



## Technology Development Group

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### Compound Library Made Through Phosphine-Catalyzed Annulation/Tebbe/Diels-Alder Reaction

Tech ID: 27511 / UC Case 2012-293-0

#### SUMMARY

UCLA researchers in the Department of Chemistry and Biochemistry have developed a small molecule library consisting of a large variety of stereochemical variants.

#### BACKGROUND

Small molecule libraries are used for high throughput screening for any biological activity. These are used for drug discovery and to investigate mechanisms of activity. However, current libraries are composed of common molecules and their variants and do not include the vast majority of chemical conformations. There is an unmet need for libraries that sample a large number of backbone conformations and stereochemical diversity.

#### INNOVATION

UCLA researchers have developed a method to synthesize a chemical library composed of unique molecules. Their 'diversity-oriented synthesis' technique was used to generate a 91-molecule library. The library consists of heterocyclic compounds composed of 16 distinct scaffolds and samples a large variety of structural and stereochemical conformations. They have used it to screen for inhibitors of invasion properties of breast cancer cells and have discovered 3 lead compounds. Additionally, the library has been screened for inhibitors of T cell exocytosis and for IFN- $\gamma$ -like compounds.

#### APPLICATIONS

- High throughput screening for drug discovery
- High throughput screening for any chemical activity
- High throughput screening for any biological activity

#### ADVANTAGES

- Samples large number of chemical conformations and distinct scaffolds
- Improved synthesis method

#### STATE OF DEVELOPMENT

Chemical library designed and synthesized

Utilized to screen for:

- Compounds against breast cancer cell migration
- IFN- $\gamma$ -like compound
- Inhibitors of T cell exocytosis

#### RELATED MATERIALS

- Zhiming Wang, Sabrina Castellano, Sape S. Kinderman, Christian E. Argueta, Anwar B. Beshir, Gabriel Fenteany, and Ohyun Kwon 'Diversity Through a Branched Reaction Pathway: Generation of Multicyclic Scaffolds and Identification of Antimigratory Agents' Chem. Eur. J. 2011

#### CONTACT

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#### INVENTORS

- Kwon, Ohyun

#### OTHER INFORMATION

##### KEYWORDS

Chemical biology, diversity-oriented synthesis, heterocycles, synthesis design, high throughput screening, small molecule library

##### CATEGORIZED AS

- **Materials & Chemicals**
  - Chemicals
- **Medical**
  - New Chemical Entities, Drug Leads
  - Research Tools
- **Research Tools**
  - Screening Assays

##### RELATED CASES

2012-293-0

► Cruz, D.; Wang, Z.; Kibbie, J. J.; Modlin, R. L.; Kwon, O. “Diversity through phosphine catalysis identifies octahydro-1,6-naphthyridin-4-ones as activators of endothelium-driven innate immunity” Proc. Natl. Acad. Sci. U.S.A. 2011, 108, 6769–6774.

► Kibbie, J. J.; Teles, R. M. B.; Wang, Z.; Hong, P.; Montoya, D.; Krutzik, S.; Lee, S.; Kwon, O.; Modlin, R. L.; Cruz, D. “Jagged1 Instructs Macrophage Differentiation in Leprosy,” PloS Pathog. 2016, 12, e1005808.

► Florian, A. E.; Lepensky, C. K.; Kwon, O.; Haynes, M. K.; Sklar, L. A.; Zweifach, A. “Flow Cytometry Enables A High-throughput Homogeneous Fluorescent Antibody-Binding Assay for Cytotoxic T Cell Lytic Granule Exocytosis” J. Biomol. Screen. 2013, 18, 420–429.

PATENT STATUS

Country	Type	Number	Dated	Case
United States Of America	Issued Patent	8,624,032	01/07/2014	2012-293

ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

► Novel Non-Peptidomimetic Prenyltransferase Inhibitors

► Hydrodealkenylative C(Sp3)–C(Sp2) Bond Scission

► Small Molecule Agonists of VDAC2 to Treat Cardiac Arrhythmias and Heart Failure

Gateway to Innovation, Research and Entrepreneurship

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