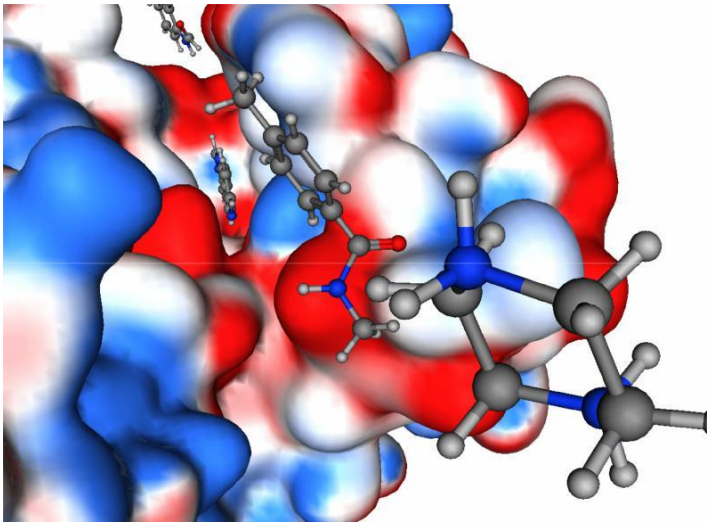
"drug discovery through chemical biology"

The "IOTA Diverse" Fragment Library



Fragment-based Drug Design

Fragment-based drug design - FBDD - is a paradigm shift for drug discovery.

Out! with expensive, million-component, high-throughput screening and combichem libraries.

In! with low complexity, target-focussed chemical libraries, tailored to specific medchem and chembio applications.

Fragment libraries are a tried and tested starting point for pharma discovery. A multitude of recent publications illustrate their successful use in drug discovery - for details, see:

www.iotapharma.com/literature

Leveraged by smart screens, chemical fragments open an easy and productive way to develop chemical probes and valuable drugs in your therapeutic programs.

The "IOTA Diverse" Fragment Library

The IOTA fragment libraries have been carefully assembled in collaboration with an expert in the FBDD area, Dr Iwan de Esch, head of Drug Design and Synthesis in the Medicinal Chemistry Department at the Free University in Amsterdam [1-6].

IOTA Diverse, IOTA's first Fragment Library, contains 1500 compounds rigorously selected for their suitability for

- fragment-based screening applications
- coverage of chemical space
- subsequent elaboration into drug-like molecules for organic chemistry.

Many of these molecules are currently being used as building blocks for drug discovery programs.

Others are totally novel compounds designed by computational chemists for specific medchem applications.

Key Features of "IOTA Diverse"

The majority of the compounds in IOTA Diverse conform to the criteria defined in the "Rule of 3" [7]. The only exception to this is the inclusion of certain compounds of ~350 MW which reflect unique chemical series whose SAR could be instructive for discovery applications.

There are no reactive functionalities such as aldehydes, sulphonyl chlorides, acid chlorides, etc. Many of the compounds are unique heterocycles which cannot be obtained through other commercial channels.

The Pedigree of "IOTA Diverse"

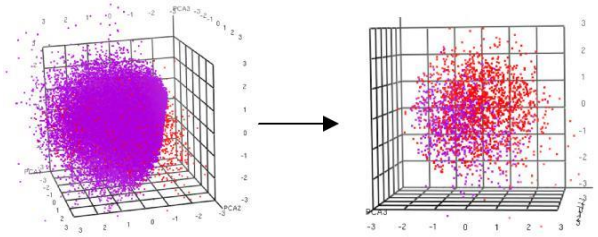
The IOTA Diverse fragment library has evolved from 50 years of medicinal chemistry and organic synthesis research.

Most of the fragments have served as synthetic precursors of existing NCEs and novel drug candidates, each with its associated route of synthesis and purification protocol, making the collection a valuable practical R&D tool.

IOTA Diverse represents a very small fraction of the total commercial synthetic universe (A). It occupies similar chemical property space to other "Rule of 3" fragment libraries (B), but covers chemical space comprehensively (C), uniquely containing almost 700 different scaffolds (D). This makes IOTA Diverse a very valuable drug discovery resource.

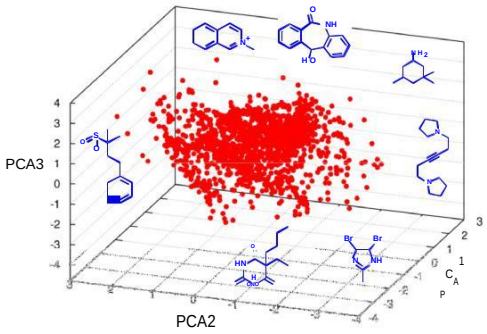
(A) Synthetic Universe

(B) Two Ro3 Libraries



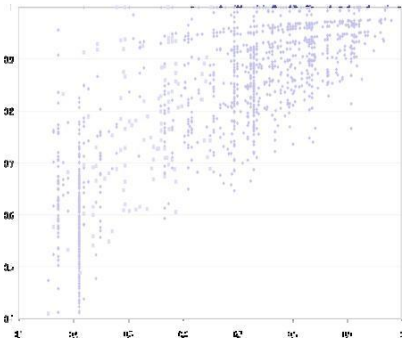
(C)

Coverage of Chemical Space [8]
by "IOTA Diverse"



(D)

"IOTA Diverse" Scaffold Space [9]



Prices and Availability

A full description of the IOTA Diverse Fragment Library, with chemical structures and property analyses, is available, under confidentiality, from IOTA.

Contact us at info@iotapharma.com for more information.

References

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2. Orrling et al. (2012) J Med Chem. 55, 8745-56.
3. Blaazer et al.(2015) J Biomol Screen. 20,131-40.
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7. Congreve et al. (2003). Drug Discovery Today. 8, 876-77.
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IOTA

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IOTA's Discovery Team

IOTA Pharmaceuticals has been built by experienced drug discovery scientists.

Dr Susan Boyd, leading IOTA's computational chemistry, has worked at Pfizer, Celltech and Scynexis and continues to consult for industry computational chemistry teams.

Dr Paul England, leading IOTA's screening activities, was head of Smith-Kline's high-throughput screening operation and was one of the senior executives at the Californian biotechnology company Aurora Biosciences.

Dr David Bailey, leading IOTA's business team, previously headed up Pfizer's Molecular Sciences Department in Sandwich, was Vice President at Incyte Pharmaceuticals, and Founding CEO at De Novo Pharmaceuticals in Cambridge.

IOTA's Discovery Strategy

IOTA believes that new chemical tools and genomic technologies are urgently required to accelerate drug discovery - today.

We aim to position ground-breaking technologies - such as FBDD - at the forefront of pharmacological research in every laboratory, making them available to researchers in formats appropriate to their widespread use.

Over the coming years, IOTA will develop a series of technology platforms to make "drug discovery though chemical biology" a reality.

We encourage you to visit IOTA's website for more information:

www.iotapharma.com