

Compound Management Service



Compound Management Service

Key Organics can support some or all your key compound management activities including compound procurement, receipt, storage, formatting and distribution needs. We provide both standalone activities on a fee-for-service basis, as well as fully integrated compound management services. Our services include:

- Compound Procurement, via preferred suppliers
- Compound Weighing
- Compound Dissolution
- Automated Reformatting & Plating
- Compound Shipping & Logistics to in-house & partner testing laboratories
- Quality Control
- Reaction ready precursors and reagents
- Assay ready formats
- Computational chemistry

Compound Storage and Stability Testing

Using our storage space and facilities in both Europe and the United States, we are ready to store your powder and liquid samples, format them on demand into the required format and distribute them to your site locations around the world. This service eliminates the need to have an organized compound repository on site while keeping your libraries easily accessible. Our storage conditions range from storage at ambient temperature to a cooled and refrigerated environment. We can also perform regular QC checks to monitor compound integrity during storage and provide valuable stability data.

Compound ordering, handling, reformatting, plating, quality control, storage; Key Organics can take care of it all.

Please contact us for further information on how we can add value to your projects and programmes.

Reaction ready precursors and reagents

Key Organics can provide reaction ready pre-weighed reagents and precursors for your in-house chemistry programs.

Your reagent and precursor needs:

- Customer supplied CAS numbers or Structures
- Functional Group(s) with/without MW cut-offs (we'll send you an SDF offering to choose from)

We can supply from, which can be filtered by price and availability:

- Customer supplied reagents and precursors
- The BIONET Collection
- Our trusted network of Partners

'Reaction Ready Reagents' can be weighed by our expert team into:

- Our standard vials with standard labels
- Customer vials with custom labels
- 'Reaction Ready' microwave tubes in specific molar amounts

With our 'Mix & Match' philosophy you have the flexibility to choose what suits your needs best and Key Organics has the experience to deliver.

Assay ready formats

Key Organics can provide assay ready formats for your in-house chemistry programs.

You tell us:

- The exact compounds
- The plate type (96 or 384 well)
- The plate sealer (cap mats, adhesive etc)
- The plate layout (columns or rows left blank)
- The Volume and Concentration (i.e. 100 μ L of 10mM DMSO)

Additional services provided include:

- Cold Shipment with Temperature Data Logger
- Data provision (Plate Maps, QC Data, Physiochemical properties of the compounds)
- Storage of stock solutions
- Cheminformatics
- Quality Control

Case Study – Reaction Ready and Restocking

Request for Reaction Ready and Restocking Compound Management Services from Sygnature Discovery Limited

Sygnature Discovery sought Compound Procurement Services for the sourcing, procurement, reformatting into 20ml and 7ml vials and shipment of commercially available compounds. Sygnature were interested in procurement of a set of around 293 x 2g reagents and 586 x 100mg reagents. Sygnature supplied a list of structures, CAS numbers and Sygnature IDs.

Tasks & Logistics

- 1 Key Organics searched for the reagents from within the BIONET Collection and from reliable partner sources and prepared SD files that contained compound structures, CAS number, Sygnature ID and cost for the required reagents. Delivery agreed to be in 2 shipments for each order.
- 2 Sygnature selected a set of the 249 x 2g and 212 x 100mg compounds for procurement
- 3 Key Organics processed the BIONET compounds and acquired the partner compounds
 - a. 100mg reformatted into the 7ml vials labelled with CAS and Sygnature ID
 - b. 2g reformatted into the 20ml vials labelled with CAS, Name and Sygnature ID
- 4 Key Organics sent the 1st shipment for each order to end user after approximately 2 weeks and the 2nd and final shipment after 5 weeks
- 5 Documents supplied to Sygnature by email with each shipment included:
 - a. SD file for each shipment with CAS, Name and Sygnature ID
 - b. UPS tracking number

"We provided Key Organics with an SD file containing structures and required quantities and they quickly supplied us with quotes for the individual products. They were happy to format into our vials and provided two shipments, with 98% supplied within our required timeframe. A great service from our preferred partner."

Chris Pearce,
Senior Scientist 2



Case Study – Assay Ready and QC

GreyWolf Therapeutics were interested in procurement of a library of 100 – 200 analogues based around three small molecules of interest.

GreyWolf Therapeutics sought a compound management service for the sourcing, procurement, QC analysis, reformatting into 96 well plates and cold shipment of commercially available compounds.

Tasks & Logistics

- 1 Key Organics searched for analogues that were genuinely available from reliable sources and prepared a spreadsheet that contained compound structures, source, cost, physiochemical properties and information on lead times for 2103 analogue compounds.
- 2 GreyWolf selected a subset of the 2103 compounds for procurement
- 3 Key Organics placed compound orders with several suppliers and consolidated shipments
- 4 Key Organics performed QC of the subset:
 - a. LC-MS m/z to confirm parent ion and purity
 - b. ¹H NMR to confirm structure
- 5 Key Organics reformatted compounds into 96-well plates, 100µL of a 10mM DMSO stock of each compound
- 6 Key Organics made a frozen shipment to end user.
- 7 Documents supplied to GreyWolf Therapeutics included:
 - a. Plate maps in excel and sd file format
 - b. Pdf of all LC-MS and ¹H NMR experiments
 - c. Excel file detailing QC data

"Like other leading biotechs, we rely on integrating key CROs into our drug discovery and development activities to deliver complex logistical solutions to meet our project requirements. Key Organics provided outstanding quality and value in this request, successfully delivering the chosen analogues with QC in an assay ready format."

Dr Martin Quibell,
Director of Medicinal Chemistry



Quality control

Our compound management service is supported by Key Organics analytical services. Compounds can be QC checked by any combination of LC-MS, NMR or GC to ensure they meet the required purity and to confirm the correct structure.

Our dedicated team of experienced and highly qualified staff can provide the following services:

- Compound identification and structure elucidation
- Compound purity screening
- Compound purification
- HPLC and GC method development and/or optimisation



Our analytical department is equipped with the following instrumentation;

- **NMR:** Bruker 400MHz AVIII NMR equipped with a 1H/13C multinuclear probe capable of performing routine 1D experiments plus variable temperature experiments
- **LCMS:** Agilent LCMS, consisting an Agilent 1260 LC multiple wavelength UV/Vis detector and ELSD Coupled to an Agilent 6130 Single Quadrupole Mass Spectrometer
Waters LCMS with multiwavelength uv/vis detector and coupled to a Micromass ZQ 2000 mass spectrometer
- **Preparative LC:** Our Waters LCMS can perform mass-directed fraction collection
- **Gas Chromatography:** Agilent 7890 GC, with flame ionisation detector

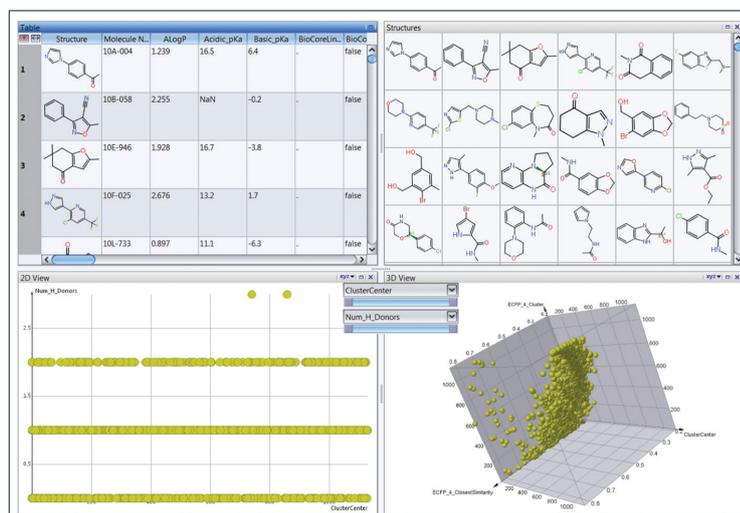
Whatever your requirement; from single analyses to more complex projects, we will be happy to review your request and provide a quotation.

Computational Chemistry

Key Organics can filter compound libraries using a range of software tools. These filtering tools 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.

Our capabilities include:

- Detecting and filtering Pan Assay Interference compounds (PAINS)
- Detecting and filtering compounds with undesirable, toxic or reactive moieties
- Generating clusters and diverse sets of compounds
- Calculating physicochemical properties





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