#### キシダ化学株式会社 企業セミナー要旨

**Title:** MCE-18 - a novel molecular descriptor to reveal current medicinal chemistry trends in Big Pharma.

#### Author:

Dr. Bogdan Zagribelny, Senior Medicinal Chemistry at ChemDiv.Inc.

Dr. Yan Ivanenkov, Head of CADD at ChemDiv.Inc.

#### Summary:

The paradigm of "drug-like-ness" dramatically altered the behavior of the medicinal chemistry community for a long time. In recent years, scientists have empirically found a significant increase in key properties of drugs that have moved structures closer to the periphery or the outside of the rule-of-five "cage". Herein, we show that for the past decade, the number of molecules claimed in patent records by major pharmaceutical companies has dramatically decreased, which may lead to a "chemical singularity". New compounds containing fragments with increased 3D complexity are generally larger, slightly more lipophilic, and more polar. A core difference between this study and recently published papers is that we consider the nature and quality of sp3-rich frameworks rather than sp3 count. We introduce the original descriptor MCE-18, which stands for medicinal chemistry evolution, 2018, and this measure can effectively score molecules by novelty in terms of their cumulative sp3 complexity.

# ご存知ですか…?

## キシダ化学の創薬支援事業

- ・キシダオリジナル ビルディングブロック(K-BB)
- ・キシダオリジナルライブラリー(K-LB)
- ・合成化学(ライブラリー合成事業)
- ・非天然アミノ酸(合成研究・製造販売)

創薬支援商品

- ・海外サプライヤー代理店事業
  - ⇒ライブラリー化合物
- ⇒ライフサイエンス商材
- ⇒海外CROへの委受託業務の仲介

### 商社事業

- ・**化合物BANKシステム** (ケミカルバンク、ライブラリーバンク)
- ・化合物管理サポート(各種小分け、プレート作成)
- ・ラボ・サポート(お客様研究所内で創薬支援)・輸入代行、法規制チェック



創薬支援サービス

# ChemDiv 新規トピック・トレンド2020



## Focused & Targeted Libraryに新デザイン追加!

### 2020年度 新デザイン追加!

- \*General Antiviral library \*MCL1 library
- \*Covalent inhibitors library \*Ion Channels library \*HDAC library
- \*PTPN library \*Lipid metabolism library \*F atom library

### ☆コロナウイルス研究関連ライブラリー

- \*PLpro library \*3CLpro library\*ACE2 library
- \*Sting agonist library \*Coronavirus library



Representative Examples of the Selected Componeds
(Included Acceptors/Disrupplities)

Annotated Libraryが16品目に増加!

生物活性やターゲットに対する実際の活性値付きライブラリーです。

Human GPCR Annotated Library Phosphatases Reference Compounds Library Transcription Factors Reference Compounds Library Ion Channels Reference Compounds Library

CNS targets activity set Therapeutical Diversity Annotated Library 3D-Biodiversity Library Launched & Clinically Evaluated Drugs Library

CNS Reference Compounds Library Receptors Reference Compounds Proteases Reference Compounds Library

reference Compounds Library Selective Target Activity Profiling Library

ChemoGenomic Annotated library for Phenotypic Screening Target Identification, Phenotypic Screening library(TIPS)

Antiviral Annotated Library



(資料請求・お問い合わせ先)

キシダ化学株式会社 ライフサイエンス推進部 探索支援グループ

Tel: 03-5625-5595 Tax: 03-5625-5596、ホームページ: http://www.kishida.co.jp/