LICHAINED LABS

Big Kahuna Small molecule preformulation

Big Kahuna lets you run hundreds of experiments in parallel with way less material, so deep exploration of your preformulation space is totally doable. Pick your variables, map out your workflow and get it all done on one system. See the big picture more clearly, discover clues and spot more advantageous variables and conditions.

Applications

- Solubility screening
 - Chiral resolution
 - LogP and LogD determinations
- Polymorph screening
 - Solvent screening
 - Salt selection/solvent screening
 - Cocrystal screening
- Powder dispensing
- Reaction screening

Key features

- Evaluate up to 384 crystallizations per run
- Analyze samples by birefringence, XRD and Raman spectroscopy without wrecking a single crystal
- Transfer and filter 96 solutions at elevated temperatures with no API precipitation
- Heat, cool, and mix on-deck, and perform parallel slurry, precipitation, cooling, and evaporation experiments on a single platform
- Design complex experiments quickly using LEA's logical recipe-oriented approach
- Add process chemistry screening capabilities and screen up to 96 reactions in parallel



Big Kahuna configured for small molecule preformulation





Heated dispense element with septum-piercing tips

Crystallizer block for polymorph screening



Example Big Kahuna deck configured for small molecule preformulation

- 1 Vial/plate gripper
- 2 Balance with visual inspection
- 3 Powder dispense hopper rack
- 4 Passive rack

- 5 Tip rack
- 6 3-position heating/stirring7 3-position heating/stirring
- 7 3-position heating/stirring8 Heated filter block
- 9 Heated 4-tip liquid
 - dispenser

Available options

Vial/plate gripper

Plate size: Standard microtiter Vial size: 1–125 mL Total mass: Up to 3 kg

Heated 4-tip liquid dispenser – extended tip

Heated reservoir volume per tip: 1 mL Reservoir temperature: Up to 120 °C Temperature uniformity: ±2 °C (across tips) Tip pitch: 9 mm Extendible tip: 1 Syringe sizes: 50 µL – 10 mL Needle size: 22 gauge, piercing

Heating/cooling/stirring station

Temperature range: -20-180 °C Mixing: Up to 750 rpm Mixing type: Magnetic tumble stirring

Heated filter block

Vial operating temperature: Ambient to 120 °C Temperature controller accuracy: ±1 °C Heater temperature ramp rate: 2 °C/min while heating Cooling: By convection Vial temperature uniformity: ±6 °C @ 60 °C Filter: High efficiency 0.7 µm binder-free glass microfiber

Crystallizer

Format: 96 independent crystallizations, with a universal substrate

pH measurement

Configuration: Single or 4-channel probe Measurement time per 96-well plate: <90 minutes Range: 1–13 pH units Resolution: 0.05 pH units Repeatability: ±0.1 pH units

Vortexing station - 3 positions

Orbital: 60–3570 rpm Maximum vortexing mass: 2268 g (5 lb/plate)

Deck screening pressure reactor (DSPR)

Max pressure rating: 200 psi @ 180 °C Pressure drop: <5 psi/hr

Viscous liquid dispenser

Technology: Positive displacement tip (PDT) **Disposable tips:** 10–10,000 μL, from Eppendorf and Rainin **Viscosity:** 1–1,000 cP



Unchained Labs

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Solid dispense

Dispense technology: Dispense algorithm dynamically controls the dispensing head to adjust for powders with different densities, particle sizes, particle shapes and static charges

- Classic powder dispense: Traditional stirrer dispense mechanism
 Hopper volume range: 10–100 mL
- Storage vial (SV) powder dispense: Unique vibratory dispensing mechanism for highly precise dispensing of small amounts as low as 0.5 mg
 - Hopper volume: 4 mL

Balance with integrated camera

- Maximum weight:
 - **Standard**: 1200 g
 - High-sensitivity option: 220 g
- Sensitivity:
 - Standard: 0.1 mg
- High sensitivity option: 0.01 mg
- Resolution:
 - Standard: 0.1 mg
 - High-sensitivity option:
 - 0.01 mg (0-110 g)
 - 0.1 mg (110-220 g)
- Repeatability:
- Standard:
 - High weight (measured >200 g): 0.25 mg
 - Low weight (measured up to 200 g): 0.15 mg
- High-sensitivity option:
 - High weight (measured at 200 g): 0.15 mg
 - Low weight (measured at 10 g): 0.04 mg

Response time: <22s

Camera resolution: 1032 pixels (max wide) x 779 pixels (tall)

Vial capping/de-capping station

Vial range: 2–125 mL

Off-deck third-party instrument integration

- XRD
- Birefringence microscope
- Raman

Other systems available for virtual integration. Please contact Unchained Labs for a full list of systems.

Facilities requirements

Physical:

Without enclosure: 156 cm W x 90.8 cm D x 140 cm H, ~300 kg With integrated enclosure:

193 cm W x 152.4 cm D x 220 cm H, ~612 kg

Electrical:

Big Kahuna: 208–220 V ±10 %, 50–60 Hz, 20 A

Computer:

US: 115 V ±10 %, 60 Hz

EU: 220 V ±10 %, 50 Hz

Compressed dry air: 0.5–0.9 MPa (70 psi to 130 psi), 4 L/min (8 mm hose)

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