otava
NEW SUBSTANCES FOR NEW RESEARCH

www.otavachemicals.com

The Art of Organic Chemistry

CUSTOM SYNTHESIS SERVICES

OTAVA has extensive experience in the synthesis of highly valuable products for biotech and pharmaceutical applications around the world. Our company helps companies around the world to advance their projects by synthesizing:

- **Starting materials, intermediates, and/or final products**
- **Advanced intermediates in drug synthesis**
- **Combinatorial chemistry templates and building blocks**

We also offer custom synthesis on the basis of our rare scaffolds. Our unique scaffold database was prepared using comparative analysis of worldwide suppliers of compound libraries.

This is your opportunity to get novel compounds for screening!

OFF-THE-SHELF BUILDING BLOCKS

Our company offers more than 40,000 Building Blocks in multi-gram quantities and purity higher than 95%.

These diverse compounds could be used for high-throughput and combinatorial synthesis of pharmaceutical libraries or scale-up of lead compounds for further development.

IN-HOUSE STOCK COMPOUNDS FOR PROMPT DELIVERY

Our In-house Stock Collection contains about 100,000 compounds and ALL compounds have undergone quality control to confirm their chemical structures. All compounds are for prompt delivery. We offer the possibility to re-supply compounds purchased from us.

GREEN COLLECTION

The Green Collection compound library (about 70,000 compounds total) was prepared on the basis of In-house Stock library and pre-formatted by Lipinski's Rules of Five:

- **LogP from 0 to 5**
- **MW from 160 to 500**
- **Number of H-donors from 0 to 4**
- **Number of H-acceptors from 0 to 7**
- **Nnumber of NO_2 groups from 0 to 2**

SEARCH NOW!

Our compounds can now be found in the eMolecules online substructure searchable database at **http://otava.emolecules.com**

Our compounds can also be searched in the SPRESI^{web} online structure and reaction database at **http://www.spresi.de**

Our compound libraries can be downloaded for free at the company's web site **http://www.otavachemicals.com** or requested directly by e-mail in suitable format. Please send your requests to **info@otavachemicals.com**

LIST OF SELECTED PUBLICATIONS

[1] Shaitanov et al. Synthesis of 4-substituted 1-arylhexahydrothieno[3,4-b]pyrazin-2(1H)-one 6,6-dioxides. *Ukrainica Bioorganica Acta.* 2006, 4 (2), 40-46.

[2] Prykhodko et al. Synthesis of 7-(3-dialkylamino-2-hydroxypropoxy)-3-aryloxychromones. *Ukrainica Bioorganica Acta.* 2005, 1 (1), 33–39.

[3] Prykhod'ko et al. Antiproliferative activities of some 7-hydroxy-3-aryloxy-2-trifluorometthyl-4H-4-chromenone derivatives against 60 human cancer cell lines. *Biopolymers and Cell.* 2004, 20 (1–2), 159–163.

[4] Lesyk et al. Synthesis of potential biologically active substances on the base of 5-carboxymethylidene-2,4-thiazolidinedione. *Pharmaceutical Journal.* 2003, 1, 51–56.

[5] Dubinina et al. Interaction of 3,4-dichloromaleimides with N- and S-nucleophiles. *Ukr. Khim. Zh.* 2002, 68 (8), 47-51.

[6] Dubinina et al. Reaction of N-substituted 3,4-dichloromaleimides with a-mercaptoazaheterocycles. *Heterocycles.* 2001, 11, 2189-2198.

[7] Alekseeva et al. The N4-aminoacid derivatives of 6-azacytidine: Syntheses and biological activity. *Biopolymers and Cell.* 1997, 13 (4), 285-290.

[8] Ognyanik et al. The synthesis and spectroscopic investigations 3-thio-6-alkylamino derivaties 1.2.4-triazinone-5. *Ukr. Khim. Zhurn.* 1988, 11, 1197-1199.

Contact us:

Tel.:/Fax: + 44 5222458
info@otavachemicals.com

OTAVA – North American Division
Tel.: 1-416-305-9979
Fax: 1-866-881-9921 (Toll-free in US & Canada)
north.america@otavachemicals.com

COMPOUND LIBRARIES AND BUILDING BLOCKS
COMPOUND LIBRARIES AND BUILDING BLOCKS

otava
NEW SUBSTANCES
FOR NEW RESEARCH

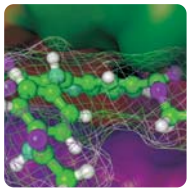
www.otavachemicals.com

The Art of Molecular Modeling

KINASE ProHit COMPOUND SETS

Effective hit compounds are essential for successful drug discovery. OTAVA offers unique ProHit compounds displaying inhibitory activity (< 1μM for the most active compounds) against distinct protein kinases. The compounds of each Kinase ProHit set are free of Intellectual property and belong to the single chemical class. ProHit compound sets can be used in the development of drugs targeting protein kinase enzymes.

OTAVA'S FOCUSED LIBRARIES



OTAVA, Ltd. offers unique Receptor-Based Target-Focused libraries.

These libraries are created from an extensive compound stock collection (490,000 compounds) and a rigorous process of refinement that involves harnessing the most current methods of theoretical medicinal chemistry.

OTAVA's Receptor-Based Target-Focused libraries are generated through Sharp Focusing approach: each molecule's interaction is measured with only a single target in a protein family.

Sharp Focusing approach is implemented as following:

- **Filtering of stock collection according to the Lipinski and Veber rules**
- **Flexible molecular docking**
- **Re-scoring according to the ligand's structural features**
- **Scanning of each docking complex for key contacts**

This in-depth analysis of each protein-ligand complex allowed designing unique target-focused libraries.

We would like to offer these products to our customers.

More libraries are on the way!

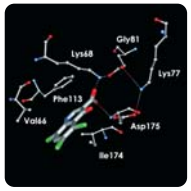
Currently available focused libraries:

- **p38 MAP Kinase Alpha**
- **Vascular Endothelial Growth Factor Receptor 2 (VEGFR2)**
- **Aurora B Kinase**
- **Janus Kinase 2 (JaK2)**
- **Phosphatidylinositol 3-Kinase (PI3K)**
- **3-phosphoinositide-dependent Kinase-1 (PDK-1)**
- **Fibroblast Growth Factor Receptor 1 Tyrosine Kinase (FGFR1K)**
- **cAMP dependent Protein Kinase (PKA)**

All of the Receptor-Based Target-Focused libraries of compounds are available in-house, and come with docking scores and values for drug-like properties.

Using Sharp Focusing approach, we could focus our combined 490,000-compound stock collection on your specific target(s), on an exclusive basis.

Our company can also create an exclusive receptor-based target-focused library based on your own collection of compounds!

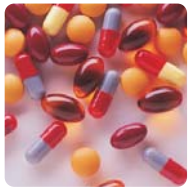


OTAVA'S APPROACH IN ACTION

Using molecular modeling techniques, chemical synthesis and biological in vitro tests, OTAVA's scientists discovered several new classes of potent human protein kinase CK2 inhibitors. One of the classes, 3-carboxy-4(1H)-quinolones, has been disclosed [1]. This class of inhibitors was discovered through receptor-based virtual screening of the OTAVA's 70,000-compound library, on the basis of OTAVA's CK2 focused library.

1. Golub et al. *J Med Chem.* 2006, 49, 6443-50.

CONTRACT RESEARCH AND DRUG DISCOVERY EXPERIENCE



Contract research is one of the main activities of OTAVA. Many leading pharmaceutical and chemical companies choose OTAVA as a reliable partner for collaboration in research and development of high-tech products.

Recently, in collaboration with ADAMED, one of the leading pharmaceutical producers, OTAVA launched integrated drug discovery project focused on protein kinases as drug targets.

OTAVA offers its facilities and experience for contract research projects in the fields of lead discovery, organic chemistry and fluorescent probes. We are always open for collaboration.

LIST OF SELECTED PUBLICATIONS

[1] Yakovenko et al. The new method of distribution integrals evaluations for high throughput virtual screening. *Ukrainica Bioorganica Acta.* 2007, 5 (1), 52-63.

[2] Golub et al. Evaluation of 3-Carboxy-4(1H)-quinolones as Inhibitors of Human Protein Kinase CK2. *J Med Chem.* 2006, 49 (22), 6443-6450.

[3] Prykhod'ko et al. Evaluation of 4H-4-chromenone derivatives as inhibitors of protein kinase CK2. *Biopolymers and cell.* 2005, 21 (3), 287-292.

[4] Sapelkin et al. Application of 4-substituted 3-carboxyquinolines as protein kinase CK2 inhibitors. Pat. UA68984 A, C07D215/00, 2004-08-16.

[5] Prykhod'ko et al. Application of 4,5,6,7-tetrahalogeno-1,3-isoindolinediones as protein kinase CK2 inhibitors. Pat. UA69165 A, C07D215/00, 2004-08-16.

Contact us:

Tel.:/Fax: +380 44 5222458
info@otavachemicals.com

OTAVA – North American Division
Tel.: 1-416-305-9979
Fax: 1-866-881-9921 (Toll-free in US & Canada)
north.america@otavachemicals.com

FOCUSED LIBRARIES AND MOLECULAR MODELING
FOCUSED LIBRARIES AND MOLECULAR MODELING