

Big Kahuna

Process chemistry

Big Kahuna lets you make additions and grab samples from your reactions while they're happening. You'll have a whole new level of insight into what your small process tweaks do in real time. Take it to the next level and screen both discrete variables like catalyst precursors and ligands and continuous variables like temperatures, pressures and time. Pinpoint key process variables, map out reaction profiles, identify high yield and selectivity conditions, and optimize synthetic routes – all on the same system.

Applications

- Process optimization
 - Identify high yield conditions
 - Reaction screening and optimization
- Screen continuous variables such as equivalents, concentrations, temperatures, pressures and time
- Screen discrete variables such as catalyst precursors, ligands and solvents
- Optimize and screen new synthetic routes
- Improve yields and impurity profiles
- Optimize catalyst loading
- Map process robustness

Key features

- Rapid, real-time reaction kinetics
- Process control of 8 individual reactions with independent pressure and temp control
- Fully automated *in-situ* reagent addition and slurry sampling under pressure
- Execute up to 96 pressurized reactions such as hydrogenation (with optional SPR or DSPR)
- Overhead stirring for complete reaction mixing
- Accurate and automated dosing of small quantities of solid, liquid or slurry reagents
- Control heating, stirring, and vortexing in vials or microtiter plates
- Provide an inert atmosphere for air-sensitive chemistries



Big Kahuna configured for reaction screening



Optimization sampling reactor (OSR)



Example Big Kahuna deck configured for reaction screening

- | | |
|----------------------------------|--------------------------------|
| 1 Vial/plate gripper | 5 Vortexing station |
| 2 Waste bin | 6 Solid dispensing tool rack |
| 3 Balance with integrated camera | 7 Heating/cooling/stir station |
| 4 PDT rack | 8 Capping/decapping station |
| | 9 1-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
Extendable tip: 1
Syringe sizes: 50 μ L–2.5 mL (standard supplied)

1-tip liquid dispenser

Dimensions (OD, ID, L): 2.03 mm x 0.76 mm (18–19 gauge) x 323 mm
Syringe sizes: 50 μ L–10 mL

Viscous liquid dispenser

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

Heating/cooling/stirring station

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

Vortexing station – 3 positions

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

pH measurement

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

Heated single-tip liquid dispenser

Heated reservoir volume per tip: 1 mL
Reservoir temperature: Up to 120 °C
Syringe sizes: 1–2.5 mL (standard)
Needle size: 16 gauge, non-piercing

Deck screening pressure reactor (DSPR)

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

Optimization sampling reactor and sampling arm

Temperature rating: –20–200 °C
Reactors: 8 independent reactors
Possible delta between adjacent reactors: 50 °C
Heating rate: Up to 5 °C/min
Cooling rate: Up to 2 °C/min
Pressure rating: 30–400 psi
Maximum overhead stirring speed: 750 rpm
Reactor total volume: 40 mL
Reactor working volume: 5–25 mL

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

- HPLC
- GC

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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