

# High throughput library synthesis with online NMR

FLEX ISYNTH for library synthesis and reaction screening with online/offline NMR



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Automated, parallel library synthesis and reaction screening with online benchtop NMR (e.g. automated synthesis, online characterization, data analysis, AI / ML closed loop).

# Solution overview

Molecules discovery (e.g. in medicinal chemistry) is driven more and more by the demand for innovative medicines which involves molecular diversity and novel routes, meaning more and more experiments typically with the same resources.

Chemspeed's fully automated, integrated FLEX ISYNTH stands for a flexible, modular, and uncompromising automated solution that:

Unlocks the chemical space via faster, better, virtually unrestricted "off-road" chemistry investigation of the reaction space, reagent space and molecule space.

Chemspeed's ISYNTH deck modularity provides unrivalled versatility to execute and perform a variety of synthesis workflows (conventional, MW-assisted, photochem, reactive gas) in a fully automated fashion, including reaction preparation, multistep synthesis, work-up, purification, analysis and product transfer to storage.

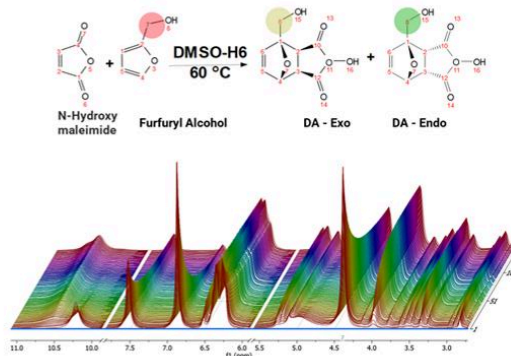
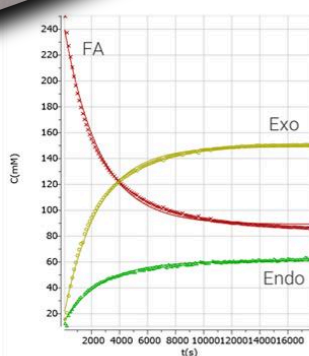
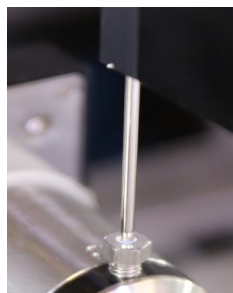
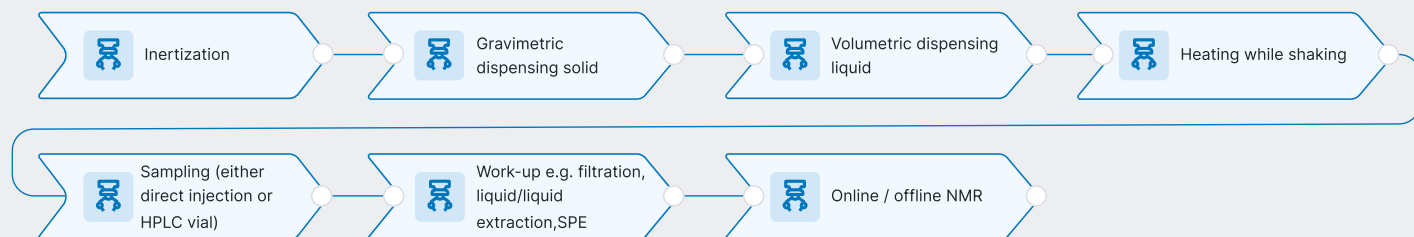
Enhances your efficiency and productivity by a factor of up to 100 in, for example: C-C / C-N coupling reactions, organometallic reactions (e.g. Grignard), alkylations, Diels-Alder reactions and transfer hydrogenations.

## Key advantages & features

- Fully automated, integrated reaction preparation, synthesis, work-up, analysis, output to storage vials for solid- and liquid-phase library synthesis as well as reaction screening.
- Easy-to-use disposable multi-functional, high-precision glass reactor arrays, available reaction scales from  $\mu\text{L}$  to mL.
- Glass reactor arrays with screwless and self-sealing opening / closing, mixing by shaking (up to 1'000 rpm), heating (up to 150°C) and cooling (-20°C), refluxing, vacuum, inertization, evaporation, L/L extraction, filtration, solid-phase extraction, crystallization and drying.
- Proprietary robotic tool exchange.
- Gravimetric solid handling from  $\mu\text{g}$  to g.
- Gravimetric liquid handling from mg to g /  $\mu\text{L}$  to mL.
- Chemistry proven liquid handling with e.g. pH, filtration, heated needle extension.
- Throughput, e.g. 24 / 48 / 96 / ... parallel reactions per run based.
- Sampling and various integrated analytics such as benchtop online NMR, HPLC (MS), UPLC (MS), GC (MS), UV-VIS, NIR / MIR / DLS measurement cell.
- Ventilated hood for safety and conditioned operation.
- AUTOSUITE SOFTWARE - drag & drop experimentation with easy interface (e.g. python custom device) to e.g. LIMS, ELN, data analysis, AI / ML closed loop.
- Exemplary integrated benchtop NMR with available operating frequency ranges of e.g. 80 / 90 MHz such as Bruker Fourier Rxn Lite, Magritek Spinsolve, incl
  - NMR device
  - Sample injection port, software and hardware integration
  - H, F, C, P, Si, B
  - 1D and 2D spectra
  - online data acquisition via flow cell or offline via standard 5 mm sample tubes
  - permanent magnet - no liquid nitrogen or helium required
  - 2 Gauss line inside NMR device housing.

## Example workflow

Chemspeed solutions can be configured to your exact workflow; here is an example of our high throughput library synthesis for innovative, better medicines workflow.



## Accelerating your existing workflows

This example solution showcases one possible workflow using Chemspeed's technologies, but the possibilities are almost endless. Building your ideal platform has never been simpler with Chemspeed. From powder dispensing to chromatography, our configurable solutions are modular and constructed to suit your exact needs.

Combine a Chemspeed base platform, robotic tools from our extensive library, reactors, vessels, racks, vials and software to create a system that compliments and enhances your workflow.



### Platforms

House your chemistry instrumentation in a solid platform. The nature of your project will decide the scale of system you require. Chemspeed offer three highly-versatile platforms as the basis for every possible instrumentation to be housed in: SWING, FLEX and FLEXSHUTTLE.



### Tools

Chemspeed's extensive tool library contains more than 70 robotic tool-features that can be integrated with Chemspeed's unique robotic tool exchange technology, including unrivalled overhead gravimetric dispensing, which can operate while mixing, heating, refluxing and cooling. Virtually any combination of these robotic tools is possible.



### Software

Quickly design, execute, analyze and report experiments with our AutoSuite software. Coordinate and orchestrate larger laboratory workflows with ArkSuite, or even digitalize your entire workflow, including manual tasks, using ArkSuite Sofia.

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## Automate and digitalize your laboratory with Chemspeed.

