC(=O)c3ccc(cc3)C(C)(C)C | C36H37O3N4Cl1 |
| 30335319 | ChemDiv, Inc | K781-1690 | ethyl 4-(4-(8-oxo-1,5,6,8-tetrahydro-2H-1,5-methanopyrido[1,2-a][1,5]diazocin-3(4H)-yl)-3-(3-(trifluoromethyl)benzamido)benzamido)piperidine-1-carboxylate | FC(F)(F)c1cc(ccc1)C(=O)Nc2c(ccc(c2)C(=O)NC6CCN(CC6)C(=O)OCC)N3CC4CN5C(=CC=CC5=O)C(C3)C4 | C34H36O5N5F3 |
| 30335447 | ChemDiv, Inc | K781-1931 | N-(5-(4-benzylpiperidine-1-carbonyl)-2-(8-oxo-1,5,6,8-tetrahydro-2H-1,5-methanopyrido[1,2-a][1,5]diazocin-3(4H)-yl)phenyl)-3-(trifluoromethyl)benzamide | FC(F)(F)c1cc(ccc1)C(=O)Nc2c(ccc(c2)C(=O)N6CCC(CC6)Cc7ccccc7)N3CC4CN5C(=CC=CC5=O)C(C3)C4 | C38H37O3N4F3 |
| 34713223 | **ChemDiv, Inc** | **K788-1241** | **N-(4-isopropylphenyl)-3-{[4-(2-methoxyphenyl)-1-piperazinyl]carbonyl}-4-oxo-1,4-dihydro-6-quinolinesulfonamide (G2iG)** | **[S](=O)(=O)(Nc5ccc(cc5)C(C)C)c1cc2c(ncc(c2O)C(=O)N3CCN(CC3)c4c(cccc4)OC)cc1** | **C30H32O5N4S1** |
| 111278730 | **ChemDiv, Inc** | **F228-0561** | **1-(5,6-dimethylfuro[2,3-d]pyrimidin-4-yl)-N-[2-(5-methyl-1H-indol-3-yl)ethyl]-3-piperidinecarboxamide (G2iK)** | **N3(CC(CCC3)C(=O)NCCc4c5c([nH]c4)ccc(c5)C)c1ncnc2[o]c(c(c21)C)C** | **C25H29O2N5** |
| 185953192 | ChemDiv, Inc | G435-0034 | (4-(2,5-dimethylphenyl)piperazin-1-yl)(1-(2-phenylpyrazolo[1,5-a]pyrazin-4-yl)piperidin-4-yl)methanone | [n]21nc(cc2C(=NC=C1)N4CCC(CC4)C(=O)N5CCN(CC5)c6c(ccc(c6)C)C)c3ccccc3 | C30H34O1N6 |
| 237221619 | ChemDiv, Inc | G435-0553 | (1-(2-(2,4-dimethylphenyl)pyrazolo[1,5-a]pyrazin-4-yl)piperidin-4-yl)(4-(2-methoxyphenyl)piperazin-1-yl)methanone | [n]21nc(cc2C(=NC=C1)N4CCC(CC4)C(=O)N5CCN(CC5)c6c(cccc6)OC)c3c(cc(cc3)C)C | C31H36O2N6 |
| 237187975 | ChemDiv, Inc | L390-0507 | N-(2-(1H-indol-3-yl)ethyl)-7-(3,4-dimethylphenyl)pyrazolo[1,5-a]pyrimidine-3-carboxamide | [n]21ncc(c2N=CC=C1c5cc(c(cc5)C)C)C(=O)NCCc3c4c([nH]c3)cccc4 | C25H23O1N5 |
| 237189315 | ChemDiv, Inc | L483-0680 | 4-(4-(4-benzylpiperidine-1-carbonyl)piperidin-1-yl)-6-ethoxyquinoline-3-carbonitrile | N3(CCC(CC3)C(=O)N4CCC(CC4)Cc5ccccc5)c1c2c(ncc1C#N)ccc(c2)OCC | C30H34O2N4 |
| 90394475 | ChemDiv, Inc | V005-9064 | 6-methoxy-2-[4-(trifluoromethoxy)benzoyl]-1-{5-[2-(trifluoromethyl)phenyl]-2-furyl}-2,3,4,9-tetrahydro-1H-beta-carboline | FC(F)(F)Oc1ccc(cc1)C(=O)N2CCc3c4c([nH]c3C2c5[o]c(cc5)c6c(cccc6)C(F)(F)F)ccc(c4)OC | C31H22O4N2F6 |
| 90317639 | ChemDiv, Inc | V007-0482 | 8-(4-{[(2-tert-butylphenyl)sulfanyl]methyl}benzoyl)-3-(2-isopropylphenoxy)-8-azabicyclo[3.2.1]octane | S(Cc2ccc(cc2)C(=O)N3C4CCC3CC(C4)Oc5c(cccc5)C(C)C)c1c(cccc1)C(C)(C)C | C34H41O2N1S1 |
| 121116441 | ChemDiv, Inc | V003-6571 | 4-fluoro-N-isobutyl-N-[2-oxo-2-({4-phenyl-1-[4-(trifluoromethyl)phenyl]-1H-imidazol-2-yl}amino)ethyl]benzamide | FC(F)(F)c1ccc(cc1)[n]2c(nc(c2)c4ccccc4)NC(=O)CN(CC(C)C)C(=O)c3ccc(cc3)F | C29H26O2N4F4 |
| 121285335 | ChemDiv, Inc | V007-7958 | 6-benzyl-4-{4-[(4-tert-butylphenyl)sulfonyl]-1-piperazinyl}-1-(3-chlorophenyl)-1H-pyrazolo[3,4-d]pyrimidine | [S](=O)(=O)(N2CCN(CC2)c3nc(nc5[n](ncc53)c6cc(ccc6)Cl)Cc4ccccc4)c1ccc(cc1)C(C)(C)C | C32H33O2N6Cl1S1 |
| 234347154 | ChemDiv, Inc | V008-7832 | N,3-bis(4-fluorobenzyl)-8-(trifluoromethyl)-2,3,4,4a,5,6-hexahydro-1H-pyrazino[1,2-a]quinoline-5-carboxamide | FC(F)(F)c1cc2c(cc1)N3C(CN(CC3)Cc5ccc(cc5)F)C(C2)C(=O)NCc4ccc(cc4)F | C28H26O1N3F5 |
| 49282656 | ChemDiv, Inc | V009-0402 | N-(4-tert-butylbenzyl)-2-[(4-chlorobenzyl)(cyclopropyl)amino]-N-[2-(1H-indol-3-yl)ethyl]acetamide | Clc1ccc(cc1)CN(C5CC5)CC(=O)N(CCc3c4c([nH]c3)cccc4)Cc2ccc(cc2)C(C)(C)C | C33H38O1N3Cl1 |
| 154638968 | ChemDiv, Inc | V009-3943 | 2-{[(4-tert-butylbenzyl)(3,3-diphenylpropyl)amino]methyl}-N-(2-furylmethyl)-1,3-thiazole-4-carboxamide | [s]1c(nc(c1)C(=O)NCc5[o]ccc5)CN(CCC(c4ccccc4)c3ccccc3)Cc2ccc(cc2)C(C)(C)C | C36H39O2N3S1 |
| 90386568 | ChemDiv, Inc | V011-3487 | 1-({1-[3',5'-bis(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1H-imidazol-5-yl}carbonyl)-4-(4-tert-butylbenzyl)piperidine | FC(F)(F)c1cc(cc(c1)c2ccc(cc2)[n]3cncc3C(=O)N4CCC(CC4)Cc5ccc(cc5)C(C)(C)C)C(F)(F)F | C34H33O1N3F6 |
| 154930032 | ChemDiv, Inc | V014-0753 | 2-[[3-(benzyloxy)-2-hydroxypropyl](butyl)amino]-N-(4-tert-butylbenzyl)-N-[2-(1H-indol-3-yl)ethyl]acetamide | [nH]1c2c(c(c1)CCN(Cc4ccc(cc4)C(C)(C)C)C(=O)CN(CC(O)COCc3ccccc3)CCCC)cccc2 | C37H49O3N3 |
| 121204288 | ChemDiv, Inc | V014-1570 | 2-methyl-N-(2-{[1-(4-methylphenyl)-4-phenyl-1H-imidazol-2-yl]amino}-2-oxoethyl)-N-[2-(4-morpholinyl)ethyl]benzamide | [n]2(c(nc(c2)c5ccccc5)NC(=O)CN(CCN4CCOCC4)C(=O)c3c(cccc3)C)c1ccc(cc1)C | C32H35O3N5 |
| 234333487 | ChemDiv, Inc | V014-8901 | 1-benzhydryl-4-{[1-(2,5-dimethylphenyl)-3-(3-methoxyphenyl)-1H-pyrazol-5-yl]carbonyl}piperazine | [n]2(nc(cc2C(=O)N4CCN(CC4)C(c6ccccc6)c5ccccc5)c3cc(ccc3)OC)c1c(ccc(c1)C)C | C36H36O2N4 |
| 372736109 | ChemDiv, Inc | V015-4774 | (4-(2-fluorophenyl)piperazin-1-yl)(4-((5-isopropyl-4-p-tolyl-4H-1,2,4-triazol-3-ylthio)methyl)phenyl)methanone | Fc1c(cccc1)N2CCN(CC2)C(=O)c3ccc(cc3)CSc4[n](c(nn4)C(C)C)c5ccc(cc5)C | C30H32O1N5S1F1 |
| 154643154 | ChemDiv, Inc | V020-4178 | 4-fluoro-N-isobutyl-N-({1-[3-(trifluoromethyl)benzyl]-4-[3-(trifluoromethyl)phenyl]-3-pyrrolidinyl}methyl)benzamide | FC(F)(F)c1cc(ccc1)C2CN(CC2CN(CC(C)C)C(=O)c4ccc(cc4)F)Cc3cc(ccc3)C(F)(F)F | C31H31O1N2F7 |
| 344693638 | ChemDiv, Inc | V025-8637 | 3-({4-[(4-fluorophenyl)acetyl]-1-piperazinyl}methyl)-6-(3-methylphenyl)-2-phenylimidazo[1,2-a]pyridine | Fc1ccc(cc1)CC(=O)N2CCN(CC2)Cc3[n]4c(nc3c6ccccc6)C=CC(=C4)c5cc(ccc5)C | C33H31O1N4F1 |
| 121097081 | **ChemDiv, Inc** | **V025-9097** | **N-benzyl-N-(2-{[4-(4-chlorophenyl)-1-(3,4-dimethoxyphenyl)-1H-imidazol-2-yl]amino}-2-oxoethyl)-4-methylbenzamide (G2iB)** | **Clc1ccc(cc1)c2nc([n](c2)c5cc(c(cc5)OC)OC)NC(=O)CN(Cc4ccccc4)C(=O)c3ccc(cc3)C** | **C34H31O4N4Cl1** |
| 344695929 | ChemDiv, Inc | V026-6880 | 2-[(4-{[2-(4-chlorophenyl)-6-(3-methylphenyl)imidazo[1,2-a]pyridin-3-yl]methyl}-1-piperazinyl)sulfonyl]benzonitrile | [S](=O)(=O)(N2CCN(CC2)Cc3[n]4c(nc3c6ccc(cc6)Cl)C=CC(=C4)c5cc(ccc5)C)c1c(cccc1)C#N | C32H28O2N5Cl1S1 |
| 344693629 | ChemDiv, Inc | V027-0500 | 2-(4-methylphenyl)-3-({4-[4-(trifluoromethyl)benzoyl]-1-piperazinyl}methyl)-6-[3-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridine | FC(F)(F)c1cc(ccc1)C2=C[n]3c(nc(c3CN5CCN(CC5)C(=O)c6ccc(cc6)C(F)(F)F)c4ccc(cc4)C)C=C2 | C34H28O1N4F6 |
| 344693828 | ChemDiv, Inc | V027-0530 | 6-(3-ethoxyphenyl)-3-{[4-(3-fluorobenzoyl)-1-piperazinyl]methyl}-2-(4-methylphenyl)imidazo[1,2-a]pyridine | Fc1cc(ccc1)C(=O)N2CCN(CC2)Cc3[n]4c(nc3c6ccc(cc6)C)C=CC(=C4)c5cc(ccc5)OCC | C34H33O2N4F1 |
| 344693645 | ChemDiv, Inc | V027-1389 | 3-({4-[(4-fluorophenyl)acetyl]-1-piperazinyl}methyl)-2-(3-methoxyphenyl)-6-[3-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridine | FC(F)(F)c1cc(ccc1)C2=C[n]3c(nc(c3CN5CCN(CC5)C(=O)Cc6ccc(cc6)F)c4cc(ccc4)OC)C=C2 | C34H30O2N4F4 |
| 344693525 | ChemDiv, Inc | V027-1402 | 6-(1-benzothien-2-yl)-2-(4-chlorophenyl)-3-[(4-{[3-(trifluoromethyl)phenyl]sulfonyl}-1-piperazinyl)methyl]imidazo[1,2-a]pyridine | FC(F)(F)c1cc(ccc1)[S](=O)(=O)N2CCN(CC2)Cc3[n]4c(nc3c7ccc(cc7)Cl)C=CC(=C4)c5[s]c6c(c5)cccc6 | C33H26O2N4Cl1S2F3 |
| 154821145 | ChemDiv, Inc | V027-1461 | 2-(4-chlorophenyl)-3-({4-[(4-fluorophenyl)sulfonyl]-1-piperazinyl}methyl)-6-phenylimidazo[1,2-a]pyridine | Fc1ccc(cc1)[S](=O)(=O)N2CCN(CC2)Cc3[n]4c(nc3c6ccc(cc6)Cl)C=CC(=C4)c5ccccc5 | C30H26O2N4Cl1S1F1 |
| 344693835 | ChemDiv, Inc | V027-4749 | 4-(6-(1-benzothien-2-yl)-3-{[4-(3-fluorobenzoyl)-1-piperazinyl]methyl}imidazo[1,2-a]pyridin-2-yl)phenyl methyl ether | Fc1cc(ccc1)C(=O)N2CCN(CC2)Cc3[n]4c(nc3c7ccc(cc7)OC)C=CC(=C4)c5[s]c6c(c5)cccc6 | C34H29O2N4S1F1 |
| 90368846 | ChemDiv, Inc | V027-7169 | 1-(diphenylacetyl)-4-(3,5-diphenyl-1H-pyrazol-1-yl)piperidine | [n]4(nc(cc4c6ccccc6)c5ccccc5)C1CCN(CC1)C(=O)C(c3ccccc3)c2ccccc2 | C34H31O1N3 |
| 344696025 | ChemDiv, Inc | V029-3339 | 6-(3-ethoxyphenyl)-2-(4-fluorophenyl)-3-({4-[(4-fluorophenyl)sulfonyl]-1-piperazinyl}methyl)imidazo[1,2-a]pyridine | Fc1ccc(cc1)[S](=O)(=O)N2CCN(CC2)Cc3[n]4c(nc3c6ccc(cc6)F)C=CC(=C4)c5cc(ccc5)OCC | C32H30O3N4S1F2 |
| 332647939 | ChemDiv, Inc | V029-3540 | 3-[4-(benzyloxy)phenyl]-3-[1-(4-fluorobenzyl)-1H-indol-3-yl]-N-[2-(2-pyridinyl)ethyl]propanamide | Fc1ccc(cc1)C[n]2c3c(c(c2)C(CC(=O)NCCc6ncccc6)c4ccc(cc4)OCc5ccccc5)cccc3 | C38H34O2N3F1 |
| 344693512 | ChemDiv, Inc | V029-8627 | 3-{[4-(4-tert-butylbenzoyl)-1-piperazinyl]methyl}-6-(2,5-dimethylphenyl)-2-phenylimidazo[1,2-a]pyridine | [n]21c(nc(c2CN5CCN(CC5)C(=O)c6ccc(cc6)C(C)(C)C)c4ccccc4)C=CC(=C1)c3c(ccc(c3)C)C | C37H40O1N4 |
| 154819933 | ChemDiv, Inc | V029-9895 | 8-[(4-{[2-(4-chlorophenyl)-6-phenylimidazo[1,2-a]pyridin-3-yl]methyl}-1-piperazinyl)sulfonyl]quinoline | [S](=O)(=O)(N3CCN(CC3)Cc4[n]5c(nc4c7ccc(cc7)Cl)C=CC(=C5)c6ccccc6)c1c2ncccc2ccc1 | C33H28O2N5Cl1S1 |
| 332651912 | **ChemDiv, Inc** | **V030-0484** | **3-(5-chloro-1H-indol-3-yl)-3-[3-(4-chlorophenoxy)phenyl]-N-[2-(4-morpholinyl)ethyl]propenamide (G2iI)** | **Clc1ccc(cc1)Oc2cc(ccc2)C(CC(=O)NCCN5CCOCC5)c3c4c([nH]c3)ccc(c4)Cl** | **C29H29O3N3Cl2** |
| 372880764 | ChemDiv, Inc | V030-1419 | (3-((4-(4-fluorophenyl)-5-(furan-2-yl)-4H-1,2,4-triazol-3-ylthio)methyl)phenyl)(4-(2-fluorophenyl)piperazin-1-yl)methanone | Fc1c(cccc1)N2CCN(CC2)C(=O)c3cc(ccc3)CSc4[n](c(nn4)c6[o]ccc6)c5ccc(cc5)F | C30H25O2N5S1F2 |
| 344693633 | ChemDiv, Inc | V030-2174 | 6-(1-benzothien-2-yl)-2-(4-chlorophenyl)-3-({4-[4-(trifluoromethyl)benzoyl]-1-piperazinyl}methyl)imidazo[1,2-a]pyridine | FC(F)(F)c1ccc(cc1)C(=O)N2CCN(CC2)Cc3[n]4c(nc3c7ccc(cc7)Cl)C=CC(=C4)c5[s]c6c(c5)cccc6 | C34H26O1N4Cl1S1F3 |
| 344696239 | ChemDiv, Inc | V030-2573 | 1-{4-[3-({4-[(2-chloro-5-nitrophenyl)sulfonyl]-1-piperazinyl}methyl)-2-phenylimidazo[1,2-a]pyridin-6-yl]phenyl}ethanone | [S](=O)(=O)(N2CCN(CC2)Cc3[n]4c(nc3c6ccccc6)C=CC(=C4)c5ccc(cc5)C(=O)C)c1c(ccc(c1)[N+](=O)[O-])Cl | C32H28O5N5Cl1S1 |
| 344696238 | ChemDiv, Inc | V030-2628 | 3-({4-[(2-chloro-5-nitrophenyl)sulfonyl]-1-piperazinyl}methyl)-2-(3-methoxyphenyl)-6-(3-methylphenyl)imidazo[1,2-a]pyridine | [S](=O)(=O)(N2CCN(CC2)Cc3[n]4c(nc3c6cc(ccc6)OC)C=CC(=C4)c5cc(ccc5)C)c1c(ccc(c1)[N+](=O)[O-])Cl | C32H30O5N5Cl1S1 |
| 344696332 | ChemDiv, Inc | V030-2674 | 2-(4-fluorophenyl)-3-({4-[(3-nitrophenyl)sulfonyl]-1-piperazinyl}methyl)-6-[3-(trifluoromethyl)phenyl]imidazo[1,2-a]pyridine | FC(F)(F)c1cc(ccc1)C2=C[n]3c(nc(c3CN5CCN(CC5)[S](=O)(=O)c6cc(ccc6)[N+](=O)[O-])c4ccc(cc4)F)C=C2 | C31H25O4N5S1F4 |
| 344696242 | ChemDiv, Inc | V030-2685 | 3-({4-[(2-chloro-5-nitrophenyl)sulfonyl]-1-piperazinyl}methyl)-2-(4-fluorophenyl)-6-(3-methylphenyl)imidazo[1,2-a]pyridine | Fc1ccc(cc1)c2nc3[n](c2CN5CCN(CC5)[S](=O)(=O)c6c(ccc(c6)[N+](=O)[O-])Cl)C=C(C=C3)c4cc(ccc4)C | C31H27O4N5Cl1S1F1 |
| 332657079 | ChemDiv, Inc | V030-2767 | 3-[3-(4-chlorophenoxy)phenyl]-3-(1H-indol-3-yl)-N-(4-pyridinylmethyl)propanamide | Clc1ccc(cc1)Oc2cc(ccc2)C(CC(=O)NCc5ccncc5)c3c4c([nH]c3)cccc4 | C29H24O2N3Cl1 |
| 344696288 | ChemDiv, Inc | V030-5887 | N-{4-[(4-{[6-(3-chlorophenyl)-2-(4-chlorophenyl)imidazo[1,2-a]pyridin-3-yl]methyl}-1-piperazinyl)sulfonyl]phenyl}acetamide | [S](=O)(=O)(N2CCN(CC2)Cc3[n]4c(nc3c6ccc(cc6)Cl)C=CC(=C4)c5cc(ccc5)Cl)c1ccc(cc1)NC(=O)C | C32H29O3N5Cl2S1 |
| 344693611 | ChemDiv, Inc | V030-8097 | 3-({4-[(benzyloxy)acetyl]-1-piperazinyl}methyl)-6-(2,5-dimethylphenyl)-2-(4-nitrophenyl)imidazo[1,2-a]pyridine | [N+](=O)([O-])c1ccc(cc1)c2nc3[n](c2CN5CCN(CC5)C(=O)COCc6ccccc6)C=C(C=C3)c4c(ccc(c4)C)C | C35H35O4N5 |
| 117452839 | ChemDiv, Inc | L227-0253 | 1-(2-(4-chlorophenyl)-5-methylene-4,5-dihydropyrazolo[1,5-a]pyrimidin-7-yl)-N-((3-methyl-1H-pyrazol-4-yl)methyl)piperidine-4-carboxamide | Clc1ccc(cc1)c2n[n]3c(c2)NC(=C)C=C3N4CCC(CC4)C(=O)NCc5c[nH]nc5C | C24H26O1N7Cl1 |
| 40717273 | ChemDiv, Inc | C380-0602 | 10-(2-chloro-6-fluorobenzyl)-8-(3,4-dihydro-2(1H)-isoquinolinylcarbonyl)dibenzo[b,f][1,4]thiazepin-11(10H)-one | Fc1c(c(ccc1)Cl)CN2c3c(ccc(c3)C(=O)N5CCc6c(cccc6)C5)Sc4c(cccc4)C2=O | C30H22O2N2Cl1S1F1 |