



TimTec LLC

Harmony Business Park Bldg 301-A
Newark DE 19711, USA
Phone: 1-302-292-8500 Fax: 1-302-292-8520
[://www.timtec.net](http://www.timtec.net) e-mail info@timtec.net

TimTec in Publications

Below are some independent reference materials that position and differentiate TimTec as one of the leading designers and suppliers of compound library collections on the market.

TimTec is well-established supplier of compound library collections on the market. Number of independent sources recommend our company and value our approach to libraries design:

Kirpotina L.N., et al. Identification of Novel Small-Molecule Agonists for Human Formyl Peptide Receptors and Pharmacophore Models of their Recognition. Molecular Pharmacology February 2010 vol. 77 no. 2, p 159-170

Filhoulaud, G., et al. The hexosamine biosynthesis pathway is essential for pancreatic beta cell development. J Biol Chem. 2009 Sep 4;284(36):24583-94.

Holder S., et al., Characterization of a potent and selective small-molecule inhibitor of the PIM1 kinase. Mol Cancer Ther. Jan. 2007, 6(1), 163-172

Jadhav A., et al. Quantitative analyses of aggregation, autofluorescence, and reactivity artifacts in a screen for inhibitors of a thiol protease. J Med Chem. 2010 Jan 14;53(1):37-51.

Pedersen, J.M., et al. Molpro-Prediction and Identification of Drug Interactions with the Human ATP-Binding Cassette Transporter Multidrug-Resistance Associated Protein 2 (MRP2; ABCG2). J. Med. Chem., 2008, 51 (11), pp 3275–3287

Auld, D. S., et al. Characterization of Chemical Libraries for Luciferase Inhibitory Activity. J. Med. Chem., 2008, 51 (8), pp 2372–2386

Yang P., et al. Multiplexed Detection of Protein–Peptide Interaction and Inhibition Using Capillary Electrophoresis. Anal. Chem., 2007, 79 (4), pp 1690–1695

Leone S., et al. SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington's disease. Bioorg Med Chem. 2008 May 15;16(10):5695-703.

Zhu P.J., et al. Quantitative high-throughput screening identifies inhibitors of anthrax-induced cell death. Bioorg Med Chem. 2009 Jul 15;17(14):5139-45.

Vicini P., et al. 2-Heteroarylrimino-5-benzylidene-4-thiazolidinones analogues of 2-thiazolyrimino-5-benzylidene-4-thiazolidinones with antimicrobial activity: synthesis and structure-activity relationship. *Bioorg Med Chem.* 2008 Apr 1;16(7):3714-24.

Buckner D., et al. Use of early passage fetal intestinal epithelial cells in semi-high-throughput screening assays: an approach to identify new innate immune system adjuvants. *J Biomol Screen.* 2006 Sep;11(6):664-71.

Park J.Y., A simple, no-wash cell adhesion-based high-throughput assay for the discovery of small-molecule regulators of the integrin CD11b/CD18. *J Biomol Screen.* 2007 Apr;12(3):406-17.

Moy, T.I., et al. High-Throughput Screen for Novel Antimicrobials using a Whole Animal Infection Model. *ACS Chem. Biol.*, 2009, 4 (7), pp 527–533

Small-Molecule Screening: It Takes a Village. *ACS Chem. Biol.*, 2007, 2 (1), pp 9–16

Kim, D.Y., et al. Design and Biological Evaluation of Novel Tubulin Inhibitors as Antimitotic Agents Using a Pharmacophore Binding Model with Tubulin. *J. Med. Chem.*, 2006, 49 (19), pp 5664–5670

Perez-Pineiro R., et al. Development of a Novel Virtual Screening Cascade Protocol to Identify Potential Trypanothione Reductase Inhibitors. *J. Med. Chem.*, 2009, 52 (6), pp 1670–1680

Kiss R., et al. Discovery of Novel Human Histamine H4 Receptor Ligands by Large-Scale Structure-Based Virtual Screening. *J. Med. Chem.*, 2008, 51 (11), pp 3145–3153

Yang H. and Liebeskind N.S., A Concise and Scalable Synthesis of High Enantiopurity (-)-d-erythro-Sphingosine Using Peptidyl Thiol Ester–Boronic Acid Cross-Coupling. *Org. Lett.*, 2007, 9 (16), pp 2993–2995

Zhong, S., et al. Identification and Validation of Human DNA Ligase Inhibitors Using Computer-Aided Drug Design. *J. Med. Chem.*, 2008, 51 (15), pp 4553–4562

Rella M., et al. Structure-Based Pharmacophore Design and Virtual Screening for Novel Angiotensin Converting Enzyme 2 Inhibitors. *J. Chem. Inf. Model.*, 2006, 46 (2), pp 708–716

Krier, M, et al. Assessing the Scaffold Diversity of Screening Libraries. *J. Chem. Inf. Model.*, 2006, 46 (2), pp 512–524

Mallya M., et al. Small Molecules Block the Polymerization of Z • 1-Antitrypsin and Increase the Clearance of Intracellular Aggregates. *J. Med. Chem.*, 2007, 50 (22), pp 5357–5363

Szewczuk L. M., et al. De Novo Discovery of Serotonin N-Acetyltransferase Inhibitors. *J. Med. Chem.*, 2007, 50 (22), pp 5330–5338

Feng B. Y., et al. A High-Throughput Screen for Aggregation-Based Inhibition in a Large Compound Library. *J. Med. Chem.*, 2007, 50 (10), pp 2385–2390

Graves A. P., et al. Decoys for Docking. *J. Med. Chem.*, 2005, 48 (11), pp 3714–3728

Huang JW. H., et al. Fragment-Based Design of Small Molecule X-Linked Inhibitor of Apoptosis Protein Inhibitors. *J. Med. Chem.*, 2008, 51 (22), pp 7111–7118

- Spycher S., *Toward a Class-Independent Quantitative Structure–Activity Relationship Model for Uncouplers of Oxidative Phosphorylation*. *Chem. Res. Toxicol.*, 2008, 21 (4), pp 911–927
- Schepetkin, I., et al. *Novel Small-molecule Inhibitors of Anthrax Lethal Factor Identified by High-throughput Screening*. *J. Med. Chem.*, 2006, 49: 5232-5244
- Shaneyfelt, M. E., et al. *Natural products that reduce rotavirus infectivity identified by a cell-based moderate-throughput screening assay*. *Virology Journal*, 2006, 3:68doi:10.1186/1743-422X-3-68
- Gross, B.J, et al. *Discovery of O-GlcNAc Transferase Inhibitors*. Department of Microbiology and Molecular Genetics, Harvard Medical School. *JACS Communications*, published on Web 09/29/05; *J. Am. Chem. Soc.* 2005, 127, 14588-14589.
- Zeng G, et al. *Validation of BKV large T-antigen ATP-binding site as a target for drug discovery*. *Antiviral Res.* 2008 Dec 11. [E-pub ahead of print]
- Schepetkin IA, et al. *Identification of novel formyl peptide receptor-like 1 agonists that induce macrophage tumor necrosis factor alpha production*. *Mol Pharmacol.* 2008 Aug;74(2):392-402.
- Pan, N.J., et al. *Targeting Type III Secretion in Yersinia pestis*. *Antimicrob. Agents and Chemother.* 2009, Feb: 53 (2), 385-392.
- Bisson H., et al. *Modeling of the Aryl Hydrocarbon Receptor (AhR) Ligand Binding Domain and Its Utility in Virtual Ligand Screening to Predict New AhR Ligands*. *J. Med. Chem.* 2009 Sept, 52 (18), 5635-5641.
- Lin G., et al. *Inhibitors selective for mycobacterial versus human proteasomes*. *Nature* 2009 Oct, 621-626.
- Schuffenhauer A., et al. *between Molecular Complexity, Biological Activity, and Structural Diversity*. *J. Chem. Inf. Model.*, 2006, 46 (2), pp 525–535
- Schepetkin, I. A., et al. *-Benzoylpyrazoles Are Novel Small-Molecule Inhibitors of Human Neutrophil Elastase*. *J. Med. Chem.*, 2007, 50 (20), pp 4928–4938
- Schepetkin, I., et al., *High-throughput Screening for Small-molecule Activators of Neutrophils: Identification of Novel N-Formyl Peptide Receptor Agonists*. *Mol. Pharmacol.* 71: 1061-1074 (2007)
- Sirois S., et al. *Screening for SARS-CoV Protease Based on KZ7088 Pharmacophore Points*. *J. Chem. Inf. Comput. Sci.*, 2004, 44 (3), pp 1111–1122
- Ciustea M., et al. *of Non-Nucleoside DNA Synthesis Inhibitors of Vaccinia Virus by High-Throughput Screening*. *J. Med. Chem.*, 2008, 51 (20), pp 6563–6570
- Li, Weizhong. *Fast Clustering Algorithm for Analyzing Highly Similar Compounds of Very Large Libraries*. *J. Chem. Inf. Model.*, 2006, 46 (5), pp 1919–1923
- Bullock, A. N., et al. *Basis of Inhibitor Specificity of the Human Protooncogene Proviral Insertion Site in Moloney Murine Leukemia Virus (PIM-1) Kinase*. *J. Med. Chem.*, 2005, 48 (24), pp 7604–7614
- Clark, D. E., et al. *Virtual Screening Approach to Finding Novel and Potent Antagonists at the Melanin-Concentrating Hormone 1 Receptor*. *J. Med. Chem.*, 2004, 47 (16), pp 3962–3971

Lawrence M. Szewczuk L. M., et al. *Novo Discovery of Serotonin N-Acetyltransferase Inhibitors. J. Med. Chem.*, 2007, 50 (22), pp 5330–5338

Ekonomiuk D., et al. *Protease Inhibitors Identified by Fragment-Based Library Docking into a Structure Generated by Molecular Dynamics. J. Med. Chem.*, 2009, 52 (15), pp 4860–4868

Simeonov A., et al. *Spectroscopic Profiling of Compound Libraries. J. Med. Chem.*, 2008, 51 (8), pp 2363–2371

Füllbeck M, et al. *Natural products: sources and databases. Highlight Nat. Prod. Rep.* 2006 April 10; 23, 347 – 356

Broom W.J., et al. *Two approaches to drug discovery in SOD1-mediated ALS. J Biomol Screen.* 2006 Oct;11(7):729-35

Bodner R.A., et al. *Pharmacological promotion of inclusion formation: A therapeutic approach for Huntington's and Parkinson's diseases. Proc Natl Acad Sci USA.* 2006 Mar 14;103(11):4246-51

Independent study says TimTec compound collection has “the best diversity”:
[://www.timtec.net/news/articles/timtec-has-the-best-diversity](http://www.timtec.net/news/articles/timtec-has-the-best-diversity).

Above is not the complete list of available and published results. We do not disclose research results from industry clients.

Our compound collections offer greater diversity since we have balanced combination of in-house synthesis and outside sourcing. There is high diversity score from collection to collection. We do not use combinatorial chemistry approach in library design and all our molecules are hand-synthesized. TimTec compounds are stored in dry form only and are freshly prepared in DMSO. TimTec offers a variety of screening collections to suit different in capacity and design/purpose assays. We do custom formatting and offer cherry picking. Compounds in our library collections are available for re-supply from our US stock.

