

# 1 An affordable platform for automated synthesis and 2 electrochemical characterization

3 Sergio Pablo-García<sup>1,2</sup>, Ángel García<sup>3,\*</sup>, Gun Deniz Akkoc<sup>4,5</sup>, Malcolm Sim<sup>1,2</sup>, Yang  
4 Cao<sup>1,2,6</sup>, Maxine Somers<sup>1,2</sup>, Chance Hattrick<sup>1,2</sup>, Naruki Yoshikawa<sup>2,7</sup>, Dominik  
5 Dworschak<sup>4</sup>, Han Hao<sup>1,2,6\*</sup>, Alán Aspuru-Guzik<sup>1,2,6,7,8,9,10,\*</sup>

6 <sup>1</sup>Department of Chemistry, University of Toronto, Lash Miller Chemical  
7 Laboratories 80 St. George Street, Toronto, ON, M5S 3H6, Canada

8 <sup>2</sup>Department of Computer Science, University of Toronto, Sandford Fleming  
9 Building, 10 King's College Rd., Toronto, ON, M5S 2E4, Canada

10 <sup>3</sup>Senior electrical engineer, Badalona, Catalonia, Spain

11 <sup>4</sup>Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for  
12 Renewable Energy (IEK-11), Cauerstraße 1, 91058 Erlangen, Germany

13 <sup>5</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Chemical and  
14 Biological Engineering, Egerlandstraße 3, 91058 Erlangen, Germany

15 <sup>6</sup>Acceleration Consortium, 80 St George St, Toronto, ON, M5S 3H6, Canada

16 <sup>7</sup>Vector Institute for Artificial Intelligence, 661 University Ave. Suite 710, Toronto,  
17 ON, M5G 1M1, Canada

18 <sup>8</sup>Department of Materials Science & Engineering, University of Toronto, 184  
19 College St., Toronto, ON, M5S 3E4, Canada

20 <sup>9</sup>Department of Chemical Engineering & Applied Chemistry, University of Toronto,  
21 200 College St. Toronto, ON, M5S 3E5, Canada

22 <sup>19</sup>Lebovic Fellow, Canadian Institute for Advanced Research (CIFAR), 661 University  
23 Ave., Toronto, ON, M5G 1M1, Canada

24 \* Corresponding authors email: ag1289@gmail.com , hann.hao@utoronto.ca

25 [alan@aspuru.com](mailto:alan@aspuru.com)

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# 1 Abstract

2 Electrochemical techniques are pivotal for material discovery and renewable energy;  
3 however, often the extensive chemical spaces to be explored require high-throughput  
4 experimentation (HTE) to ensure timely results, which are costly both for instrument and  
5 materials/consumables. While self-driving laboratories (SDL) promise efficient chemical  
6 exploration, most contemporary implementations demand significant time, economic  
7 investment, and expertise. This study introduces an open and cost-effective autonomous  
8 electrochemical setup, comprising a synthesis platform and a custom-designed  
9 potentiostat device. We present an SDL platform that offers rapid deployment and  
10 extensive control over electrochemical experiments compared to commercial  
11 alternatives. Using ChemOS 2.0 for orchestration, we showcase our setup's capabilities  
12 through a campaign in which different metal ions reacts with ligands to form  
13 coordination compounds., yielding a database of 400 electrochemical measurements.  
14 Committed to open science, we provide a potentiostat design, campaign software, and  
15 raw data, aiming to democratize customized components in SDLs and ensure transparent  
16 data sharing and reproducibility.

# 1 Introduction

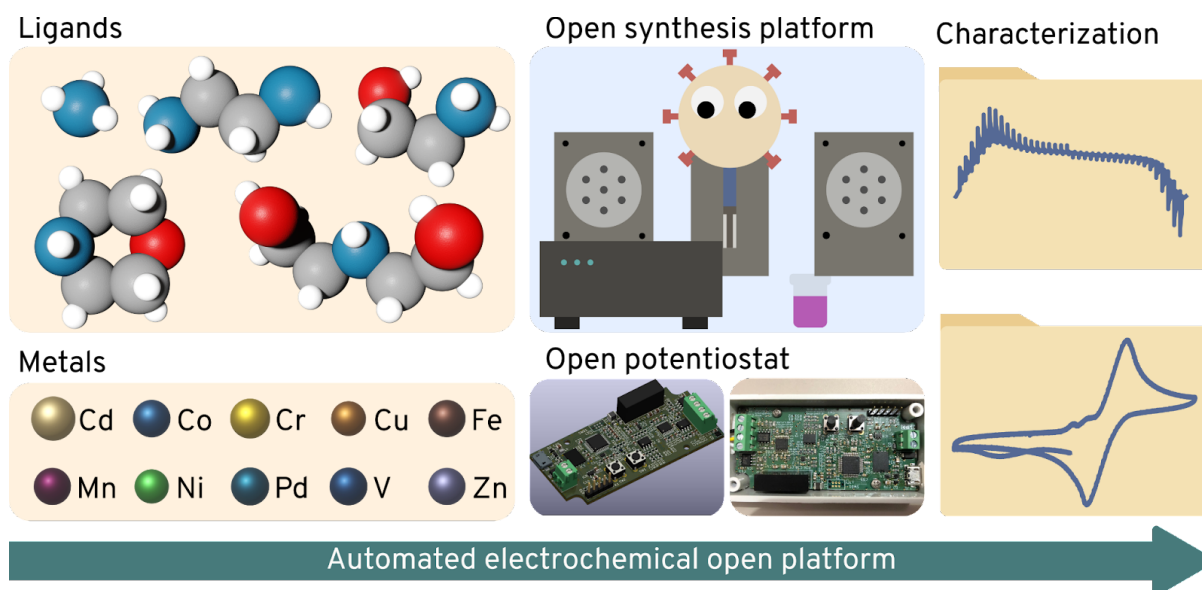
2 Self-driving laboratories<sup>1-3</sup> (SDLs) represent a paradigm shift in chemical research,  
3 integrating three key components:<sup>4</sup> (i) automated laboratory equipment,<sup>5</sup> (ii)  
4 experimental planners,<sup>6,7</sup> and (iii) orchestration software,<sup>8,9</sup> with seamless communication  
5 among these elements. Automated procedures enhance throughput and, once  
6 established, easily lend themselves to parallelization in a reproducible fashion, provided  
7 instrument choices and operational know-how are in place. While parallelization is well  
8 adapted to automated high-throughput calculations, device costs, access to  
9 reagents/consumables, and space limitations generally impede the broad application of  
10 parallelised automated experimentation. Recent initiatives within the open-source  
11 hardware and software community,<sup>10</sup> in tandem with the “maker movement”,<sup>11</sup> offer  
12 promising solutions, emphasizing customizability and cost-effectiveness. The  
13 computer-driven, self-diagnosing nature of SDLs facilitates on-the-fly decision-making,  
14 potentially generating consistent and reproducible experimental data in both human and  
15 machine-readable formats.<sup>12-14</sup>

16 In recent years, SDLs have found wide-ranging applications in material discovery,<sup>15-17</sup>  
17 renewable energy production,<sup>18,19</sup> energy storage,<sup>20</sup> and synthetic chemistry.<sup>21,22</sup>  
18 High-throughput methodologies, particularly in material synthesis and testing, have  
19 become pivotal, with electrochemical techniques playing a central role in characterizing  
20 candidate materials.<sup>23</sup> Importantly, electrochemistry SDLs have demonstrated their  
21 supremacy over traditional workflows in the pace and quality of generating  
22 electrochemistry data.<sup>24-27</sup> Nevertheless, most examples still rely on commercial  
23 potentiostats to carry out experiments, with applications that range from fundamental  
24 cyclic voltammetry to more advanced techniques.<sup>28</sup> Despite the common use of  
25 commercial potentiostats, their accessibility is hindered by their proprietary software,  
26 obfuscated data format, and, more importantly, the elevated financial cost coming along  
27 with high-precision commercial platforms. Conventional single-channel desktop  
28 potentiostats are not designed for parallel analysis, facing challenges in high-throughput  
29 analyses, while multi-channel instruments compound expenses.

30 In response, the scientific community has endeavored to develop open-design  
31 potentiostat solutions since the early 1970s.<sup>29-32</sup> The more recent attempts aimed to  
32 further lower the economic barriers and enhance their compatibility with automated  
33 setups<sup>33-37</sup> whereas some developed potentiostats focused on wireless capabilities,  
34 portability and point-of-care applications.<sup>38-40</sup> All these progress were made possible by  
35 taking advantage of the improvements in electronic parts of potentiostats, such as  
36 microprocessors, analog-to-digital converters (ADC), digital-to-analog converters (DAC)

1 and operational amplifiers (Op-amp). Nevertheless, open source devices that provide  
2 advanced functionalities inherent to their commercial counterpart and an easy  
3 integration with orchestration frameworks, are still lacking for SDLs.

4 Another crucial aspect of electrochemical SDL setups involves automated synthesis and  
5 sample transfer capabilities. While many commercial solutions are readily available, the  
6 advent of SDLs has sparked interest in open-source and cost-effective alternatives  
7 designed with modularity and adaptability in mind.<sup>14</sup> Although previous attempts have  
8 been made to integrate electrochemical systems with synthesis platforms, these solutions  
9 often tend to be confined to specific setups, missing the essential traits of generality and  
10 modularity. Previously, taking the advances in automating organic chemistry established  
11 by the Burke group<sup>41</sup> while further implementing modular design principles and  
12 open-source software, we introduced an extendable multipurpose platform, MEDUSA, as  
13 the next generation of “The Machine”.<sup>7,42</sup> Specifically, it has full potential to incorporate  
14 both post-synthesis/processing analysis in automation workflows, therefore is ideal for  
15 establishing end-to-end automated electrochemistry platforms.



16

17 **Figure 1.** Schematic of this work. Given a set of ligands and metals, mix them using our open synthesis platform  
18 “MEDUSA” and characterize them using our open design potentiostat. Finally, store the raw characterization data in our  
19 database.

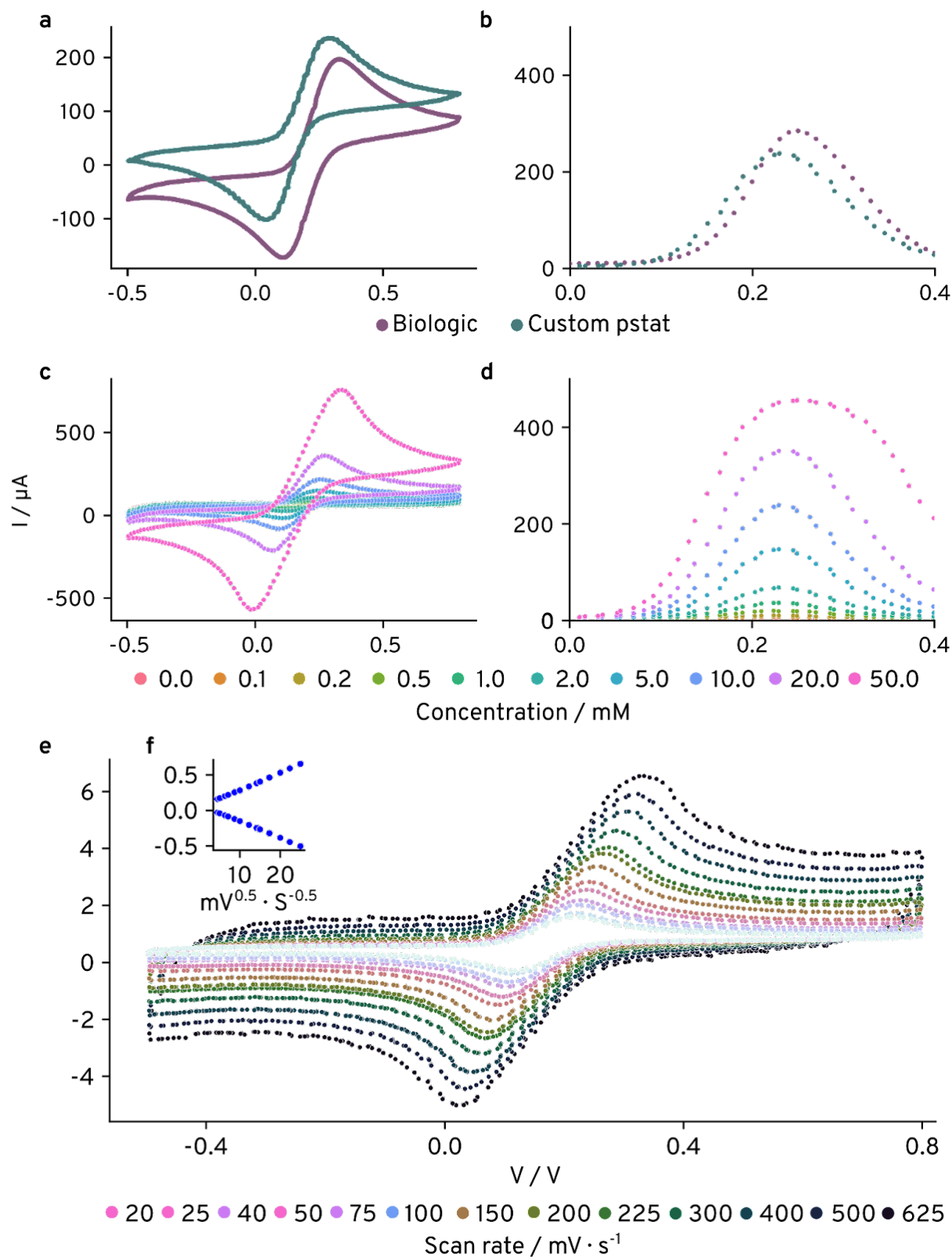
20 Further elaborating our proof-of-concept prototype for open and affordable SDL,<sup>7</sup> this  
21 work integrates an automated laboratory framework that combines an in-house designed,  
22 compact potentiostat device with a basic version of MEDUSA (**Figure 1**). The primary goal  
23 is to demonstrate the capabilities of this integrated setup by streamlining the generation  
24 of a comprehensive database containing metal/ligand complexes of electrochemical  
25 interest. The framework's affordability and open-source architecture make it an  
26 attractive option for electrochemical researchers seeking a flexible, cost-effective

1 platform for high-throughput chemical screening. Integrating SDLs into advanced  
2 workflows can unleash end-to-end automation, facilitate high-throughput  
3 experimentation, and enable active decision-making, thereby producing the high-quality  
4 datasets essential for both experimental and machine-learning communities.<sup>43</sup> This  
5 adaptability positions the framework as a valuable tool for generating reproducible and  
6 reliable data, with potential applications spanning redox flow batteries, environmental  
7 toxin detection, and beyond.

## 8 Results

### 9 Potentiostat design and benchmarking

10 Potentiostats are essential characterization tools for electrochemical studies. However,  
11 most labs use potentiostats from commercial vendors are a) controlled by proprietary  
12 software; b) using graphic user interfaces (GUI); and c) generate post-processing  
13 post-processing data. Because of these limitations, these potentiostats leave aside full  
14 control via an application programming interface (API) and direct access to raw  
15 measurements. While user-friendly for manual operations, the three features mentioned  
16 above pose challenges when integrating into automated platforms, therefore calling for  
17 potentiostats well digitized to support data-rich experiments and electrochemical process  
18 analysis in modern SDLs. Applying the basic principles of electronics,<sup>44</sup> we have designed  
19 an open-source potentiostat using a STM32 chipset, together with open source firmware  
20 and interface. Notably, the instrument benefits from its low cost (*circa* CAD 120/device,  
21 see **Note S1**) and compact size (2 cm x 5 cm x 10 cm), consequently it can be easily  
22 parallelized to enable high-throughput experiments (HTE) even for groups with a limited  
23 budget or are starting their first SDL setup. The potentiostat can be operated with a single  
24 USB cable for power and data transmission. The software design allows seamless  
25 implementation of highly customizable electrochemical protocols in addition to readily  
26 provided standard techniques. The detailed design of the potentiostat can be found  
27 attached as supporting information. **Figure S1** shows a 3D render of the device. **Note S2**  
28 contains a comprehensive description of the design and the firmware implementation.



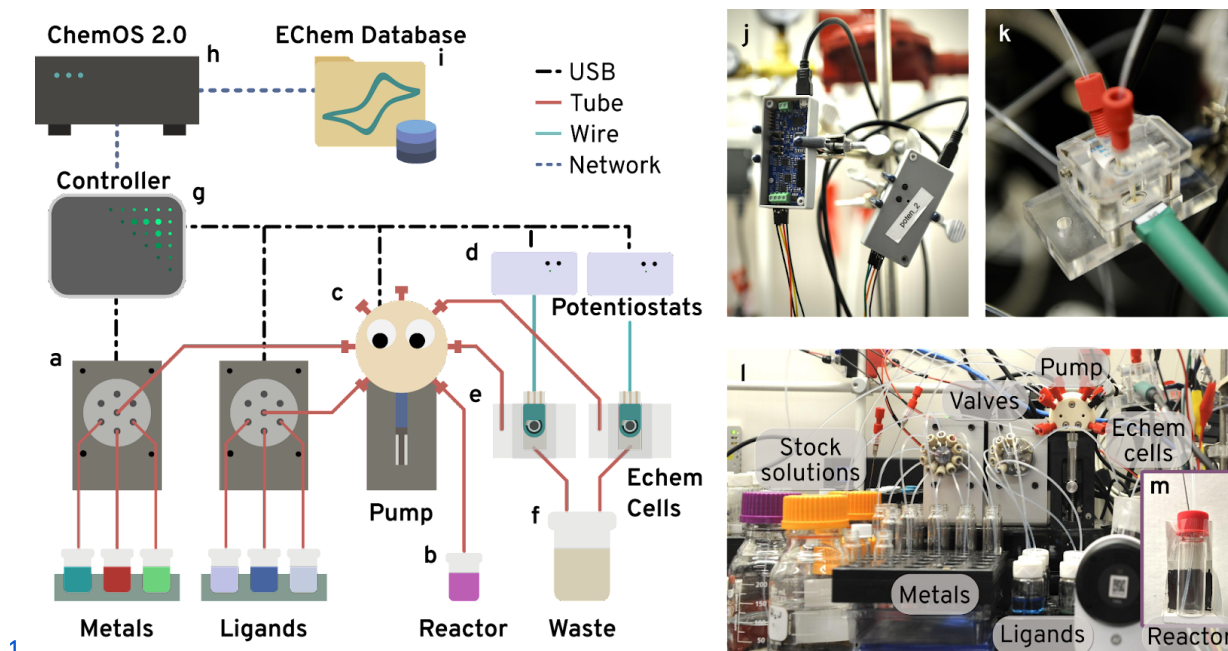
1  
 2 **Figure 2.** Benchmark of our custom potentiostat using  $K_4[Fe(CN)_6]$  as reference and NaCl 1 M as electrolyte. **a-b**  
 3 Comparison of CV (a) and DPV (b) techniques employing both a commercial potentiostat with a traditional setup (blue)  
 4 and our custom platform (orange) at a reference concentration of 10 mM. **c-d** Results of CV (c) and DPV (d)  
 5 measurements at various reference concentrations using our custom platform. **e-f** Characterization of the reference  
 6 compound at different scan rates, maintaining a fixed reference concentration of 10 mM, utilizing our custom platform.  
 7 Measurement parameters can be found in the Methodology-Electrochemical Measurement section.

1 In addition to low-cost potentiostats, the introduction of disposable printed electrodes  
2 and miniature flow cells has greatly changed electrochemical analysis as it liberates  
3 human operators from tedious surface treatment of electrodes, while significantly  
4 reducing material cost.<sup>45-47</sup> To demonstrate the capability of a low-cost electrochemistry  
5 platform, we benchmarked our homemade potentiostat against a commercial  
6 electrochemistry workstation (Biologic SP-300) using screen-printed electrodes  
7 (Dropsense, see **Supporting Information** for details). For both Cyclic Voltammetry (CV)  
8 and Differential Pulse Voltammetry (DPV) experiments with a 10 mM  $K_4[Fe(CN)_6]$  standard  
9 solution, the performance of our low-cost platform and that of a traditional platform are  
10 comparable. (**Figure 2a-b**) We further performed variable concentration experiments to  
11 investigate the sensitivities of our platform (**Figure 2c-d**), suggesting a detection limit of  
12 1 mM for CV and 0.1 mM for DPV techniques, which lies in the common range of both  
13 techniques. In variable scan rate experiments, a linear relationship could be identified  
14 between the peak current against the square root of the scan rate (**Figure 2e-f**), in line  
15 with expected diffusion-controlled redox events. In both variable concentration and scan  
16 rate experiments, the performance of our low-cost platform is competitive to the  
17 traditional platform based on a commercial potentiostat. Further benchmarks can be  
18 found in **Figures S2-S5**.

## 19 Experimental setup

20 Our experimental setup, as illustrated in **Figure 3**, comprises an integrated framework  
21 for synthesis/characterization and orchestration components. In the synthesis  
22 component, we have: (a) two selection valves, each linked to either metal or ligand  
23 solutions. (b) A reactor designed to mix the metal and ligand candidates effectively and  
24 (c) a syringe pump, connecting the aforementioned components to the electrochemical  
25 cells. The electrochemical setup consists of: (d) Two potentiostats, each individually  
26 connected to an independent printed electrode. (e) These electrodes are housed within  
27 acrylic flow cells, connected to a (f) waste vessel. Coordination and control of these  
28 systems are orchestrated by: (g) A mini-PC, which oversees and manages their operations  
29 and (h) a running SiLA2 server, enabling the exposure of synthesis and characterization  
30 processes to (i) ChemOS 2.0, facilitating remote automation and data collection. The raw  
31 data acquired from the potentiostat devices is collected by ChemOS 2.0, processed, and  
32 stored within an (i) internal SQL database situated on an external device.





1  
2 **Figure 3:** Design of our automated framework divided in a-c automated synthetic platform (MEDUSA), d-f  
3 electrochemical setup, g-i orchestration j-l actual experimental setups. The components are the following: a selection  
4 valves, b chemical reactor, c syringe pump, d potentiostats, e electrochemistry cells, f waste, g driver controller, h  
5 orchestration software, i database. The (solid) physical connections between the components are (red) tubes and (teal)  
6 wires, and the (discontinued) information transfer connections are (black) USB and (blue) network. j-k show the photos  
7 of the actual platform: j potentiostat devices, k Echem cell and l the general setup.

8 Automated electrochemistry experimentation is made possible through an iterative  
9 workflow, as depicted in **Figure 4**. This workflow encompasses the following key steps: (a)  
10 The pump transfers reference solution (10 mM  $K_4[Fe(CN)_6]$ , 1 M NaCl) to Echem cells. (b)  
11 The potentiostats conduct CV and DPV experiments, and results are processed on the  
12 edge. (c) The server actively decides for continuing loop or human intervention  
13 notification based on processed data. (d) The pump transfers metal/ligand pairs with a  
14 specific ratio to the reactor for complexation. (e) The pump sends the reaction mixture to  
15 Echem cells. (f) The potentiostats conduct CV and DPV experiments. (g) Subsequently,  
16 cleaning is applied to eliminate any residual chemicals on the cell. (h) Finally, the server  
17 reports the results to the user. The detailed complexation and electrochemical  
18 procedures are described in the **Experimental Methodology** section. While the  
19 coordination of ligands to metals involves various kinetic profiles and complicated  
20 thermal dynamic equilibriums, here we only measure the electrochemical profile of  
21 well-mixed reaction mixtures after staying at room temperature for ~5 min without  
22 extensively optimizing the reaction conditions and purifying the products.<sup>48</sup>





1 respectively. Each complex was prepared at 1:7 metal/ligand concentration ratios to  
2 ensure complete complexation, utilizing 1.0 M NaCl in water as the electrolyte/solvent,  
3 and 1:1 HOAc/NaOAc as the buffer solution. Subsequently, comprehensive  
4 characterizations were conducted, employing CV and DPV techniques. This thorough  
5 investigation resulted in a substantial database encompassing 400 voltammetry data.  
6 Noteworthy, the workflow embraces the potential to expand to a broader space including  
7 additional ligands, different metal/ligand ratios, mixed ligands and addition orders,  
8 buffer pH, and reaction time. The accumulation of data points is still ongoing.

9 To derive meaningful insights from the CV and DPV measurements, advanced data  
10 processing techniques were applied. For CV, a window average was utilized to rectify  
11 noisy data. In the case of DPV, the results were fitted to a Gaussian equation to enhance  
12 the signal's shape. Furthermore, a peak-finding algorithm, implemented in Scipy, was  
13 employed to identify the key peaks in both sets of measurements. To enhance the  
14 transparency, reproducibility, and overall clarity of our dataset, we have included both  
15 the raw and processed versions of the characterization measurements.

## 16 Discussion

### 17 Framework

18 While most parts of the experiments were performed without human intervention, the  
19 screen-printed electrodes degraded throughout the experiments, which is indicated by  
20 an increase of voltammogram baseline and diminishing of peaks corresponding to redox  
21 events (**Figure S6**). For reversible electrochemistry systems such as  $K_4[Fe(CN)_6]$ , the  
22 lifetime of a typical electrode could reach up to 12 hours of operation. However, the  
23 lifetime may be significantly reduced due to irreversible processes (e.g. metal reduction  
24 and coating on the electrode) and heterogeneous samples (e.g. precipitation formation in  
25 reaction). In a typical example, one electrode can be used for 10 metal/ligand  
26 combinations. An estimation of the experimental cost can be found on **Note S6**.

27 During the experiment, several issues have been identified, which will be improved in our  
28 future work: (i) While the synthesis platform was assembled by an undergraduate student  
29 in our research group within 2 h, it might be challenging for inexperienced researchers  
30 new to the system. We plan to prepare a protocol describing the assembly and usage of  
31 the platform in detail. (ii) Potentiostats have a relatively high power draw of 600 mA each,  
32 which precluded the use of a Raspberry Pi 4 as the controller as they have has a power  
33 limit of 1.2 A. Future iterations will include a separate external power supply to increase

1 the number of supported frameworks. (iii) The communication between the mini-PC and  
2 the potentiostats is implemented using serial protocols without error detection, which  
3 occasionally leads to corrupt data. We are currently including verification methods such  
4 as checksum/CRC or Modbus protocols to improve reliability. The improved versions will  
5 be included in future versions of the firmware.

## 6 Auto complexation and electrochemical measurement capabilities

7 Despite the challenges encountered, our framework exhibited remarkable efficiency,  
8 executing 400 electrochemical measurements in a semi-automated mode. This  
9 achievement not only underscores the robustness of our approach but also highlights the  
10 promising potential of cost-effective setups for conducting diverse coordination  
11 chemistry and electrochemical experiments.

12 Integral to this adaptability is the modular architecture of MEDUSA, enhancing the  
13 overall extensibility of our system. This modularity facilitates ease of integration and  
14 positions our setup to navigate more complex electrochemical configurations, especially  
15 those necessitating multiple stations. Our autocomplexation capabilities not only meet  
16 the demands of conventional electrochemical techniques but also set the stage for  
17 exploration and innovation in more intricate electrochemical setups.

18 While our focus is centred on CV and DPV, the potentiostat's adaptability allows for the  
19 utilization of dynamic voltage shapes (**Note S1**). For instance, a current hold function was  
20 easily implemented in the firmware, unlocking the chronopotentiometry (CP) analysis.  
21 Further inclusion of advanced electrochemistry techniques, including AC voltammetry  
22 (ACV), squarewave voltammetry (SWV), electrochemical impedance spectroscopy (EIS),  
23 as well as utilizations in electrolysis and electrosynthesis studies, is ongoing and will be  
24 supported in future firmware versions.

## 25 Efficient data generation

26 Human operators, susceptible to stress and errors during repetitive tasks, pose challenges  
27 to the robustness of experimental campaigns, introducing uncertainties into  
28 measurements. Despite the initial investment in time and resources for our experimental  
29 setup, the enhanced reliability and robustness it brings significantly outweigh these  
30 costs. Automated logging capabilities within our setup play a crucial role. The data  
31 obtained is seamlessly stored and organized in an internal database, providing easy  
32 access and expediting the process of failure debugging. This not only ensures cleaner data  
33 management but also accelerates the identification and resolution of issues.

1 Moreover, the low-level access to the code of both the auto-complexation platform and  
2 the potentiostat amplifies the benefits. The unprocessed data can be readily shared,  
3 fostering transparency and collaboration. By benefiting from this open approach,  
4 external researchers can detect errors, audit our code, and, in terms of Linus's Law,<sup>49</sup>  
5 contribute to its continuous improvement over time. This collaborative cycle ensures not  
6 only precision and reliability in our data generation but also promotes the perpetual  
7 enhancement of the system's quality.

## 8 Automated data management

9 Our data management strategy integrates with ChemOS 2.0, serving as a centralized  
10 orchestrator. The SiLA2 server within our framework enhances reliability and simplifies  
11 data curation, embodying our commitment to human-readable and efficient  
12 experimental workflows. Key to this integration is using a JSON schema in the job file  
13 (**Note S5**), structured hierarchically to represent experimental variables. The SiLA2 server  
14 parses and translates this schema to the internal workflow operations, ensuring precise  
15 execution of experimental protocols. Characterization results are presented in a universal  
16 CSV format, facilitating compatibility with various external data analysis tools.

17 The coupling of job/result pairs with detailed logging information is systematically  
18 stored in the orchestrator's database. This structured approach allows for easy querying  
19 of experimental results, promoting accessibility and data-driven analysis. For a  
20 comprehensive understanding of the database schema, refer to **Note S3**.

## 21 Active decision making

22 Within our setup, alongside the firmware and automation code, a minimal but effective  
23 active decision-making algorithm (**Figure 4**) serves to alert users in case of reference  
24 measurement failures. Despite its simplicity, this feature enhances the robustness of our  
25 system by notifying users of potential issues promptly.

26 As we designed our framework, we identified diverse areas that stand to benefit  
27 significantly from the integration of active decision-making algorithms. These areas  
28 include tuning DPV parameters, dynamic characterization techniques, and intricate  
29 experimental planning targeting specific observables.<sup>7</sup> Incorporating such techniques  
30 would undoubtedly elevate our framework's quality and efficiency.

31 However, we acknowledge the inherent complexity of implementing these advanced  
32 decision-making algorithms, recognizing that their integration falls outside the current  
33 scope of our work. Yet, embracing our project's *libre* nature, we invite external

1 researchers to explore and modify our existing setup and code. This collaborative  
2 approach encourages the implementation of these advanced features into diverse  
3 workflows, expanding the capabilities of our framework over time.

## 4 Data Analysis

5 Out of the 100 duplicates of CV experiments, only two pairs of voltammograms exhibit  
6 significant shape differences in the terms of peak numbers and/or positions, while the  
7 same number of different pairs exists in the DPV experiments. Meanwhile, pairs  
8 exhibiting differences in peak intensities can be identified. These results suggest our  
9 electrochemical measurement setup and activation decision making algorithm can  
10 produce highly reliable and reproducible results, which could be challenging for manual  
11 systems. Noteworthy, although only 10 ligands and fixed conditions, including pH,  
12 metal/ligand ratios, reaction time were applied in the early phase of our data collection  
13 campaign, more complicated ligand space and complexation conditions can be easily  
14 applied to the currently ongoing project.

15 Among the successfully performed CV experiments, 16 examples do not show significant  
16 peaks corresponding to redox events within the measurement range (-1.2 to 1.1 V,  
17 electrochemical window of water). Similarly 24 DPV experiments do not show significant  
18 peaks in both cathodic and anodic scans, which contain all 16 aforementioned examples.  
19 These observations suggest that while being a more sensitive technique by principle and  
20 by benchmarking experiments with  $K_4[Fe(CN)_6]$  reference solutions, DPV measurements  
21 with unoptimized parameters may not be sufficient for more general electrochemical  
22 measurements.

23 The peaks identified in DPV experiments tend to be more symmetric and less overlapping  
24 with each other compared to the CV experiments, making it easier to identify the peak  
25 positions and intensities for quantification purpose. However, DPV experiments take  
26 longer time than CV experiments (253 s vs 115 s per experiment) even 5 cycles were  
27 performed in all CV measurements. Additionally, 16 examples show reduction of signals  
28 with increasing CV cycle numbers, suggesting coating/deposition on the electrode  
29 surface which leads to electrode degradation. Therefore, predicting the DPV and  
30 many-cycle CV results based on the initial few CV cycles would be important to save time  
31 and cost.

32

## 1 Conclusions and Outlook

2 We constructed an Echem self-driving laboratory platform to unravel the end-to-end  
3 automated synthesis and electrochemical measurements of metal complexes. Based on  
4 our homemade synthesis robot and potentiostat, as well as open-source software and  
5 hardware design, we provide a low-cost, accessible and reliable solution for automating  
6 electrochemistry data acquisition. Empowered by ChemOS 2.0 and active decision  
7 algorithm, we demonstrate the capabilities of our platform by creating a high-quality,  
8 reliable, open-source electrochemistry database containing 400 voltammograms, at a  
9 speed and cost that can hardly be achieved by human operation. The database is actively  
10 accumulating.

11 We believe this work can benefit the data-rich research focusing on electrochemistry, not  
12 only because of the impressive data volume, data consistency and the raw data  
13 accessibility. Importantly this campaign is not limited locally. Instead the low-cost and  
14 open-source nature of our solution ensures a low-barrier knowledge transfer, therefore  
15 ideal to be delivered and implemented across the world. We envision that further  
16 adaptation of such a solution will finally lead to a delocalized and democratized  
17 electrochemistry self-driving lab community.

## 18 Experimental procedures

### 19 Resources availability

#### 20 Lead contact

21 Further information and requests for resources should be directed to and will be fulfilled  
22 by Han Hao (hann.hao@utoronto.ca)

#### 23 Materials availability

24 This study did not generate new material

#### 25 Data and code availability

26 Potentiostat schematics, printed circuit board design (in gerber format), bill of materials  
27 (in bom file format), and the design file of the case are included in our Zenodo repository  
28 (DOI: 10.5281/zenodo.10633135) Current drivers of the potentiostat, as well as the Python



1 interface to control it can be found in our Gitlab repository  
2 (<https://gitlab.com/aspuru-guzik-group/potentiostat>). The generated database,  
3 containing the raw and processed CV and DPV measured results of all the measurements  
4 can be also found in our Zenodo data repository.(DOI: 10.5281/zenodo.10633135).  
5 MEDUSA drivers, Potentiostat drivers/interface and 3D printing design of potentiostat  
6 enclosures are available in our Gitlab repository. Complexation robot controlling software  
7 are available in our Gitlab repository  
8 ([https://gitlab.com/aspuru-guzik-group/self-driving-lab/instruments/e\\_complex](https://gitlab.com/aspuru-guzik-group/self-driving-lab/instruments/e_complex)).

## 9 Experimental methodology

### 10 Experiment workflow

11 The complexation reactions were conducted on “MEDUSA”, a robotic platform for  
12 automated chemistry synthesis. The platform is based on syringe pumps and selection  
13 valves and has a modular design for easy expansion and adaptation to downstream  
14 sample preparation and characterization. In the context of this manuscript, two  
15 electrochemistry characterization modules, each containing an Echem flow cell and a  
16 potentiostat, were directly connected to the synthesis module, and all the syntheses and  
17 measurements were performed on a single platform automatically without human  
18 intervention except for refilling stock solution and changing electrodes.

### 19 Active quality control

20 The screen-printed electrode has a limited lifetime. To ensure the reliability and quality of  
21 data and avoid artifacts from surface degradation and/or coating on the electrode, we  
22 implemented an active decision-making strategy. We base this strategy on measurement  
23 and on-the-edge (controller device) analysis of the reference solution (10 mM  $K_4[Fe(CN)_6]$ ,  
24 1.0 M NaCl) and on-the-fly workflow management on the server.

25 The reference solution was transferred to the Echem cells followed by DPV and CV  
26 measurements (see **Electrochemical measurement** subsection for parameters). An x64  
27 mini-PC processes the DPV results as the edge device to generate the plot and  
28 corresponding Gaussian fitting, which are streamed to the server. Based on the stress  
29 testing, an arbitrary threshold of 0.20-0.25 V for peak center ( $x_0$ ) and <0.1 V for deviation  
30 ( $\sigma$ ) was chosen. The server actively made decisions on continuing or halting experiments.  
31 In the case of an experiment halt, a message was pushed to notify a human chemist using  
32 Slackbot (**Note S7**).

## 1 Complexation reactions and clean-up

2 Metal-ligand complexation reactions were performed in the following manner:

- 3 1. Add 0.25 mL of 1.0 M HOAc/NaOAc buffer solution.
- 4 2. Add 0.75 mL of 3.0 M NaCl solution.
- 5 3. Add 0.35 mL of 0.3 M ligand solution.
- 6 4. Add 0.15 mL of 0.1 M metal solution.
- 7 5. Purge 1.0 mL N<sub>2</sub> through the reaction mixture, then draw-and-dispense 1 mL of
- 8 the reaction mixture; this step is repeated 3 times to ensure a good mix.

9 Clean-up was performed in the following manner:

- 10 1. Pass 0.25 mL of water through each Echem cell for 5 times.
- 11 2. Fully empty the reaction vial and discard the residue to waste.
- 12 3. Add 0.9 mL H<sub>2</sub>O to the reaction vial then fully empty to waste, repeat this step 3
- 13 times to ensure thorough cleaning of the reaction vial.

## 14 Electrochemical measurements

15 Both DPV and CV experiments were performed for the reference and the reaction  
16 mixtures. Notably, to reduce the degradation of the electrode and avoid current spike at  
17 the onset, DPV experiments were performed in one cycle, starting from open-circuit  
18 potential (OCP) towards minimum voltage ( $V_{\min}$ ), then raising to maximum voltage ( $V_{\max}$ ),  
19 finally returning to OCP.

20 Two sets of parameters were chosen for reference and reaction, respectively. The  
21 reference DPVs were measured in the range of -0.1 - 0.5 V at 100 mV pulse voltage and 10  
22 mV step voltage with 50 ms pulse width and 500 ms period, and CVs were measured in  
23 -1.2 - 1.1 V for 3 cycles at 200 mV/s. The reaction mixtures DPVs were measured in the  
24 range of -1.2 - 1.1 V at 100 mV pulse voltage and 10 mV step voltage with 50 ms pulse  
25 width and 500 ms period, and CVs were measured in -1.2 - 1.1 V for 5 cycles at 200 mV/s.

## 26 Computational tools

27 The coordination and management of the experimental processes were executed using  
28 ChemOS 2.0<sup>8</sup>, which was integrated into the laboratory's local network. We employed an  
29 x64 mini-PC with the Debian Linux system and a virtual Python 3.11.2 environment to  
30 control the potentiostat, selection valves, and syringe. Communication between the  
31 controller and the potentiostat was established through a serial communication protocol,

1 aided by a Python interface built on top of Pyserial 3.5,<sup>50</sup> enhancing user interaction. In a  
2 similar fashion, we enabled communication between the selection valves and the syringe  
3 pump, utilizing MEDUSA drivers. Regarding the hardware connections, the valves, pumps  
4 and potentiostats were directly connected to the USB ports of the PC. To ensure seamless  
5 recognition, udev rules were implemented to correctly identify the pumps and  
6 potentiostats. The Python interface of the potentiostat was designed with the capability  
7 to transmit target voltages in real-time or buffered mode. To create the voltage  
8 waveforms essential for CV and DPV measurements, we utilized Numpy 1.26.1<sup>51</sup> and Scipy  
9 1.11.3.<sup>52</sup> Additionally, for data analysis, we employed pandas 2.1.1<sup>53</sup> and Matplotlib 3.8.0.<sup>54</sup>

10 For remote operation control, a SiLA2<sup>55</sup> server was deployed using the SiLA2 Python  
11 implementation 0.10.5. The client operates as a SystemD service and offers four distinct  
12 methods: (i) Mixing the compounds and conveying them to the reactor, (ii) Performing  
13 CV, (iii) Executing DPV, and (iv) Cleaning. All methods accept input in the form of JSON  
14 with operation-related parameters. Methods (ii-iii) return measurement results in CSV  
15 format, while methods (i, iv) return None. An error is reported in case of a failure. To  
16 enable concurrent operations within the workflow, we leveraged the asyncio<sup>42</sup> Python  
17 library. Before starting the orchestration with SiLA2, the robustness of the setup was  
18 tested by using simpler bash scripts running both potentiostats in parallel *via* subshells.  
19 The results of those tests have also been incorporated into the database. A Slack bot has  
20 been used to report the incidents and warnings regarding the process. The bot has been  
21 implemented sending requests *via* curl 7.88.1 to the rest API provided by Slack.

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## 1 Author contributions

- 2 S. P.-G., methodology, writing of the first draft, firmware and software development,
- 3 conceptualization, supervision.
- 4 A. G., hardware design and firmware development.
- 5 A. D., firmware and software development, writing.
- 6 S. M., workflow development, orchestration, writing.
- 7 C. Y., methodology, conceptualization, editing.
- 8 S. M., preparation of experimental workflows, editing.
- 9 H. C., firmware development.
- 10 N. Y., experimentation, 3D design of the case.
- 11 D. D., review, editing, funding acquisition
- 12 H. H., methodology, writing of the first draft, data analysis, preparation of experimental
- 13 workflows, conceptualization, supervision.
- 14 A. A.-G., conceptualization, funding acquisition, supervision, project administration,
- 15 writing review & editing.

## 16 Competing interest statement

- 17 The authors declare no competing interests.

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