Issue 10 | April 2015

Key Organics Newsletter

Chemistry | Innovation | Quality

Our Q2 Newsletter features our new co-marketing collaboration with the University of Nottingham and the launch of our 2nd Generation Premium Fragment library. We also profile our capabilities for filtering and screening our BIONET libraries for more defined physico-chemical properties. We present details of over 600 compounds from our proprietary collection of 5-trifluoromethyl-2,3-disubstituted pyridines and their *N*-substituted analogues that are precursors to the broad-spectrum fungicide Fluazinam and useful precursors to other alkyl and arylaminopyridines. Our interview is with Key Organics Managing Director, Dr Joe Carey and we also profile our forthcoming exhibition and conference attendance for Q2.

New Co-Marketing Collaboration

New product innovation continues to be a strategic priority for our future growth as we seek to further build our successful BIONET product portfolio that now contains over 93,000 intermediates, fragments, biochemicals and screening compounds. BIONET is now one of the fastest growing and valuable global compound collections and our recent investments in new, data-verified, fragment libraries is unrivalled. As well as our internal synthetic chemistry efforts, we seek to establish mutually beneficial co-marketing programmes with selected partners that provide new products, methodology and customer-solutions that are applicable to both research and development across the markets we serve (i.e. pharmaceuticals, agrochemicals and material sciences). Our access to global markets supports the expedient delivery of our BIONET products to meet and exceed our customers' needs.

The University of Nottingham

UNITED KINGDOM · CHINA · MALAYSIA

We are therefore pleased to announce our new co-marketing collaboration with the University of Nottingham. The focus of this partnership will be to commercialize new products emerging from the vast and high value research that is undertaken at the University of Nottingham which continues to rank among the UK's leading Universities for chemistry research. The University will benefit from having access to Key Organics' compound handling unit (CHU) and global sales channels, and also enjoy an additional revenue stream for continued investment. Forthcoming newsletter and product launches will feature a selection of new products from this collaboration.

BIONET Fragment Libraries

As reported in our last newsletter, Key Organics entered into a collaboration with the Broad Institute, (Cambridge, MA) and NMX Research and Solutions, (Montreal, Canada) in order to produce our new **2nd generation BIONET Premium Fragment Library**. This unique library builds upon our previous CNS and Premium Fragment libraries and is now due for release.

Please contact Andrew Lowerson (andrewl@keyorganics.net) for further details.

North American Customers

Our Bedford, MA warehouse and Compound Handing Unit is able to supply our BIONET product range directly to our USA and Canadian customers.
Please visit our website at www.keyorganics.net or contact our US Office Manager, Steven Brouillette at: stevenbrouillette@keyorganics.net

Key Organics
Chemistry Services

Looking for FTE & Custom Chemistry Services?

Our Services team offers a wide range of integrated FTE and custom chemistry services from medicinal and discovery chemistry to process R&D/scale-up and toxicity batch supply. With over 28 years' expertise, we have an excellent track record and continue to add value through our creative input. Our chemists make full use of the Accelrys e-notebook platform to facilitate information exchange, data compliance and efficient project management. We can provide further comprehensive development support throughout the pre-clinical phase.

Our new Key Organics Services brochure is now available in either hard copy or PDF versions. It profiles how our CRO service offerings can make a difference to your drug discovery and development programmes through either accessing our Key Finder™ library design service or our isotope-labelled expertise.

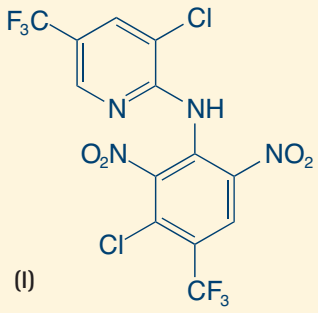
Please visit our website at:
www.keyorganics.net
to download a pdf copy.

New 5-trifluoromethyl-2,3-disubstituted pyridine precursors

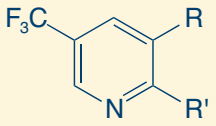
Fluazinam-(I) (3-chloro-*N*-(3-chloro-2,6-dinitro-4-trifluoromethylphenyl)-5-trifluoromethyl-2-pyridinamine) is a broad-spectrum fungicide and is classed as an arylaminopyridine. It acts by inhibiting the germination of spores and the development of infection structures where its mode of action involves the compound being an extremely potent uncoupler of oxidative phosphorylation in mitochondria and also having high reactivity with thiols. It is unique amongst uncouplers in displaying broad-spectrum activity against fungi and also very low toxicity to mammals due to it being rapidly metabolised to a compound without uncoupling activity.

Key Organics has synthesized a collection of over 600 5-trifluoromethyl-2,3-disubstituted pyridines-(II) and its *N*-substituted analogues-(III) that are now available within our BIONET portfolio. Compounds can be purchased as single entities or as functional group classes, please contact us for more information prior to the SD and PDF files being made available on-line.

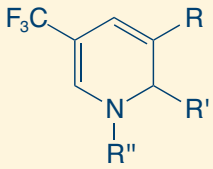
Figure 1. Fluazinam-(I), 5-trifluoromethyl-2,3-disubstituted pyridines-(II) and its N-substituted analogues-(III)



(I)



(II)



(III)

Compound filtering and selection, offering more focused products to meet your needs

For over 28 years, Key Organics has supplied quality intermediates (16k), screening compounds (50k) and fragment libraries (24k) to the international Life Science industry. Our focus has and continues to be on quality, expedient delivery and value to our customers.

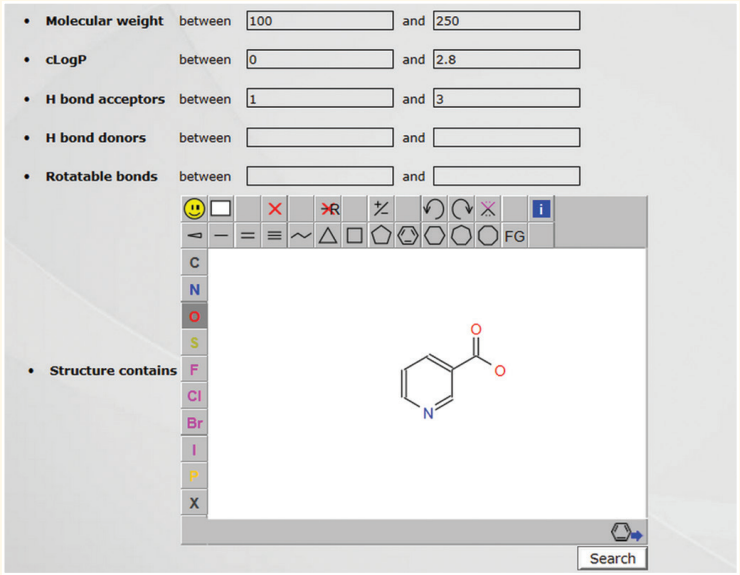
To aid our customers select the compounds of interest for their projects, intermediates are separated out by functional group and also by substructure *(Table 1)*.

Table 1. Functional Group and Substructure Group Classes

BIONET Functional Groups	BIONET Substructure Groups	
Alcohols	Anilines	Naphthyridines
Aldehydes	Azaindoles	Other Ring Systems
Amines	Benzimidazoles	Oxadiazoles
Amino Acids	Benzodioxepines	Oxazoles
Aromatic OH	Benzodioxines	Piperidines
Boron Compounds	Benzodioxoles	Pyrans
Carboxylic Acids	Benzofurans	Pyrazoles
Diamines	Benzothiadiazole	Pyrazolopyridines
Dicarbonyls 1,3	Benzothiazines	Pyridines
Esters	Benzothiazoles	Pyrimidines
Fluorinated Compounds	Benzothiaphenes	Pyrroles
Hydrazides	Benzoxazines	Pyrrolidines
Hydrazines	Benzoxazoles/Benzisoxazoles	Quinazoline
Hydroxylamines	Furans	Quinolines
Ketones	Imidazoles	Quinoxalines
Miscellaneous Functional Groups	Indoles	Thiadiazoles
Nitriles	Isoindoles	Thiazolanes
Protected Compounds	Isoquiolines	Thiazoles
Reactive Halides	Isothiazoles	Thiaphenes
Saturated Compounds	Isoxazoles	Triazoles
Spiro Compounds	Naphthalenes	
Sulphonyl Chlorides		
Thiols		

Customers can also use our advanced on-line search facility to find compounds with specific physicochemical properties such as cLogP (Figure 1).

Figure 1. Search criteria functionality



However, if more advanced refinement is required, Key Organics chemists use a range of software tools to apply further filters, which can also generate clusters and diverse sets of compounds to the customer's specification. We can also filter against PAINS and REOS (Pan Assay Interference compounds and Rapid Elimination Of Swill, respectively) as already applied to our fragment libraries.

These filtering tools (*Figure 2*) can be applied to generate diverse sets of building blocks of a particular functional class for a customer's proposed library synthesis and also to generate filtered, diverse libraries of screening compounds for new lead generation or SAR by catalogue. We can also enumerate virtual libraries using this approach which can be a powerful tool in designing bespoke sets of compounds for Hit to Lead SAR exploration (*Figure 3*).

Figure 2. Set of available acids, mapped in 2D by logP and MWt and in 3D with logP, MWt and number of rotatable bonds.

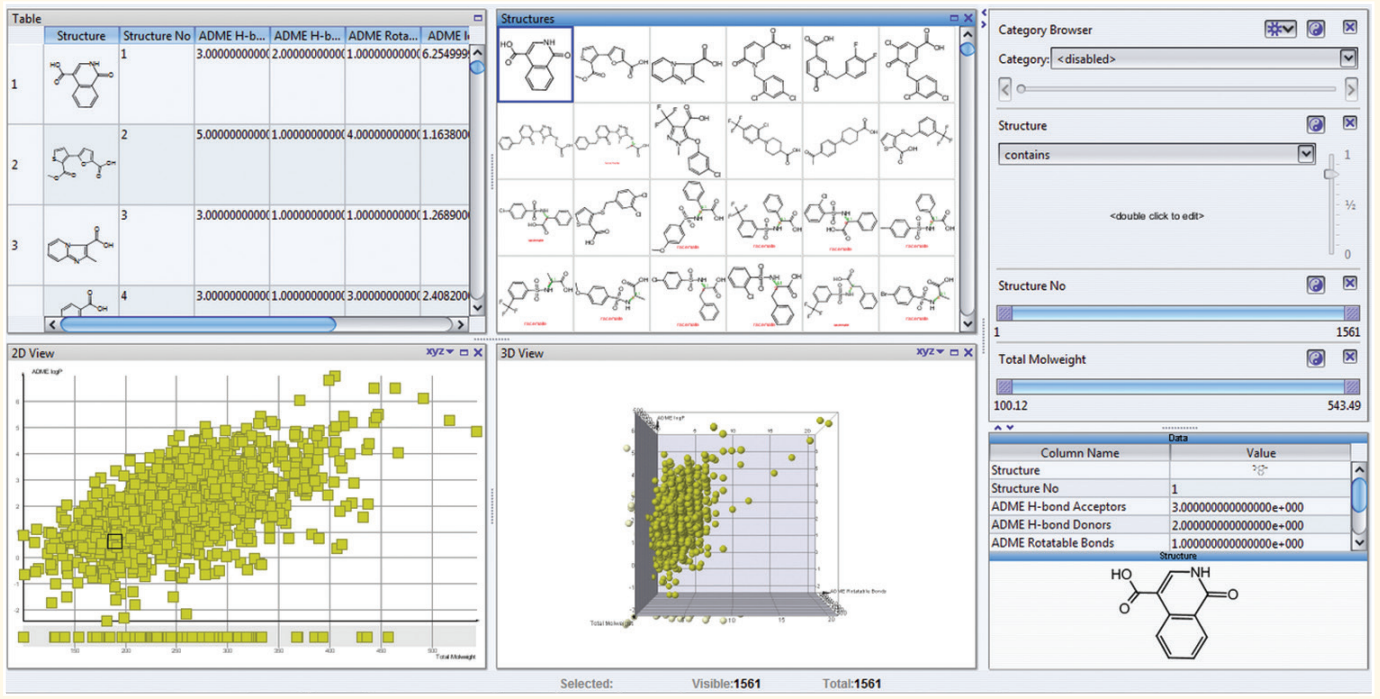
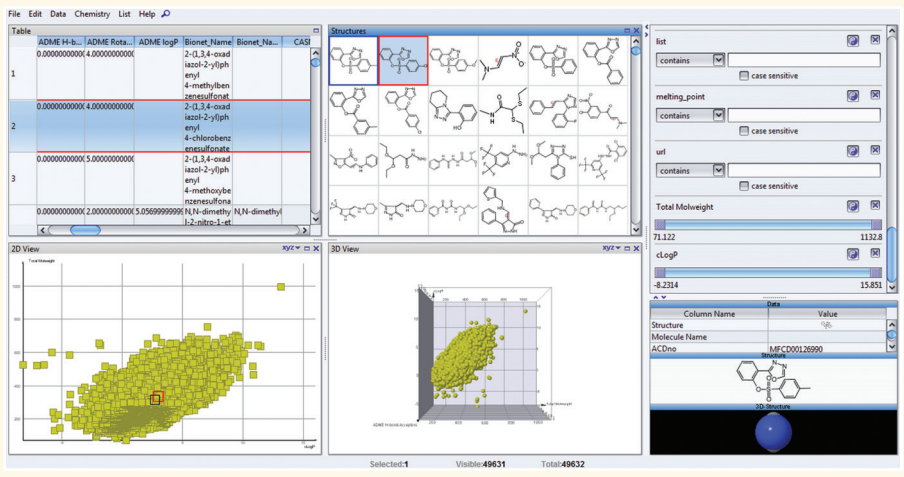


Figure 3. Available screening compounds



After applying the appropriate filters and any desired clustering or diversity, the output can be exported as an SD file which can then be used to generate a purchase list. Using this approach, Key Organics chemists can provide our customers with direct access to high quality sets of compounds that are filtered according to the their project needs. A key selling point is that >90% of our listed compounds are in stock from our unique and proprietary BIONET collection.

Key Organics will be attending the following events this quarter:

April 21st – 23rd	Drug Discovery Chemistry	San Diego, USA	http://www.drugdiscoverychemistry.com
April 22nd – 24th	CPhI	Tokyo, Japan	http://www.cphi.com/japan/home
May 11th – 13th	Biotrinity	London, UK	http://biotrinity.com
May 19th – 20th	Academic Drug Discovery 2015	Cambridge, UK	http://selectbiosciences.com/conferences/index.aspx?conf=ADD2015
June 5th	Opportunities and Challenges in Cancer R&D	Glasgow, UK	http://www.smr.org.uk/smr/Meetings/20150605/Default.asp
June 15th – 18th	BioUSA	Philadelphia PA, USA	http://convention.bio.org
June 24th – 25th	Chemspec	Cologne, Germany	http://www.chemspecevents.com/europe

Staff Interview Dr. Joe Carey, Managing Director

Q: Please tell us a bit about yourself?

A: I originally come from the Wirral and became interested in science through having some inspirational teachers at secondary School. I was fortunate enough to find a chemistry job aged 16, working for Shell Research at their Sittingbourne Research Centre where they undertook agrochemical R&D. As a research technician in their physical organic chemistry team, I enjoyed the freedom to learn and develop eventually leaving after 5 years to study chemistry at Sussex and Oxford where I obtained my D.Phil under Prof. John Brown, FRS. I live in a small village in Cornwall with my family and try to make good use of the wonderful local environment.

Q: What is your role within Key Organics?

A: My main role as MD involves delivering the strategic and business objectives of our board but we are all very much hands-on so I am involved in most operational aspects of the business, particularly marketing, sales and contractual matters. Within a growing business, our management and operational teams are encouraged to be creative and explore new ideas as we seek to build new products and services within our current and new markets. Driving change continues to be our focus and building further differentiation in our quality services and product divisions that are aligned to our customers current and future needs.

Q: What do you enjoy about working at Key Organics?

A: I enjoy working with a creative group of professionals who are passionate about all aspects of our business and willing to go the extra mile for our customers. We are also fortunate to have a strong and supportive parent company who take a long-term view, possibly not surprising since Tennants Consolidated Ltd have been in business since the 1700's! The growth of our BIONET collection from 65,000 compounds back in 2012 to now almost 93,000, together with the launch of our US office last year, means that we are now an established and global player in high value research intermediates and speciality products.

Q: What do you think is Key Organics' greatest strength?

A: As a customer-facing organisation, our people are our greatest strength since they have to translate customer needs into a service or product and deliver consistently to a very high standard. Creativity in developing new products, internally or through partnership plus finding new ways to market and deliver them has been a significant achievement for our team in the last year. Our web sales have increased by over 100% and we have successfully entered new markets and further developed existing territories while making good use of our resources.

Key Organics

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