Cooperative Mobile Robots for Autonomous Synthetic Chemistry

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Autonomous laboratories can accelerate discoveries in chemical synthesis, but this requires automated measurements coupled with decision-making processes based on those data.[1] Most autonomous laboratories are highly engineered[2] and the measurement instruments are integrated directly with the synthesis platforms.[3] The associated cost and complexity favours the use of a single, fixed characterisation technique rather than drawing on the wide range of instrumentation available in a standard synthetic laboratory. Any decision-making algorithms must then operate using this narrow range of characterisation data.4 As a result, closed-loop autonomous chemical synthesis bears little resemblance to human experimentation, either in the infrastructure required or in the decision-making steps. Here we show that a synthesis laboratory can be integrated using two cooperative mobile robots that perform measurements and make decisions in a more human-like way. Our modular and flexible workflow features two mobile robots, a Chemspeed synthesis platform, a liquid chromatography-mass spectrometer (LC-MS), and a benchtop nuclear magnetic resonance (NMR) spectrometer. This collaborative robotic approach allows for the autonomous use of existing specialized equipment without monopolizing it or requiring extensive redesign. A heuristic decision-maker processes the measurement data, selecting successful reactions to advance further and automatically checking their reproducibility. We exemplify this approach in the areas of medicinal chemistry-inspired structural diversification, supramolecular host-guest chemistry, and photochemical synthesis. More generally, the inherently modular nature of this strategy allows the easy integration of other characterization methods and other chemistries.
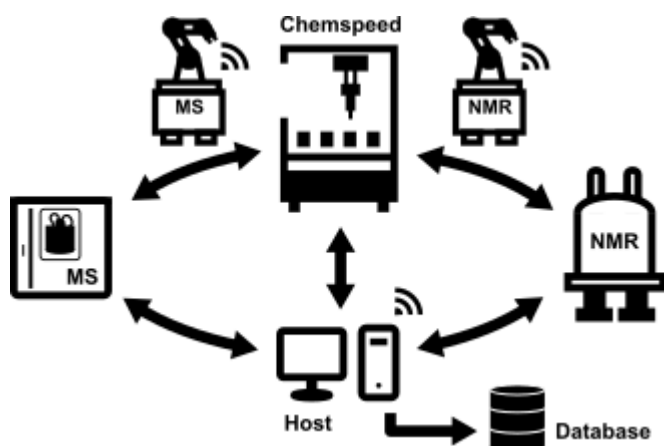
Figure 1: Workflow design for an autonomous synthesis platform utilizing two mobile robots for sample transportation between a Chemspeed synthesizer and a benchtop NMR spectrometer and an ESI-MS spectrometer.

Bibliography :

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