Communications in Computational Chemistry
Commun. Comput. Chem., Vol. 7, No. 3, 226–242
doi: 10.4208/cicc.2025.90.03

Review

Recent Progress in Autonomous Laboratories for Chemical Synthesis

Zhenyu Jiang[1,†], Yubang Liu[1,†] and Zhuofeng Ke[1,*]

[1]*School of Materials Science and Engineering, PCFM Lab, The Key Laboratory of Low-carbon Chemistry & Energy Conservation of Guangdong Province, Sun Yat-sen University. Guangzhou 510275, P. R. China.*

[†] Z.J. and Y.L. contributed equally

[*]Corresponding author: kezhf3@mail.sysu.edu.cn

Received on 31 March 2025; Accepted on 05 May 2025

Abstract: The integration of artificial intelligence (AI) and robotics into chemical synthesis has given rise to autonomous laboratories, transformative systems designed to overcome limitations in traditional experimental approaches. This review synthesizes recent advancements in autonomous laboratory systems, highlighting their applications in chemical synthesis and the innovations driving their evolution. Autonomous laboratories combine automated hardware, intelligent software, and adaptive systems to optimize experimental workflows, reduce human intervention, and enhance efficiency in complex reaction environments. Key developments include AI-driven reaction pathway planning, closed-loop optimization frameworks, and robotic platforms capable of executing multi-step synthesis with minimal expert oversight. Leading research groups have demonstrated significant progress, such as AI-guided discovery of functional materials, automated photocatalytic reaction optimization, and self-learning microfluidic systems. This review provides a comprehensive analysis of current achievements and remaining gaps, offering insights for researchers and policymakers in advancing this transformative technology.

Key words: autonomous laboratory, chemical synthesis, artificial intelligence, machine learning.

1. Introduction

Global challenges in energy development, healthcare, and food safety have underscored the limitations of traditional chemical synthesis processes, particularly their slow experimental throughput, high trial-and-error costs, and poor adaptability to complex reactions [1]. To circumvent these hurdles, next-generation autonomous laboratories have arisen, synergizing automated robotic workstations with advanced artificial intelligence (AI) decision-making systems [2]. In these laboratories, experimental protocols are first designed by artificial intelligence, then implemented by robotic platforms, with data analysis performed concurrently. This closed-loop system achieves significant time reduction and efficiency gains [3], and empowers researchers to investigate more extensive and complicated experimental setups, transforming the creation and improvement of sophisticated experiments into attainable objectives [4].

Autonomous laboratory systems are built upon three fundamental elements: physical equipment, digital program, and integrated platform. The physical apparatus manages chemical transformations, carries out synthetic procedures, and performs material characterization. This component comprises dedicated synthesis and analysis tools for routine operations, versatile robotic manipulators capable of adaptive tasks, modular devices including additive manufacturing systems [5,6] and liquid handling workstations [7]. These tools reduce hardware procurement costs and enable autonomous device construction. The digital program concentrates on planning optimal experimental protocols and controlling robotic activities, merging: (1) device communication, (2) data management, (3) AI decision-making, and (4) experimental planning modules [8]. The modular architecture is further augmented through the integration of advanced probabilistic optimization frameworks and machine learning paradigms. Specifically, Gaussian process-based Bayesian Optimization (BO) facilitates efficient exploration of high-dimensional experimental parameter spaces by constructing surrogate models that balance the exploitation of known optima with an exploration of uncertain regions [9]. Reinforcement learning (RL) algorithms, implemented through Markov decision processes, enable autonomous policy optimization by maximizing cumulative reward signals derived from experimental outcomes [10]. Deep neural network architectures, particularly attention-based transformer models, provide robust pattern recognition capabilities for multivariate experimental data analysis, enabling the prediction of complex structure-property relationships [11]. This synergistic integration of machine learning methodologies significantly enhances the system's capacity for autonomous experimental design and closed-loop optimization while maintaining rigorous statistical foundations. The integrated platform serves as the laboratory's "brain", physical sensors, executing algorithmic decisions, and delivering accurate operational commands. The platform simultaneously serves as a bidirectional communication interface, permitting investigators to conduct remote experiment supervision, access instantaneous measurement data, and execute necessary manual override [12].

To date, several research teams globally have effectively implemented self-operating laboratory systems in synthetic chemistry applications (Figure 1), demonstrating substantial advancements. Nevertheless, current automated research platforms continue to face considerable challenges, including underdeveloped algorithms for complex chemical processes, exorbitant costs of research and development as well as maintenance, and unavoidable human participation in select procedural stages [3]. These limitations impede the broad adoption and continued evolution of autonomous laboratories. Consequently, this review seeks to analyze state-of-the-art innovations in automated synthesis technologies, define their operational frameworks and characteristic features, and evaluate their successes and ongoing challenges, providing references for future research on autonomous laboratories.

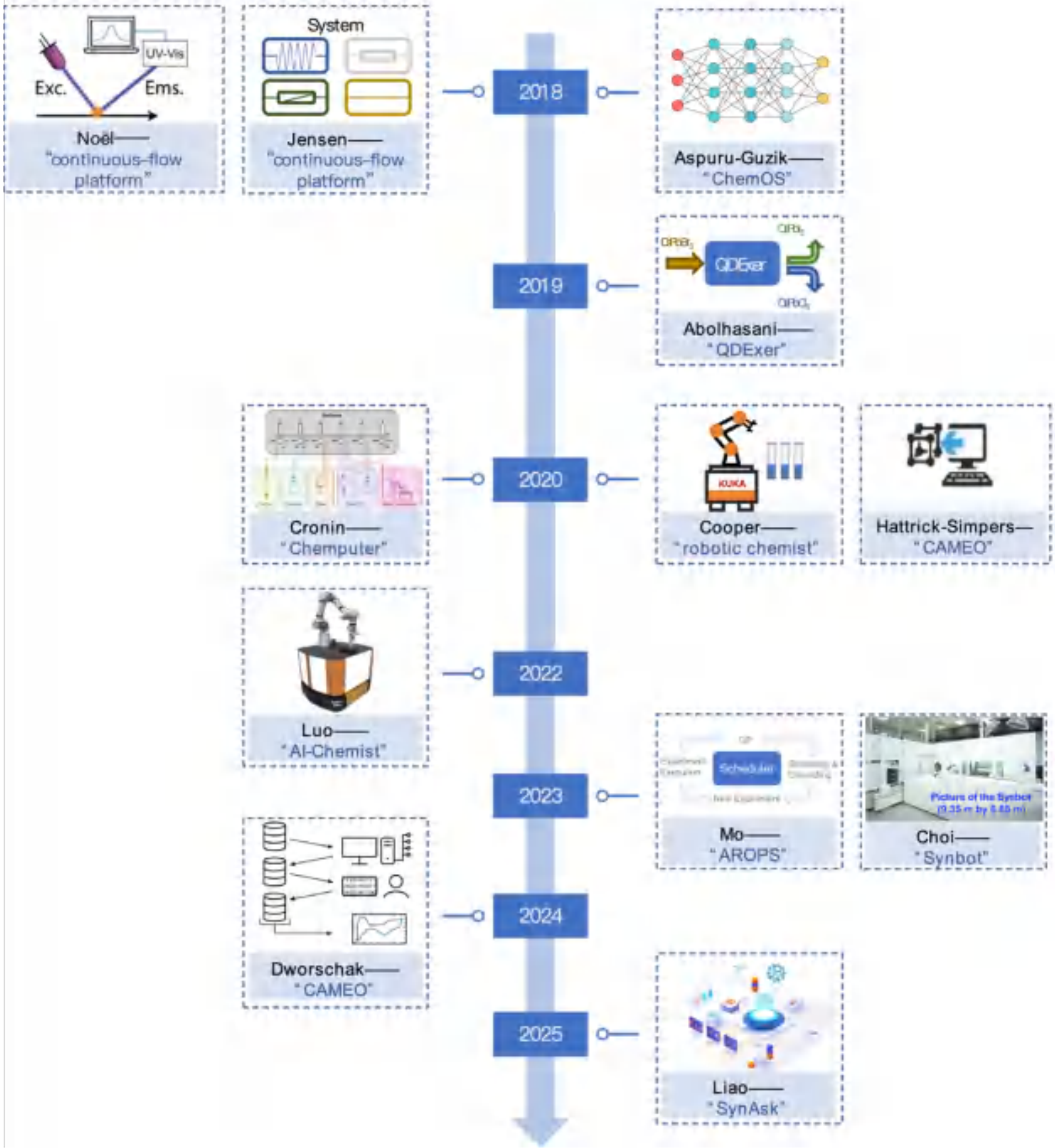

Figure 1. Timeline of the publication of the first key achievements by various research teams [13-24]. Panels reproduced/adapted with permission. Copyright: Refs 13,15,18 © AAAS; 14,17 © Wiley (CC-BY); 16 © Wiley-VCH; 19 © Nature Communications (CC-BY); 20 © National Science Review (CC-BY); 21 © ACS; 22 © Science (CC-BY); 23 © J. Mater. Chem. A (CC-BY); 24 © Chem. Sci. (CC-BY). Full license links in Supporting Information.