



React
ALL

THE FUTURE OF REACTION SCREENING

Speed up your product development

ReactALL is an innovative benchtop multi-reactor system with novel automated sampling and overhead stirring for medium-throughput experimentation. This cutting-edge device is specifically designed to address the needs of chemical reaction screening and optimization - route scouting as well as process development and optimization. It fills the gap between high-throughput screening and larger laboratory reactors by providing high-quality, data-rich experimentation with low material needs at medium-throughput. Heterogeneous reactions are well accommodated by the sampling mechanism which representatively captures solids, the stirring mechanism which suspends but does not grind solids, and the integrated cameras which see and profile particle sizes and shapes. This is all achieved in standard vials with 5-10 mL working volume through Technobis' SmartCap™ technology.

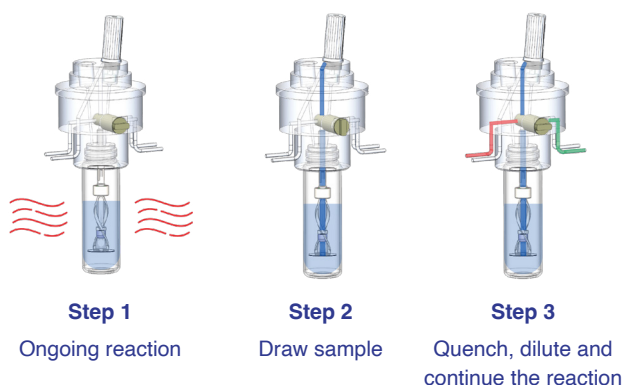
Features

- Five independently controlled reactors with 5-10 mL working volumes
- Integrated automated sampling, quench, and dilution directly into HPLC vials with up to 18 samples per reactor
- Sample heterogeneous reactions with representative sampling of the solid and liquid components without piercing reactor septa
- Overhead stirring with novel helical stirrers designed with the aid of CFD to evenly suspend solids without grinding
- Uses standard vials with SmartCaps™ with novel sampling and stirrer mechanisms
- Integrated color cameras to see and profile particle sizes, shapes and turbidity within the reactors
- Open API - ready for robotics integration
- High-quality, data-rich experimentation with higher throughput and lower material needs

Integrated automated sampling, quench, and dilution directly into HPLC vials

The system comprises five small-scale reactors, each equipped with fully automated sampling. Representative samples are immediately quenched, diluted, and transferred to standard HPLC vials on the *ReactALL*.

The sample, quench and dilution volumes are precisely controlled by the system for quantitative analysis. Wide bore tubing and streamlined pump-free fluidics assure robust sample transfer, even for heterogeneous samples. And the novel SmartCap™ sampling technology does not pierce reactor septa, so there are no pierced holes for losing solvent. The diluted samples are held in HPLC vial racks which are compatible with common HPLCs for easy transfer to the HPLC for a streamlined workflow.



Reclaim up to 76% of your experiment time

Speed your product's time to market, saving precious time, resources and cost along the way. Start running your experiments overnight and find out the results the next morning.

Utilize the power of the SmartCap™ Technology

Fully automated, unattended sampling in each reactor.

Controlled sequencing perfection

Flawlessly executed Sample-Quench-Dilute-Rinse sequence, without the need for additional probes or internal pumps.

Crafted for homogenous mixing

Attain uniform mixing with specifically designed stirrers.

Maximise insights with minimal material usage

ReactALL empowers you to explore multiple experimental conditions with data richness, all while saving resources.

Minimal working volume, maximum output

Operate with a mere 5 to 10 mL of reaction volume.

Versatile screening

Ideal for organic synthesis and multi-condition screening.

Independent temperature control

Take full control of your experiment temperature in each of the 5 reactors. From -10°C to 150°C , no chiller required. Achieve even lower temperature down to -25°C with the optional chiller.





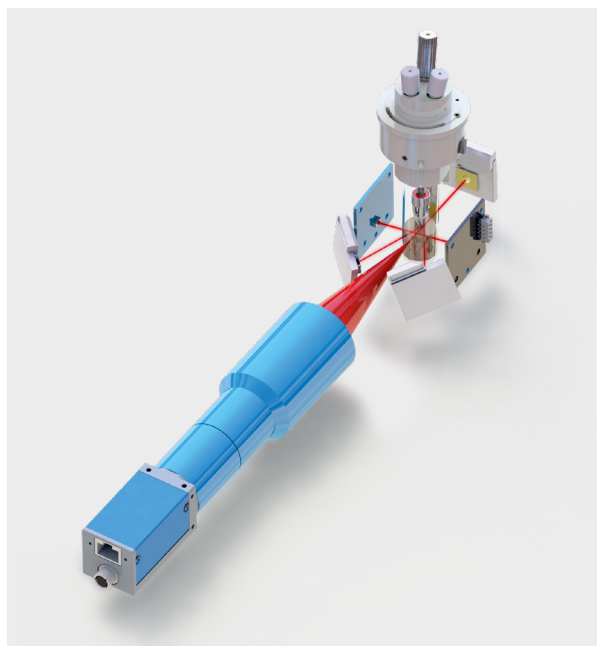
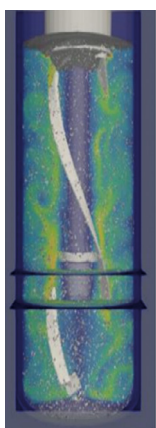
Overhead stirring without grinding solids

The SmartCap™ suspends the innovative stirrers which were designed with the aid of Computational Fluid Dynamics to evenly suspend solids without grinding. The helical shape above a pitch blade creates small eddies which promote mixing and homogenous distribution of solids, even at these small reactor diameters. Importantly, the agitators do not grind solids, a distinct advantage over stir bars which can grind solids and alter chemistry.

Impeller



Helix



Achieve research excellence with next-gen analytics

ReactALL is equipped with integrated colour cameras, which provide invaluable insights into particle shape and size, and allow you to continuously monitor the ongoing reaction.

The instrument's in-line analytics do not require probes, wires, or conduits, and have no contact with the reaction mixture, avoiding potential perturbations or cross-contamination.

Next to this, profile transmissivity comes as a standard feature. It can be used as a simple indicator of texture and changes in texture, within or across reaction conditions.

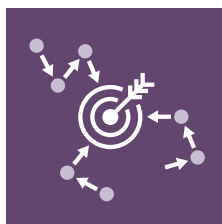
Would you like to use a Raman spectrometer to follow in-line chemical reactions? **ReactALL** is equipped for this as well.

Designed for the Lab of the Future

Save time and materials while increasing insights and results. **ReactALL** is designed to integrate in the Lab of the Future to provide a user-friendly and intuitive experience when you streamline your experiment process.

- Precise, reproducible, standardized and scalable data
- Connectivity to other devices thanks to open APIs
- Compact-sized instrument, optimized for productivity

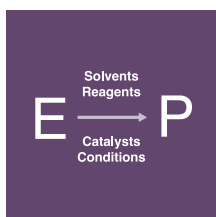
Applications



Route scouting

Route Scouting is an essential step in the chemical development process for the manufacturing of a drug substance. After the preclinical stage, the route of synthesis used in the drug discovery phase may not

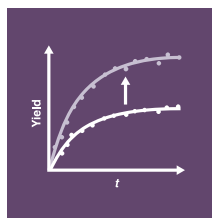
be feasible or optimum for large scale manufacturing. A wide range of factors such as safety, environmental, economic, control, and throughput are considered before establishing the final route for synthesis. **ReactALL** offers the unique advantage of considerably greater data richness and much higher quality experimental control than high-throughput screening. It also offers greater throughput at a significantly lower scale than typical automated laboratory reactors. This allows truly doing more with less, by applying high-quality, data-rich experimentation earlier in the process development timeline when custom synthetic intermediates are in limited supply and very expensive. For example, more efficient synthetic routes may be enabled sooner by getting key but difficult reactions to work by studying more conditions in greater detail more quickly.



Reaction screening

Screening reactions for the best catalyst, reagent, or solvent is often done with high-throughput robotic platforms at very small scale. While these systems can explore a wide range of variables, the experimental

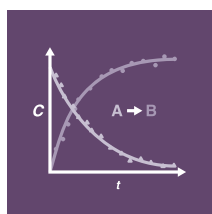
conditions may not be scale predictive, and each reaction gives very little data, typically just reaction endpoint analysis. Confirmational experiments are required at larger scale under more scale predictive conditions, especially for heterogeneous reactions which includes about 70% of reactions. **ReactALL**'s facility with heterogeneous reactions makes it ideal for confirmatory screening experiments. Moreover, **ReactALL** can be used to screen for scalability, i.e., sensitivity to scale up parameters: stoichiometry variations (e.g. from local concentration gradients on scale), temperature variations (e.g. from local hot spots on scale) and lot-to-lot variability of reagents, starting materials, and solvents. Importantly, the smaller scale and higher throughput of **ReactALL** relative to typical automated laboratory reactors allows performing these key experiments earlier in the process development timeline when custom synthetic intermediates are in limited supply and very expensive.



Reaction optimization

The optimization of reaction yield, selectivity, and impurity control with respect to continuous variables such as temperature and stoichiometry requires quality data-rich experimentation, ideally with

higher throughput and smaller scale for speed and efficiency as enabled by **ReactALL**. The integrated HPLC sampling within **ReactALL** is particularly valuable for profiling not only main components, but also trace impurities due to the high dynamic range of HPLC.



Reaction profiling and kinetics

Reaction profiling is valuable for both qualitative observations and quantitative kinetics modeling, both of which are enabled by **ReactALL**'s automated sampling for HPLC and

ReactALL's integrated cameras for particle size and shape. Qualitative observations are key to reaction screening (by finding good reactions which were initially run under the wrong conditions, i.e. correcting false negatives) and reaction optimization (finding the best conditions for not only high yield and selectivity, but also robust conditions where the peak yield and selectivity are a stable plateau with respect to reaction time and conditions). Profiling can also show reaction stalling or induction periods, reaction intermediates, and any product decomposition, all as a function of conditions which can be explored five at a time in **ReactALL**.

Reaction profiling is also extremely valuable for reaction kinetics and quantitative modeling by providing mechanistic understanding for reaction optimization, and reaction modeling to extrapolate from measured reaction conditions to a broader hypothetical reaction space including reaction parameters and scales which have not been studied experimentally (thus saving time and resources). Much richer models can be created from reaction profiles (e.g. from HPLC) than from just reaction end point data. Modeling the formation of impurities (detectable by HPLC) is especially important because the mechanisms which form trace species may be complex and unintuitive and the control of impurities is very important for pharmaceutical synthesis. **ReactALL** offers the particular advantage of relating reaction concentration profiles (from HPLC) with reaction texture and particle characteristic profiles (from the integrated cameras) to model and understand key but otherwise hard to see effects.

What's in the box?



ReactALL



SmartCap™

Helix stirrer

Impeller stirrer

Reservoirs for the quench-dilute-rinse-waste sequencing



Standard HPLC vials with tray



Frit filter (0.5-10 micron)

Specifications ReactALL

Reactors	5
Reactor Type	16 mL vials
Working Volume	5 - 10 mL
Temperatures profiles	5
Temperature range	-10°C to 150°C without chiller -25°C to 150°C with optional chiller*
Temperature accuracy	0.5°C
Heating/Cooling rate	0.1 - 20°C/min
Stirring modes	Impeller & helix shaped
Stirrer materials	3D printed Inconel & PTFE coated magnet
Stirring rate	0 - 1250 rpm
Turbidity	Every reactor
Reflux	0 - 35°C Overpressure relief valve
Sample pocket	12 - 15 µl
Sampling mode	Sequential
Duration sample preparation	2.5 - 4 min.
Dilution factor	70-100x
Total sample (incl. quench & dilute)	~1.2 mL
Sample vials	Std. HPLC
Fully automated sampling (sampling, quench, dilute & rinse)	16 - 18 samples per reactor
In-line analytics	5 particle view imaging cameras and/or Raman probes
Particle size and shape analysis	Yes – with particle view imaging cameras
Extra functions	Additional ports for solid and liquid dosing
Data export	Word Report, XML, CSV
Footprint (DxWxH in cm)	93 x 52 x 43
Additional software	Advanced image analysis

* When ambient temperature is 21°C ± 2°C and chiller cooling capacity at 18°C is about 1180 watt.

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