

# Automated Rapid Reaction Screening by DESI-MS

**A novel method integrates accelerated chemical reaction synthesis and online analysis using microdroplets and mass spectrometry, offering rapid, automatic, and error-free screening of numerous reaction mixtures.**

Combinatorial chemistry involves chemical synthetic methods that make it possible to prepare a large number of compounds in a single process. There are many limitations with current processes including the use of separate systems for reaction synthesis and reaction screening. Typically, a robotic instrument combines reagents and conducts reactions, which can vary from minutes to hours, to even days. Once completed, the transfer to a screening instrument, such as a mass spectrometer, takes place after the manual sample of each reaction product and the manual creation of an array of reaction products on a substrate for screening. The screening of each reaction product is time consuming. Given the reaction product is manually prepared, numerous errors, such as contaminated or mixed-up samples, leads to improper data. Repeating the entire process is the only solution.

Researchers at Purdue University have developed systems and methods for conducting reactions and screening for reaction products. This method is based on desorption electrospray ionization (DESI) of the reaction mixture to produce microdroplets containing the reagents. Within the droplets, the reagents can react at accelerated rates. The droplets are directed towards a mass spectrometer (MS) and their contents are monitored online using MS. This method offers accelerated screened reactions, with analysis performed online and in concert with reaction, and the speed of DESI analysis allows for the analysis in a single experiment of a large numbers of different reactions mixtures.

## Advantages:

- Rapid
- Automatic
- Uses existing equipment

**Technology ID**  
2017-COOK-67863

## Category

Robotics &  
Automation/Automation &  
Control  
Biotechnology & Life  
Sciences/Analytical & Diagnostic  
Instrumentation  
Chemicals & Advanced  
Materials/Materials Processing &  
Manufacturing Technologies

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## View online



Potential Applications:

-Chemical analysis

-Microfluidics

**TRL: 3**

**Intellectual Property:**

Provisional-Patent, 2017-03-22, United States | NATL-Patent, 2018-03-22, China | NATL-Patent, 2018-03-22, Europe | PCT-Patent, 2018-03-22, WO | NATL-Patent, 2019-09-17, United States | CON-Patent, 2022-05-16, United States | CON-Patent, 2023-01-25, United States | CON-Gov. Funding, 2023-10-10, United States | CON-Gov. Funding, 2024-10-07, United States | DIV-Patent, N/A, China

**Keywords:** Combinatorial chemistry, chemical synthetic methods, reaction synthesis, reaction screening, desorption electrospray ionization, DESI, microdroplets, mass spectrometer, accelerated reactions, online analysis, Chemistry and Chemical Analysis, DESI, Ionization, Mass Spectrometry