



SiriusT3 PhysChem Platform

The SiriusT3 is a fully automated solution for the physicochemical characterization of single-component organic chemicals and their salts. Integrating seamlessly with analytical workflows in drug discovery, it helps researchers to identify the most promising small molecule drug candidates rapidly and efficiently, reducing the risk of late-stage failures.

An integral tool for compound screening, the SiriusT3 measures physicochemical properties such as the ionization constant (pK_a), lipophilicity ($\log P/\log D$) and solubility of ionizable drugs using sub-mg amount of sample. Pion's unique, proprietary Cheqsol method enhances instrument capabilities enabling the accurate determination of kinetic and intrinsic solubilities for ionizable compounds, characterization of supersaturation behavior and the generation of pH-solubility profiles.

The SiriusT3 is the only commercially available fully automated system combining *in vitro* physicochemical property measurement with high-throughput screening capabilities.

ALLOWS USER TO

- Determine pK_a values rapidly and to the highest commercially accessible accuracy for both UV-active (UV-metric) and non-UV active compounds (pH-metric); complete measurements in as little as 15 minutes using the Fast UV technique.
- Generate detailed information about the extent of compounds supersaturated states, their intrinsic solubility, and pH-solubility within a single automated assay in under two hours.
- Apply high throughput pK_a screening; automated assays produce results in ~6 mins per titration.
- Validate pK_a data by applying both spectroscopic and potentiometric techniques.
- Measure $\log P/\log D$ as a function of pH quickly and easily using Pion's potentiometric technique in place of traditional shake-flask methods.
- Minimize sample requirements: Spectrometric assays are performed in solution and typically require only 1 - 2 mg of sample for pK_a and $\log P/D$ analysis and between 1 - 10 mg for solubility measurements.
- Spectrometric pK_a analysis can be conducted with as little as 5 μL of a 10mM sample stock solution.
- Produce high integrity data for regulatory submission (where required).

PRODUCT CONFIGURATIONS

DTAu: The fully automated SiriusT3 system including the dispenser module, titrator module, spectrometer and autoloader. Suited for both potentiometric and spectroscopic use with 192 automated vial positions.

DTu: A one vial only system consisting of a dispenser module, titrator module and spectrometer. This system has both potentiometric and spectroscopic assay capabilities for only 1 assay at a time to be manually replaced by the user.

DTA: A full system including the dispenser module, titrator module and autoloader with no spectrometer. This system has potentiometric assay capability only with use of 192 automated vial positions.

LITE: Also a one vial only system consisting of a dispenser module and titrator module only. This system does not contain the spectrometer and therefore allows fully automated potentiometric assay capabilities for 1 vial at a time relying on manual replacement by the user.

ACCESSORIES

Assay Expert: An optional integrated software prediction module for structural analysis and the identification of ionizable groups. Determine acidity/basicity and estimate pK_a and log P values. Use the resulting data to optimize experimental design.

TECHNICAL SPECIFICATIONS

- pH range 1.8 - 12.2, standardization by Sirius Four-Plus
- pH electrodes containing Ag/AgCl, double junction reference
- Overhead stirrer with variable speed, computer controlled
- Temperature controlled by Peltier, range 12°C to 70°C
- Pass-through light detection to monitor turbidity – percentage light detected reported to 0.1%
- Water, Acid, Base, Partition solvent and CoSolvent reagents used
- Supports 7 different partition solvents including Octanol, Dodecane and Toluene
- Supports 10 different CoSolvents including Methanol, Acetonitrile, DMSO and MDM. Six can be installed simultaneously via automated valve
- Precision dispensers, 0.5 mL syringes, multi-tip capillary bundle, minimum volume of 0.020 mL
- Fully automated probe movement X-Y axis on titrator module
- Wash station provides static and flowing washes
- Autoloader holds up to 192 samples, automatic gripper arm for transfer to sample position
- Purge gas - two internal flow meters, nitrogen or argon supply required
- Assay volumes from 1.0 to 3.2 mLs

DIMENSIONS AND WEIGHT

	Height	Width	Depth	Weight
DTAu	700 mm	825 mm	460 mm	85 kg
DTu	700 mm	475 mm	460 mm	58 kg
DTA	700 mm	825 mm	460 mm	85 kg
LITE	700 mm	475 mm	460 mm	58 kg



Pion stands behind the science

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Specifications subject to change without notice
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