



Next generation solution  
for automated physchem  
measurement

# SiriusT3 Assays

## **pK<sub>a</sub> assays:**

- Determine pK<sub>a</sub> values to the highest commercially available accuracy
- Generates distribution of species plots
- Determine buffer capacity

Understanding the ionisation state of a drug and how it varies with pH provides key information about the proportion of species available for absorption.

Running pK<sub>a</sub> determinations in different media reveals detailed information about how the pK<sub>a</sub> changes due to solvent interactions, partitioning, precipitation or binding.

## **logP assays:**

- Determine logP
- Determine logD vs. pH
- Study octanol/water & many other mixtures

Understanding the logP and logD reveal how the ionisation state of the molecule influences its lipophilicity. This information can be used to improve ADME predictions as well as evaluating how changes to the molecule can increase/decrease the lipophilicity for a desired application.

## **Solubility assays:**

- Determine intrinsic solubility
- Determine kinetic solubility
- Derive pH vs. solubility profile
- Determine supersaturation

Solubility is a complex and fundamental parameter affecting drug absorption. Understanding the full kinetics of supersaturation, precipitation, dissolution and the relationship between solubility and pH is crucial to understanding the ADME behaviour of a drug molecule.

## **Dissolution assays:**

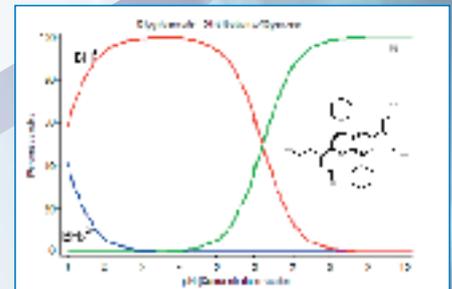
- Profile drugs for dissolution and precipitation rates
- Explore the effects of changing pH
- Run assays with excipients, additives and biorelevant media

Dissolution assays with pH control and in the presence of excipients and biorelevant media (FaSSIF/FeSSIF) can be used to evaluate the effects of different formulations on the dissolution and precipitation kinetics. This information can aid the selection of appropriate formulations for different routes of administration.

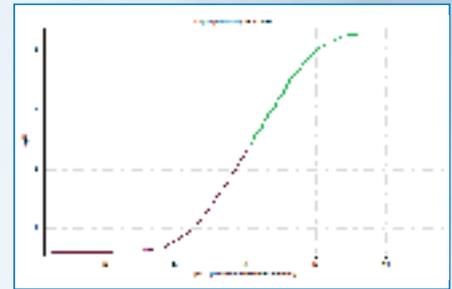
**SiriusT3 automation reduces operator time and replaces the need for time consuming shake-flask style experiments and reliance on multiple pH buffers.**

**Measuring physchem data at early stages of drug development reduces the risk of costly late stage failures.**

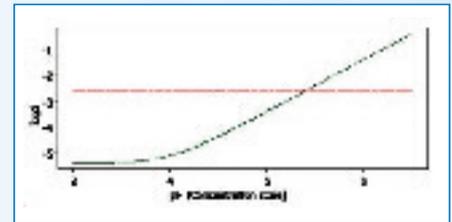
## **Distribution of species**



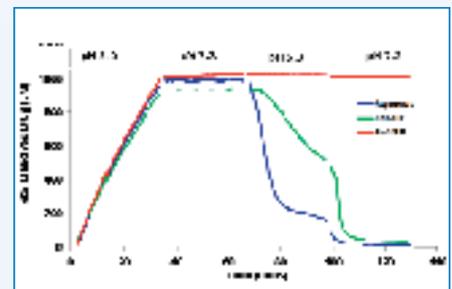
## **Lipophilicity profile**



## **pH vs. Solubility profile**



## **Dissolution profile with variable pH**



## SiriusT3 key features and benefits

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- 
- $pK_a$ , logP, logD, pH-Solubility profiling and dissolution integrated on a single system.
  - Full automation - no manual moving or cleaning of probes required.
  - Minimal running costs - uses off the shelf reagents with no special "kits" required.
  - Built in ultra-sonic bath to aid measurements of insoluble compounds.
  - 1ml assay volume, less than 1mg of sample required for most experiments.
  - Automatic calibration and cleaning protocols.
  - Built-in automatic turbidity detection - precise detection of precipitation events.
  - Computer controlled temperature management - no water circulator required.

Time & Cost Savings

Improved Efficiency

- Fully automated cosolvent assays included as standard.
- Measure under physiologically relevant conditions.
- Study effects of solvents, excipients, additives, biorelevant media.
- pH range of 1.8 - 12.2, extendable to 0.5 - 13.5 with UV options.
- Powerful software can model effects of ionisation, partitioning, precipitation and solvent shifts.

Detailed Data

Better Decisions



The SiriusT3 allows physchem measurements to be performed on sub-milligram quantities of material. This revolution allows the best quality data to be obtained even on discovery compounds where sample quantity is a limiting factor. By obtaining high quality information at an earlier stage in the discovery and development process, decisions about chemistry changes and formulation routes can be made early, saving money, and potential problem areas in other assays can be identified and resolved with ease.

**Ordering Information:**  
Interested in SiriusT3?  
Contact us to arrange a demonstration or free of charge sample evaluation

## SiriusT3 Technical Specification

<b>pH electrode:</b>	Ag/AgCl, double junction reference
<b>Stirrer:</b>	Overhead, variable speed, computer controlled
<b>Temperature probe:</b>	Thermocouple, Temperature measured with every datapoint
<b>Temperature control:</b>	Peltier, Range: 12°C to 70°C
<b>Turbidity detection:</b>	Pass-through light detection - percentage light detected reported to 0.1%
<b>Precision dispensers:</b>	Water, Acid, Base, partition solvent, CoSolvent (six-installed, via automated 6-way valve), minimum volume of 0.024 $\mu$ L
<b>MultiTip dispenser:</b>	Multi-tip capillary bundle
<b>Probe movement:</b>	Fully automated X-Y axis on titrator module
<b>Electrode storage/calibration:</b>	Home position for electrode storage and pH7 buffer positions for calibration
<b>Washes:</b>	Two static washes and flowing water wash station
<b>Autoloader:</b>	Holds up to 192 samples, automatic gripper arm for transfer to sample position
<b>Purge gas:</b>	Two internal flow meters, nitrogen or argon supply required
<b>Partition solvents:</b>	Supports 7 including Octanol, Dodecane, Toluene
<b>CoSolvents:</b>	Supports 10 including Methanol, Acetonitrile, DMSO and MDM
<b>System standardisation:</b>	Sirius Four-Plus™ procedure
<b>pH-range:</b>	1.8 - 12.2
<b>Assay volume:</b>	0.5 to 3.5mls
<b>Services required:</b>	One mains power inlet (110 or 240 V), 50-60Hz
<b>Connection to the PC:</b>	USB
<b>Computer:</b>	Intel compatible processor, 2GB Memory, 10GB Available disk space, one free USB port, CD/DVD-ROM-drive, 1280x1024 screen resolution. XP/Vista/Windows7 with IE6 or higher.
<b>Environment:</b>	For indoor use only Altitude $\leq$ 2000m Temp. 5°C to 40°C Max relative humidity 80% @ 31°C Mains voltage fluctuation +/- 10% Installation overvoltage Cat II Pollution degree 2

Physical Dimensions	Weight	Height	Width	Depth
Dispenser module	35kg/77.16lbs	700mm	260mm	460mm
Titrator	23kg/50.71lbs	490mm	215mm	460mm
Autoloader	27kg/59.52lbs	490mm	350mm	460mm
Total	85kg/187.39lbs	700mm	825mm	460mm



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