

# BIONET

## FRAGMENT LIBRARIES

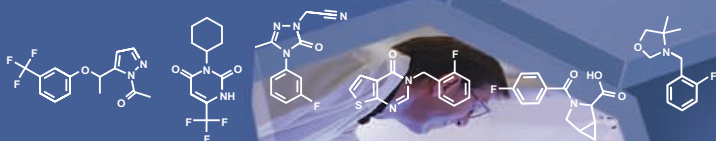
Andrew Lowerson, Dr. John Harris, Elizabeth A. Jones

Are you looking for high quality, novel fragments to complement your in-house fragment collections? Do you use the established 'Rule of 3'<sup>(1)</sup> (Ro3) or softer criteria to make your selections?

Recent scientific discussion<sup>(2)</sup> has claimed that Ro3 based collections omit fragments of pharmacological interest due to the stringent criteria imposed. Key Organics offers the Bionet Extended Fragment Library Set of 11,839 Fragments which targets the requirements of fragment optimization. This Collection has been selected using softer ADME filters. Bionet also offers its subsets of Bionet Bromo Fragments, NEW Bionet Fluoro Fragments as well as the established Bionet Fragment Library Ro3 Collection. A further CNS targeted Set is to be released shortly.

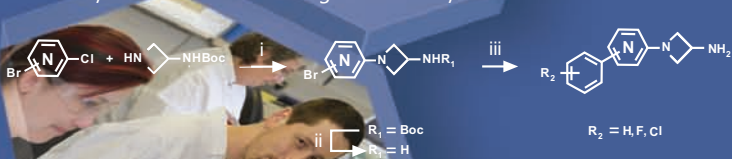
## NEW – The Bionet Fluoro Fragment Set

A collection of 1117 fluorinated Fragments, of which 636 are unique to Bionet, incorporating mono CF<sub>3</sub> and mono F compounds which allow for identification of the Fragment bound in the active site by the highly sensitive <sup>19</sup>F NMR screening technique.



## Fragment Optimization

With 25 years of versatile expertise in providing novel screening compound design and synthesis, Key Organics is well qualified to offer fragment libraries based around any fragment of interest. The example below illustrates the advantage of a fragment linkage approach combined with in-house microwave chemistry techniques for the synthesis of a small fragment library.



i) DIEA, EtOH, mw, 130°C, 10min, 92–99%; ii) HCl, dioxane, 99%; iii) R<sup>2</sup>ArB(OH)<sub>2</sub>, Pd<sup>II</sup> cat, aq. base, DME, mw, 140°C, 15–30 min, 43–47%

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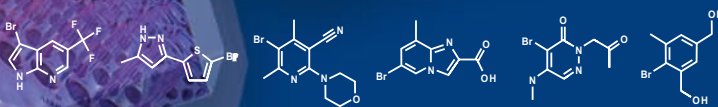
*The right side of the Equation*

## COMING SOON – The Bionet CNS Fragment Set

The Bionet CNS Fragment set comprising 250 Fragments, of which 100 are unique to Bionet, have been carefully selected for screening suitability against CNS targets. The selection has been filtered by TPSA, LogP, MW, Hydrogen Bond Donors and Acceptors, Functionality and Molecular Flexibility. Contact us to register your interest.

## The Bionet Bromo Fragment Set

The Bionet Bromo Fragment collection of 370 Fragments of which 158 are unique to Bionet. Bromo Fragments allow for easier identification of the Fragment bound in the active site of a target by X-ray crystallography.



## The Bionet Fragment Library Extended Set

The Bionet Fragment Library Extended Set encompasses 11,839 diverse fragments of which 3,546 are uniquely available\* through Bionet. All the Fragments are selected based on the softer ADME filters (MW<350, clogP<3.5, H-bond donors<4, H-bond acceptors<4 and number of rotatable bonds<4), chemical tractability and potential for Fragment evolution.

Solubility<sup>(3)</sup> and TPSA descriptors have been calculated for the Ro3, Bromo, Fluoro and CNS fragment collections. We are currently implementing experiments to assure solubility in DMSO (200mM) and KPi buffer (2mM) for all our Fragment collections. A full description of solubility methodology is available on request.

(1) Congreve, M.; Carr, R.; Murray, C.; Jhoti, H. A Rule of Three for fragment-based lead discovery?, *Drug Discovery Today*, 2003, 8, 876–877.

(2) Kenny, P.: fbdd-lit.blogspot.com.

(3) Hou, T. J.; Xia, K.; Zhang, W.; Xu, X. J.: ADME Evaluation in Drug Discovery 4. Prediction of Aqueous Solubility Based on Atom Contribution Approach, *J. Chem. Inf. Model.*, 2004, 44, 266–275.

\* Based on a comparison with commercially available libraries containing >8 million compounds.

**IOCAS** ← **Key Organics** → **BIONET**

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Key Organics



# Key Organics

*The right side of the Equation*

Key Organics offers a comprehensive range of chemistry solutions to its clients and is a leading global provider in the supply of high quality chemical products and contract services to the pharmaceutical, agrochemical, biotechnology sectors together with related industries and applications.

Key Organics has 25 years of proven expertise and competence enabling it to become a long-term strategic partner to meet all its clients' chemistry needs. Rather than just selling compounds the primary aim of Key Organics is to provide a consistent, reliable and very high quality service, with unrivalled customer support, technical back-up, guaranteed confidentiality and outstanding performance.

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Screening Compounds  
Bulk Intermediates  
Research Intermediates  
Assay Standards  
Fragment Libraries  
Core Scaffolds  
Agrimedates™

**BIONET**

**BIONET** Products

Under the BIONET brand, Key Organics offer the renowned and extensive Bionet Screening Compounds, Bionet Intermediates, Bionet Ro3 Fragments, and Bionet Assay Standards, Core Scaffolds and Agrimedates™ Collections

**Key Organics**

**KOCAS** Services

Tailor-made services under the KOCAS brand include Custom chemistry, Contract/FTE chemistry, Library development, KOCitius, KOSYnergi, and Analytical support services

**KOCAS**

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Whatever the chemistry requirements, Key Organics can be trusted to offer the best value solutions to meet individual needs.

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