Enhancing FAIRdata by providing digital workflows from data generation to the publication of data: an open source approach described for cyclic voltammetry

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# 1 General definitions and explanations of included tools

**Chemotion-ELN**<sup>1</sup>: *Chemotion ELN* is an open source software that is used in this work to execute the suggested workflow including different software components and methods. It includes different components that facilitate the work with scientific data, e.g. the *Data Collector*, *ChemSpectra*, and routines to store data and to export them.

Link to the code resource: <u>https://github.com/ComPlat/chemotion\_ELN</u>; Link to documentation: <u>https://chemotion.net/docs/eln</u>

**Shuttle:** *Shuttle* is a software that can be executed on a computer of scientific instruments, allowing the transfer of data from the device's computer to a remote location. *Shuttle* monitors the data folder of the instrument's computer. The monitoring determines, depending on predetermined criteria, which files or folders are to be transferred at what time to avoid transferring incomplete or unnecessary data. As *Shuttle* needs to be compatible with many different devices it is individually configurable per device and environment. The configuration is done via the GUI of ShuttleBuilder.

Link to the code resource: <u>https://github.com/ComPlat/shuttle</u>; Link to documentation: <u>https://chemotion.net/docs/eln/devices/configurations/data\_transfer</u>

**ShuttleBuilder:** *ShuttleBuilder* is a software that can be used to build an executable *Shuttle* file. *ShuttleBuilder* is currently offered as a self-hostable service to allow the straightforward generation of *Shuttles* which are used for transferring data from devices to another location. The *ShuttleBuilder* allows to generate a tailor-made software (*Shuttle*) for the device and environment it will be used in (depending on the device's PC, the network, the remote storage location and available transfer protocols, etc.) which can then be set up on every device where such a data transfer is to be implemented. The web-based *ShuttleBuilder*'s GUI allows the administrator to input all the parameters required by the program to transfer the files and generates an executable file as an output, ready to be placed on the device with no further installation required.

Link to the code resource and documentation: <u>https://github.com/ComPlat/shuttlebuilder</u>; Link to documentation: <u>https://chemotion.net/docs/eln/devices/configurations/data\_transfer</u>

**Data Collector**<sup>2</sup>: The *Data Collector* is part of *Chemotion ELN* and can be configured via the ELN Admin UI. The *Data Collector* feature imports data automatically from a folder which is monitored. The data is made available to the users in their inbox of the ELN following file or folder naming conventions. The data collector may collect folders or files, depending on how it is configured and whether analytical data is provided as folders or files. Alternatively, the *Data Collector* may not watch a local folder but fetch data from another storage via SFTP. Link to the code resource: is part of the Chemotion ELN source code (see above); Link to the documentation: <a href="https://chemotion.net/docs/eln/devices/configurations/local\_collector">https://chemotion.net/docs/eln/devices/configurations/local\_collector</a>

**ChemSpectra:**<sup>3</sup> *ChemSpectra* is a software that can be used as stand alone software or integrated into other systems. It can be used to view and analyze data files from analytical instruments such as NMR devices, mass spectrometers, or potentiostats (in the work described here).

Link to the code resource: App: <u>https://github.com/ComPlat/chem-spectra-app</u> and client for ELN: <u>https://github.com/ComPlat/react-spectra-editor</u>; Link to the documentation: https://www.chemotion.net/docs/repo

**ChemConverter:** *ChemConverter* converts different file formats and types from integrated devices to common and well known formats such as JCAMP-DX and JSON. It extracts columns

for x,y- data visualization and metadata and maps them to predefined structure (xy data and xy points) and metadata schemes (metadata). Currently, the *ChemConverter* can handle most text readable files like TXT, CSV or DTA, as long as the content is properly structured. Additionally, developers can create their own readers, if there is no reader available already. *ChemConverter* runs as a background process of *Chemotion ELN*, when a user or device (via *Data Collector*) provides analytical data, but may also be used as a standalone application.

Link to the code resource: <u>https://github.com/ComPlat/chemotion-converter-app;</u> Link to the documentation: <u>https://www.chemotion.net/docs/services/chemconverter</u>

**Chemotion Repository:**<sup>4</sup> The Chemotion repository is a research data repository, available as a service hosted by the Karlsruhe Institute of Technology that allows chemists and other scientists to share data from experimental chemical (molecular) research in a reusable and traceable manner, incorporating domain-specific standards. Chemotion focuses on experimental synthesis and the associated protocols, the representation of chemical compounds and their properties, and their characterization using analytical data. The chemotion repository was used (besides RADAR4Chem and Zenodo) in this work to demonstrate how CV data can be made publicly available through research data repositories.

Link to the code resource: <u>https://github.com/ComPlat/chemotion\_REPO/</u>; Link to the documentation: <u>https://www.chemotion.net/docs/repo</u>

# 2 Details and explanation for enabling the transfer of data from potentiostats to an ELN

# 2.1 Option 1, Step 1a: Unattended, automatic data transfer to a data exchange location with ShuttleBuilder

#### 2.1.1 How to get a-Shuttle by using ShuttleBuilder

General information: First, the administrator can choose from two different protocols, either SFTP (based on SSH) or WebDAV (based on HTTP(S)), and needs to enter the operating system the program is intended for, either Ubuntu x64, Windows x64 or Windows with a x32 bit architecture. Given that the Shuttle project is coded in the GO programming language, it offers the flexibility to employ SSH-based protocols across operating systems that may not inherently support such protocols. However, it's worth noting that on Windows XP-based computers, the GO SSH functionality isn't supported. In such cases, it becomes necessary to install WinSCP, which is conveniently provided by the ShuttleBuilder. The source address for the data on the device's computer must be given, and the desired target location where the data is to be transferred to must also be entered. If required by the target storage location, the username and password can also be specified. Finally, the administrator can choose between three transfer methods, either transferring only individual files or transferring an entire folder newly created by the software. A third possibility is to zip folders before their transfer. The last option the administrator has to specify is a delay time that the program will wait for before transferring them to the target. This allows integrating systems that amend data files throughout the experiment's runtime, instead of saving completed data files after an experiment has finished. The program will additionally monitor the status of the data and only transfer it after the data file has been closed and is no longer being written to. Finally, the builder GUI instructs the administrator how to install the program on the PC and the steps necessary to instruct the PC to autostart the program after booting the operating system and running the program in the background, as it requires no further user or administrator input.

**The Gamry example:** In the following section, the options that need to be set in the Builder for a Gamry device are introduced (see also Figure S1).

The computer managing the Gamry device is a modern Windows machine with an x64 architecture. Since the Gamry potentiostat produces single files as output, the transfer method can be set accordingly and as transfer protocol SFTP is used. Additionally to the protocol, architecture and transfer information, a wait time of 300 sec. and the required path information are entered into the *ShuttleBuilder*. The download of the *Shuttle* that can now be executed in the browser-based user interface of the *ShuttleBuilder* initializes the compile process at first. Once the compilation process is successfully completed, the *Shuttle* as a file called *efw.exe* is automatically downloaded.

Back						
Nam	ComPlat Gamry Potentiostat					
Unique name of the Sh	Unique name of the Shuttle instance. This name cannot be changed!					
Transfer protoco	SFTP	~				
You can either use the	VebDAV protocol or the SFTP protocol					
Use	ioc-ls-i-pot-0001					
WebDAV or STFP User						
Passwor	: [					
WebDAV or STFP Passw	ord					
Sr	C:\\Users\\Public\\Documents\\My Gamry Data\\					
Source directory to mo always use \\.	hitor. Note: If you use only single \ in the path, the build will fail. Therefore, make sure that you					
Ds	os-login.lsdf.kit.edu/lsdf01/lsdf/kit/ioc/projects/analytik/LS-I-Analytik/LS-I-nPot/ELN					
WebDAV or SFTP destin	ation URL. If the destination is on the lsdf, the URL should be as follows:					
SFTP: os-login.lsdf.k	t.edu/[OE]/[inst]/projects/[PROJECT_PATH]/					
WebDAV: https://os	webdav.lsdf.kit.edu/[OE]/[inst]/projects/[PROJECT_PATH]/					
[OE]-Organisations	einheit, z.B. kit.					
	, z.B. ioc, scc, ikp, imk-asr etc.					
[DSERIVAME]-OSEI- [PROJECT_PATH]-F	ath (directory) within the LSDF					
Тур	: File	~				
Type must be 'file'. 'fol	er' or 'zip'. The 'file' option means that each file is handled individually, the 'folder' option means					
that entire folders are l	ransmitted only when all files in them are ready. The option 'zip' sends a folder zipped, only when all					
files in a folder are read	у.					
Duratio	. 300					
Duration in seconds, i.e	, how long a file must not be changed before sent. (default 300 sec.)					
System architectur	: Windows 64 Bit	~				
Your computer archited	ture : either 64 bit or 32 bit (i386)					

**Figure S1:** The GUI of the transfer program's web-based *ShuttleBuilder* allows the administrator to input all parameters for the transfer of data from a device's PC to a target location for ELN import.

#### 2.1.2 How to use the Shuttle with a potentiostat's PC

Next it is explained how to complete the installation on the device's PC. Beforehand, however, it is worth mentioning that access rights to this device are restricted for the standard user. Hence, the installation has to be completed by an authorized system admin. The installation itself is simple and can be described in three steps. Firstly, a directory "C:\Program Files\eln\_exporter" has to be

made. Secondly, the downloaded *efw.exe* has to be copied into "C:\Program Files\file\_exporter". Finally, a *file\_exporter\_task.vbs* (Visual Basic script) has to be created in the startup directory of the device. This file exporter task.vbs can be downloaded from the builder and looks as follows:

Dim WinScriptHost Set WinScriptHost = CreateObject("WScript.Shell") WinScriptHost.Run Chr(34) & "C:\Program Files\file\_exporter\efw.exe" & Chr(34), 0 Set WinScriptHost = Nothing

This completes the installation. After the device is restarted the file\_exporter\_task.vbs will automatically trigger the monitoring and transferring of the Gamy output files.

#### 2.1.3 Dependency statement for the Shuttle

The Shuttle is developed in the Go programming language. At the time of publication Shuttle supports the latest Go version 1.23. Go is a compiled programming language that offers a simple interface for cross-compilation. This enables the Shuttle to be compiled for almost all devices with minimal effort. The ShuttleBuilder currently supports all Linux systems, as well as Windows 10 and Windows 11. Even Windows XP and Windows 7 on i386 processors are supported. If support for another system is required, the Shuttle can be compiled manually or it can be extended in consultation with the development team.

#### 2.2 Option 1, Step 1b. Transfer of data from exchange location to ELN

The configuration is done on the ELN side as described in the documentation (https://chemotion.net/docs/eln/install\_configure/configuration?\_highlight=datacollecto#datacollector-settings )

The system of the exchange location allows for sftp access. The ELN data collection is then configured accordingly using key authentication through the Chemotion ELN Admin interface.

Data Collector Configuration - Device: ComPlat Gamry 1010B

Watch method	filewatchersftp -	User	XXXXXXXXX	
Host	xxx.xxx.kit.edu			
SFTP auth. with	keyfile 🗸	Key file	000000000000000000000000000000000000000	
Watch Directory	/REMOTE/PATH/TO/WA	ATCHED/FOLDER/L	S-I-nPot/ELN	
Number of files	e.g. 10			
	Folderwatcher: set to 0 for	or a varying number of	files	

#### Figure S2: Configuration of the Data Collector in ELN

File collection is configured in the config/datacollectors.yml file to run every few minutes using a cron syntax. In our case:

```
production:
    :services:
    - :name: 'filewatchersftp'
        :cron: '03,13,23,33,43,53 5-22 * * *'
...
# Dir of ssh keys for data collection over sftp
    :keydir:
```

"config/data\_collector\_keys"

#### 2.3 Option 2, Data transfer from device using rsync and rrsync

At Leipzig University, rsync and rrsync was used to transfer data. The machine controlling the CV device runs Windows 10 22H2 with OpenSSH for Windows with PowerShell as default shell and WSL (version 2.0.9.0, Kernel 5.15.133.1-1, as of 2023-11-17) with OpenSSH with bash as default shell (as of 2023-11-17). The following data transfer routine takes a maximum of three minutes

from the start of the data transfer on the computer controlling the device until the data is available in the user's ELN inbox. The overall process is visualized in Figure S3.



Figure S3: Data transfer process from device to ELN with rsync and rrsync used at Leipzig University.

#### 2.3.1 Step 1a: Data transfer to the device to a large data storage with rrsync

Users save their analytical CV data (in the case of PalmSens EmStat3 with PSTrace software) as .pssession files on the local hard drive of the machine controlling the CV device in a designated folder, but may and tend to choose their own (sub)folder structure, hence, data is aggregated first and then pushed to the large data storage with rsync/rrsync.

PalmSens PSTrace software automatically saves a file for each run in a "autosave" folder, but a measurement including many runs is saved by the user at the end of the measurement including many runs i.e. the software does not continuously save data to a file as this is the case with the Gamry software.

The data transfer is initiated by the user via a shortcut on the desktop which runs a powershell script to start WSL, runs "find", pipes the list of files to rsync to push the CV data to a large data storage via SSH with a passwordless key file for authentication. In order to restrict any other use than rsync and access to any other folder than the designated folder for CV data on the large data employed, storage with that keyfile, rrsync was see the rrsync man page https://download.samba.org/pub/rsync/rrsync.1.

This is the slowest step of the data transfer routine, as "find" is inherently slow. The aggregation of all .pssessions and subsequent rsync took 3 sec as of 2023-12-07.

# **2.3.2** Step 1b: Transfer of new CV data from large data storage to the folder watched by Chemotion ELN's Data Collector with rsync

The server hosting Chemotion ELN holds the second copy of all research data (*cf.* 3-2-1-0 rule). In order to only copy new CV data from the large data storage to the local folder watched by Chemotion ELN's *Data Collector*, the ELN server fetches only the new CV data from the large data storage by comparing the folder on the ELN server with CV data on the large data storage via rsync's --compare-dest option. The new CV data rsynced to the folder watched by Chemotion ELN's Data Collector is then ingested by Chemotion ELN and made available to the ELN users in their inboxes.

This is automated via cron and each run takes less than a second (as of 2023-12-07).

File collection is configured in the ADM UI as well as the config/datacollectors.yml as filewatcherlocal which also specifies the time between each run and the local folder:

```
production:

:services:

- :name: "filewatcherlocal"

:every: 2 #minutes

:localcollectors:

- :path: "/chemotion/datacollector"
```

#### 2.3.3 Step 1c: Sync of CV data on large data storage and ELN server

Finally the folder holding all .pssessions files on the ELN server is synced with the corresponding folder on the large data storage, so that both servers hold a separate and identical copy of all CV data.

This is also automated via cron and each run takes less than a second (as of 2023-12-07).

# 3 Data and Metadata conversion: generating the converter's profile

The profile consists of specific rules defined with the help of drop-down menus inside the GUI and must be predefined for each measurement method and device at least once. The decision on the used profile and the mode of action is made by the admin of the system who configures both for the single ELN instance. Table 1 lists the different vendors and possible identifiers.

Manufacturer	Output File	possible identifier	additional notes
Gamry	.DTA text file	<ul><li>DTA file extension</li><li>header contains "Cyclic"</li></ul>	
PalmSens	.pssession JSON file	<ul> <li>pssession file extension</li> <li>value of "title" key is "Cyclic Voltammetry"</li> </ul>	exports in other formats (e.g.xlxs) possible with PalmSens PSTrace software but with the loss of many metadata
Metrohm	simple csv formatted .txt file	<ul> <li>titles of columns</li> <li>e.g. "Potential applied (V)" and "Scan"</li> </ul>	no metadata included

 Table 1: Conversion of data

#### 3.1 Step 2a: Data conversion with ChemConverter in detail

Cyclic voltammetry comes with different challenges with respect to the generation of a conversion profile, as the output data from devices usually contain the data of several cycles, therefore the processing of the files needs to include a separation of the content according to multiple repetitions of reduction and oxidation in one study. According to the converter's routines, each cycle (including reduction and oxidation path) is converted to one jdx-file, allowing a clear separation of the cycles while keeping the data in one container for a direct comparison. In case of non normalized CV measurements, the adjusted voltage and the measured current are plotted.

Normalization (e.g.  $\frac{I}{A}$ ) will be a feature provided by future software updates. Once the profile is created in the converter by the ELN admin, all files of the same type including the predefined identifier (Table 1), are processed automatically according the selected profile to a standardized BagIt bag including different jdx-files with xy-correlation of the single CV measurements. Altogether, we defined three profiles for the conversion of CV measurements, according to the three file types available from the aforementioned vendors. Other profiles could be configured easily in the future.



**Figure S4:** Visualization of conversion with ChemConverter from Gamry's DTA format to the open format JCAMP-DX.

#### 3.1 Step 2b: Metadata mapping with ChemConverter in detail

A key step is the definition and implementation of a target metadata scheme, to which the extracted metadata - independent of the data source - are mapped to. The integration into an ELN as Chemotion offers the option to embed those target metadata schemes and thus providing the necessary mapping target.

To visualize, edit and add additional metadata to an analysis, a JAVA Script based GUI is used by the ELN. The GUI is highly flexible but bound to a specific ontology (e.g. CV, NMR, IR ...). Users with special rights are able to build and edit the GUI with the help of a simple Web interface. Therefore buttons, fields and drop-down menus are defined and arranged. It's also possible to define rules to hide specific fields or create ones with predefined units.



Figure S5: Screenshot of the *Generic Dataset* designer, a tool built to define metadata for each measurement type used in the ELN Chemotion/LabIMotion. Fields and elements created and

designed here are presented as input fields in the GUI of the ELN and can be autofilled during the file conversion process of ChemConverter. Different types of fields can be selected e.g. simple text, "system-defined" for physical units and "select" for drop-down menus for the user to choose from a preselected list later. The JSON implementation of the *Generic Dataset* can be gained from the supporting data deposition in Zenodo (https://doi.org/10.5281/zenodo.12827203).

We collected the required metadata for cyclic voltammetry measurements with representatives of the community as a basis for metadata mapping. The collected required information was defined as metadata form in the ELN to allow users to fill this information if directly available and it is provided as a target scheme for extracting and matching metadata that comes from a measurement. The design and representation of the metadata scheme was done with the GUI described in Figure S7. The metadata scheme consists of different sections, each bearing specific information on the used samples, the preparation of samples and the setting, the used devices and equipment and other conditions and parameters of the measurement. As the required metadata consist of usually data that can be gained from a file and needs to be completed with data given by the user (e.g. data describing the setting, including e.g. the type of electrodes, the conditions and other parameters of the measurement, can be added), a combination of extracted and matched metadata and users' input seems to be suitable in most of the cases.

cyclic voltammetry (CV)								
Layer Label	Field Label	Value	Unit	Name	Туре	Source?	Source identifier	Source data
General information								
	Title			title	text			
	Data Type			data type	text			
	Date	19 9 2022		date.	text			
	Date	18.9.2023		date	text			
	Time	10:35:02		time	text			
	Contributor			contributor	text			
	Creator			creator	text			
	operator	DHM		operator	text			
	Comments			comments	text			
Sample details								
Sample details	inter a			1.1.1		44		
	label	DHM-15		label	text	Chemotion		DHM-15
	id	113176		id	text	Chemotion		113176
	Amount	1	1 mg	amount	system-defined-mass			
	Volume		DI	sample_volume	system-defined-volumes			
	Size			size	text			
Sample preparation								
andre bisharan	Cohiant	MaCN		cohuent	coloct-columnts			
	Otherstern	WIEGH		solvent attac	select-solvents			
	Other solvent			solvent_other	text			
	Volume of solvent		2 ml	amount_sol	system-defined-volumes			
	Concentration of analyte	1	1 mmol_l	concentration	system-defined-molarity			
	Supporting electrolyte	TBAPF6		salt	select-salt			
	Other salt			salt others	text			
	Amount supporting electrolyte	193	30	amount salt	system-defined-mass			
	Concentration supporting electrolyte	193	mmoll	concentration calt	natem defined melarity			
	concentration supporting electrolyte	100	" ""moi_i	concentration_sait	system-defined-molarity			
	Purge electrolyte solution	true		purge_sel	cneckbox			
	Purge gas	nitrogen		purge	select-atm			
	Other purge gas			purge_other	text			
	Purge flow rate	(	0 ul min	purge flow	system-defined-flow rate			
	Purge time		5 min	purge time	system-defined-duration			
Devices used for the measurement				here-"une				
Devices used for the measurement		-						
	Brand	Gamry		brand	text			
	Serial No	IFC1010-30	0147	serial	text			
	Instrument	Potentiosta	at	instrument	text			
Additional equipment and devices								
	Used electrodes	traditional		time	relect-type			
	CCCA method	acomoteia		cype method	second per			
	ECSA method	geometric		ecsa_method	text			
	Polishing method	8 figure-eig	ght	polishing_method	text			
	Polishing material	AI2O3		polishing_material	select-polishing_material			
	Other polishing materials			polishing_others	text			
	Particle size	(	0 mm	polishing material size	system-defined-length			
	Chip brand			ship	coloct chip brand			
	chip brand			chip has a	select-crip_orano			
	Chip type			chip_type	select-cnip_type			
	Working electrode (WE)	glassy carb	ion	working	select-working			
	Other working electrode			working_others	text			
	WE-area (mm <sup>2</sup> )	0.785		working area	text			
	Counter electrode (CE)	platinum		counter	select-counter			
	Other counter electrode			counter others	text			
	other counter electrode			counter_others	text			
	CE-area [mm <sup>-</sup> ]	2.010		counter_area	text			
	Reference electrode (RE)	others		reference	select-reference			
	Other reference electrode	Ag/AgNO3	(0.01 M AgN	Preference_others	text			
	RE-area [mm <sup>2</sup> ]			reference_area	text			
	Special coating	false		coating	checkbox			
	Centies material			seating details	tent.			
and 1 10 11	coating material			coating_details	text			
Settings describing the measurement								
	Operation mode	without me	otion	mode	select-operation_mode			
	Atmosphere	nitrogen		atmosphere	select-atm			
	Other atmosphere			atmosphere_others	text			
	Temperature	6	0 C	temperature	system-defined-temperature			
	Separation	none		separation	select-separations			
	Candidana	deals		and delega	salast an dialast			
	conditions	dark		conditions	select-conditions			
	Wavelength			conditions_ill	text			
	Comments			comments	text			
Measurement details								
	Internal reference	ferrocene		reference_internal	select-reference_measure			
	Other internal reference			reference internal others	text			
	No of cycles		2	curles	integer	Device		2
	Sean rate [V/s]	0.0000000	-	con rate	text	Davise		0.0000000
	Scan rate [v/5]	0.0999998		scan_rate	(CAL	Device		0.0533338
	Step size [V]	0.005		step_size	text	Device		0.005
	Rotational rate [rpm]			rate	text			
	iR correction value [Ohm]			ir_two	text			
	iR correction included	false		ir	checkbox			
	Voltage start [V]	3.00000F-0	001	voltage start	text	Device		3.00000E-001
	Voltage limit 1 [V]	-7.000005	.001	voltage limit one	text	Device		-7.00000E-001
	Volume Line 2 Dd	7,00000E-		to the limit one	sunt .	Device		.,,000002-001
	voitage limit 2 [V]	3,00000E-0	101	voitage_limit_two	text	Device		3,00000E-001
	Voltage limit end [V]	3,00000E-0	001	voltage_limit_end	text	Device		3,00000E-001
Plotting parameters								
	Plotting convention	IUPAC		plotting convention	select-plotting conventions			
	xunits			xunits	text			
	taunite			www.ite	text			
	former			formes .				
	xfactor			xtactor	text			
	yfactor			yfactor	text			
	resolution			resolution	text			
Software used for data generation								
	Software	Framework	2	software	text			
	Software vertice	7.9.6		roftware version	text			
	and the second sec	2.00.00			and the second			

**Figure S6:** List of metadata that is available as a basic set of metadata as \*.xlsx. The Metadata that can be extracted from the measurement file or completed manually in the ELN UI. The generated Excel file is also able to distinguish the source between device and user.

After the extraction and listing inside the Converter GUI, the desired metadata can be assigned to different key-values. This step allows the mapping of different sets of metadata from different original file types to just one standard metadata scheme.

EXPLAIN           TAG         CV           TITLE         LABEL         Cyclic Voltammetry         Test &ldentifier           DATE         LABEL         12.10.2022         Date           TITLE         LABEL         12.10.2022         Date           TIME         LABEL         12.10.2022         Date           TIME         LABEL         12.10.2022         Date           NOTES         NOTES         1         &Notes           PSTAT         PSCI010-30147         Potentiostat         YVINT           VINIT         POTEN         -3,30000E+000         F         Initial &E (V)           VLIMIT2POTEN         -3,30000E+000         F         Scan Limit &1 (V)           VFINAL         POTEN         -0,30000E+000         F           SCARRATE         QUANT 3,0000E+000         F         Scan Limit &2 (V)           VFINAL         POTEN         -0,0000E+000         F         Initial &E (V)           SCARRATE         QUANT 3,0000E+000         F         Initial &E (V)           SCARRATE         QUANT 2,0000E+001         Scan Rate (mV/s)         STEPSIZE           TIREDRARG         QUANT 7,85000E-003         Electronde Type         Electronde Type	Gamry Input .DTA File	Upload to converter software	For international and an analysis of the second and an an analysis of the second and an	
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**Figure S7:** Depicted parts of the workflow combining the selection of metadata in the training input file, the mapping of the selected metadata to a metadata scheme and the visualization of the real results (= extracted metadata) after the upload of a real input file.

#### Example for downloaded table format

The results of the analyzed data from the data plot in ChemSpectra can be downloaded as a table

format file.

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4	Analysis ID		985331						
5	Dataset ID		985332						
6	Dataset name	DHM-12-CV-1mM+1mMFc-N2_	100mVps-No9						
7	Link to sample								
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12									
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**Figure S8:** Screenshot of a csv output file from ChemSpectra. The tool produces one csv file for each curve/cycle of the experiment. It contains the peak values (potential and current) of the redox-

pairs defined by the user in the frontend as well as the calculated values (current ratio, half-wave potential and  $\Delta E_p$ ) derived from them. Each line in the table mirrors one redox-pair. In this example, the first line represents the attributes of the added ferrocene reference substance shifted to  $E_{1/2} \rightarrow 0$  V and the second line represents the features of the measured complex sample.

# **4 BagIt Implementation**

To achieve a standardized and structured output container, BagIt is used. BagIt is a hierarchical file system conventions created by the California Digital Library and the Library of Congress<sup>5</sup>. BagIt is about reliable transfer of content in a package, which are called "bags". It is also possible to serialize a bag as a zip-file if a single file for uploading is needed. According to the memo from the IETF the bag consists of required and optional elements. Required are the "bagit.txt" file and a data / payload sub-directory. The bagit.txt contains a line with the BagIt version (in our case 1.0) and a line with the used encoding (UTF-8) of the tags. Also at least one manifest tag file is needed named after the checksum algorithm and containing a checksum and path for each file in the payload directory. We decided to use sha256 and sha512 simultaneously. Two different algorithms are used for the purpose of double checking [2]. The "bagit.txt" must contain the used BagIt version and encoding which is 1.0 and UTF-8. Each recorded curve or cycle of the CV data is stored as one file in JCAMP-DX format after conversion inside the "data" folder while the converted metadata is stored as a .json-file inside "metadata/converter.json". To avoid problems with up- and downloading multiple files, the BagIt container is serialized as .zip-file.

# **5** Special features for Cyclic Voltammetry in ChemSpectra

ChemSpectra further allows the calculation and assignment of some standardized key values to describe and compare different curves of CV experiments when using different references or equipment (e.g. the voltage and current absolute values could be quite different if using other electrodes). The most common and already implemented values are

- the correction value of the capacitive background current aka  $I_{\Box 0}$  (or sometimes also  $i_{sp0}$ ). This value is currently determined graphically by the user.
- The current (I in Ampere) ratio  $i_{pa}/i_{pc}$  of a given redox-pair calculated by the approximation formula of <u>NICHOLSON, RI S. 1966</u>. Adopted to ChemSpectra's notation the formula is

calculated as:  $I_{ratio} = \frac{|I_{p,min}|}{|I_{p,max}|} + \frac{(0.485) \times |I_{\lambda o}|}{|I_{p,max}|} + 0.086$  whereby  $I_p$  are the current values of the anodic and cathodic peaks.

• The peak separation between the anodic and cathodic peak  $\Delta E_p = |E_{p,max} - E_{p,min}|$  whereby E is the voltage values of the peaks.

## 6 ChemSpectra Workflow

The interaction between users and their data files within the ChemSpectra and ELN ecosystem is illustrated in Figure S9 as a flow diagram. As an integrated application, ChemSpectra manages data transfer between the ELN, its own front-end and back-end systems, and the user interface. This process involves multiple iterations of data exchange and ensures seamless integration, traceability and functionality.



Figure S9: Complete workflow diagram of *ChemSpectra* and the interaction of its front- and backend with the ELN and the user.

## 7 Inline Notation

We also provide a draft for an inline notation to report redox potentials obtained by CV measurements, similar to the so-called NMR textual analysis, initially defined by two IUPAC Recommendations<sup>6,7</sup>. For NMR, this inline notation is generated automatically by *ChemSpectra* after analysis of NMR data in *ChemSpectra*. The same will apply to CV in an upcoming release of Chemotion ELN. After several reviews within the authors of this document we agreed on the following inline notation, taking Cu(TMGqu)<sub>2</sub>PF<sub>6</sub> as an example:

CV (1 mM in MeCN vs. Ref (Fc<sup>+</sup>/Fc) = 0.38 V, 
$$\nu = 0.1$$
 V/s, to neg.):  
 $E_{1/2} ([Cu(TMGqu)_2]^{2+}/[Cu(TMGqu)_2]^+, \Delta E_p) = -0.04$  V (80 mV).

Similar to the NMR text, the inline notation starts with the abbreviation of the method used. This is followed in parentheses by information on the concentration of the analyte and the solvent applied. In addition, the redox couple of the reference substance is mentioned together with the explicit mention of the value of the redox potential of the reference substance used for calibration i.e. to which reference the redox potentials are *reported*. The signal of the redox couple of the reference substance is regularly set to 0 V, which is common practice among some of the authors of this work, but it can be set to any other value, but this should be reported redox potentials of organic molecules are regularly reported vs. SCE, while the actual measurement was referenced with ferrocene as internal standard. Following Pavlishchuk and Addison the redox potential of the reference or quasi reference electrode (QRE)<sup>9</sup>,<sup>10</sup> used in the measurement cell is considered to be part of the metadata (see above, Generic Dataset Template), if the measurement is internally referenced using ferrocene or any other internal standard. Moreover, the inline notation provides

information on the scan rate v (lowercase Nu, following IUPAC Recommendations<sup>9</sup> and IUPAC Orange Book) as well as the direction the measurement was started (to neg./ to pos.). The latter information was considered to be important as reactive (radical) intermediates formed within the cell might induce additional redox events in CV spectra<sup>11</sup> (e.g. dehalogenation of arylhalides). Following the parentheses, the half-wave potential  $E_{1/2}$  for each redox event is provided. The redox couple is given in parentheses according to IUPAC Green Book 2007<sup>12</sup>, followed by  $\Delta E_p$ , separated by a comma. For irreversible redox events, where the potential may be determined based on half-peak potentials  $E_{p/2}^{10}$ ,  $\Delta E_p$  and the corresponding parentheses and the value are omitted. For redox quiet counter ions (if present), these counter ions may be omitted. The half-wave potential(s)  $E_{1/2}$  in V are subsequently reported after the equal sign together with the  $\Delta E_p$  in mV in parentheses. Each reported redox couple with its redox potential reported is separated with a comma plus single space and each notation ends with a full stop.

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**Figure S10:** Implementation of the inline notation in the analysis section of the Chemotion ELN and Chemotion Repository.

# 8 Representation of data in different repositories

	📦 Viewer	×
$H_{3}C H_{3}C $	<b>IUPAC Name:</b> copper(1+);1,1,3,3-tetramethyl-2-quinolin-8-ylguanidine;he (C <sub>28</sub> H <sub>36</sub> CuF <sub>6</sub> N <sub>8</sub> P)	exafluorophosphate
	Canonical SMILES: F[P-](F)(F)(F)(F)F.CN(C(=Nc1cccc2c1nccc2)N(C)C)C.CN(C(=Nc1cccc2c InChI: InChI=15/2C14H18N4.Cu.F6P/c2*1-17(2)14(18(3)4)16-12-9-5-7-11-8-6-10-15-13(11)1 +1:1:1	:1nccc2)N(C)C)C.[Cu+] 2;;1-7(2,3,4,5)6/h2*5-10H,1-4H3;;/q;;
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CH313C	Crosslinks: 🔘 🌀 1 <sup>st</sup>	
Sample Published on 20	124-03-08 🔘	
Contributor: David Herrmann		
1. Karlsruhe Institute of Technology, Germany		
Author: David Herrmann <sup>1</sup>		
1. Karlsruhe Institute of Technology, Germany		
Sample type: Consists of molecule with define	d structure	
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Sample ID: CRS-39256		
Relations of this sample:		
<ul> <li>Stanek, J., Sackers, N., Fink, F., Paul, M., P. Electron-Transfer Proteins. Chemistry – A E</li> <li>Herrmann, D., Hodapp, P., Starman, M., Huu</li> <li>Hoffmann, A., Seitz, T., Zeitler, K., Dorn, A., source approach described for cyclic voltam</li> </ul>	sters, L., Grunzke, R., Hoffmann, A., & Herres-Pawlis, S. (2017). Copper Guanidinoquinoline Complexes iropean Journal, 23(62), 15738–15745. https://doi.org/10.1002/chem.201703261 nog. PC., Lin, CL., Le, Klar, J., Bizzarri, C., Roese, P., Oppel, N., Fischer, T. G., Tremouilhac, P., Hot Jung, N., & Bräse, S. (2023). Enhancing FAIRdata by providing digital workflows from data generation to metry. American Chemical Society (ACS). https://doi.org/10.26434/chemrxiv-2023-95s19	as Entatic State Models of zhauer, L., Herres-pawlis, S., the publication of data: an open
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CV (1 mM in MeCN vs. Ref (Fc <sup>+</sup> /Fc) = 0 V, $v = 0$	1 V/s, to neg.): $E_{1/2}$ ([Cu(TMGqu) <sub>2</sub> ] <sup>2+</sup> /[Cu(TMGqu) <sub>2</sub> ] <sup>*</sup> , $\Delta E_p$ ) = -0.44 V (90 mV).	
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CV (1 mM in MeCN vs. Ref (Fc <sup>+</sup> /Fc) = 0 V, $v = 0$	1 V/s, to neg.): $E_{1/2} ([Cu(TMGqu)_2]^{2*}[Cu(TMGqu)_2]^*, \Delta E_p) = -0.44 V (90 mV).$	
Datasets		
DHM-12-CV-1mM-N2_100mVps-No6		ᆂ 🔜 💼

# Figure S11: Representation of the same dataset in three different repositories: CV dataset in the

### Chemotion

Repository

(https://dx.doi.org/10.14272/UVLHGRADYISRGZ-UHFFFAOYSA-N.10).

Published May 2024   \	/ersion v3		Dataset 🚨 Open	44	6
Analytical d	ata: cyclic voltammetry - Version 1.1			<b>VIEWS</b>	S DOWNLOADS
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Project members:	Harran Davilla, Sania? 🔿 Haffmann, Alavandar? 🔿 Einskar Tilmann O	Children Minele 1		Versions	
Bräse, Stefan <sup>1</sup> (0)	nerres-rawiis, sonja" 🥥, normann, Alexander Vo, Fischer, minann G.	, Jung, Nicole U,	Show affiliations	Version v3	May 2024
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Cyclic voltammetry exp enable a discussion at	periment of the complex [Cu(TMGqu)2]PF6, previously reported by Stanek at a bout how to report on cyclic voltammetry data - it refers to the preprint: https://	I. 2017. This dataset and its /doi.org/10.26434/chemrxiv-;	description is published as a first draft to 2023-95s19.	Version Draft v.1.0 10.5281/zenodo.8391609	Sep 29, 2023
Files				View all 2 version	ns
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DHM-12-CV	-1mM+1mMFc-N2_100mVps-No9.2_bagit.edit.png		94.4 kB	Communities	
DHM-12-CV	-1mM+1mMFc-N2_100mVps-No9.2_bagit.infer.json		37 Bytes	NFDI4Chem	
DHM-12-CV	-1mM+1mMFc-N2_100mVps-No9.2_bagit.jdx		10.6 kB		
DHM-12-CV	-1mM+1mMFc-N2_100mVps-No9.3_bagit.csv		270 Bytes 💙	Keywords and subjects	
Files (935.2 k8)			*	Cyclic voltammetry Open Science	Electrochemistry
Name		Size	Download all	Research data management Digitalia	zation
CV_with_Fc+_Fc_R md5:54d1cd24e4a6468010ddd	eferenceDHM-12-CV-1mM+1mMFc-N2_100mVps-No9.zip	511.5 kB	Preview     Lownicad		
CV_without_Fc+_Fc	_ReferenceDHM-12-CV-1mM-N2_100mVps-No6.zip	423.7 kB	Preview     L     Download	Details	
1100.1112004070714401800100				D01 10.5281/zenodo.11230180	
				Dataset	
Additional detai	IS			Publisher	
				Zenodo	
Related works	Is cited by Preprint: 10.26434/chemrxiv-2023-95s19 (DOI)			Languages English	
References	<ul> <li>Herrmann, D., Hodapp, P., Starman, M., Huang, PC., Lin, CL., L Tremouilhac, P. Holzhauer, L., Herres-pawlis, S., Hoffmann, A.,</li> </ul>	e, L., Klar, J., Bizzarri, C., Ro Seitz, T., Zeitler, K., Dorn, A.,	ese, P., Oppel, N., Fischer, T. G., Juna, N., & Bräse, S. (2023), Enhancing	Diabts	
	FAIRdata by providing digital workflows from data generation to voltammetry. American Chemical Society (ACS). https://doi.org/1	the publication of data: an op 0.26434/chemrxiv-2023-95s	pen source approach described for cyclic 19	. agino	
	<ul> <li>Stanek, J., Sackers, N., Fink, F., Paul, M., Peters, L., Grunzke, R., Complexes as Entatic State Models of Electron-Transfer Proteins doi.org/10.1002/chem.201703261</li> </ul>	Hoffmann, A., & Herres-Pav . Chemistry – A European Jo	wlis, S. (2017). Copper Guanidinoquinoline burnal, 23(62), 15738–15745. https://	Creative Commons Attribution	1 1.0 Generic
Citations @			•	Citation	
				Herrmann, D. (2024). Analytical data: cy	clic voltammetry - Version
Show only:	Literature (0) Dataset (0) Software (0) Unknown (0)		n Search	1. I [Data sel]. Zenodo, https://doi.org/10	.5261/201000.11250160
	Citations to This Version			Style APA .	<b>B</b>
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				Created May 21, 2024	
				Modified May 21, 2024	

Figure S12: Representation of the same dataset in three different repositories: CV dataset in Zenodo (<u>https://doi.org/10.5281/zenodo.11230180</u>).

RADAR Metadata	Content	Statistics	Technical Metadata	DOI: 10.22000/jSIYquBIZcUmYYJx Publication date: 2024-07-26		
lated identifier:	(Cites) 10.26434/chemsxiv-2023-95s19 - DOI (Is Variant Form Of) 10.14272/UVLHGRADYISRGZ-UHFFFA/ (Is New Version Of) 10.22000/1753 - DOI	OYSA-N.5 - DOI		Download Dataset DOWNLOAD (1.8 MB)		
ator/Author:	Herrmann, David 💿 https://orcid.org/0009-0008-1636-087	5 [Karlsruhe Institute of Technology]				
tributors:	(Project Member) Herres Pawlis, Sonja ⊙ https://orcid.org/0000-0002-4354- (Project Member) Hoffmann, Alexander ⊙ https://occid.org/0000-0002-9647	4353 [RWTH Aachen] 49532 [RWTH Aachen]		Download Metadata RADAR V DOWNLOAD Statistics		
	(Project Member) Fischer, Tillmann G. O https://orcid.org/0000-0003-4480-8	1661 [Leibniz Institute of Plant Biochemistry (IPB)]		17 0 Views Downloads		
	(Project Member) Bizzarri, Claudia <sup>©</sup> https://orcid.org/0000-0002-4077-2553 (Project Member) Jung, Nicole <sup>©</sup> https://orcid.org/0000-0001-9513-2448 [K4	[Karlsruhe Institute of Technology] arlsruhe Institute of Technology]		Rights statement for the dataset This work is licensed under CC BY 4.0		
	(Project Member) Bräse, Stefan 📀 https://orcid.org/0000-0003-4845-3191 [K	arisruhe Institute of Technology]		Cite Dataset		
e:	Analytical data: cyclic voltammetry - Version v.1.1			RADAR V COPY		
scription:	(Abstract) Cyclic voltammetry experiment of the complex ( to enable a discussion about how to report on cyclic voltam	Cu(TMGqu)2]PF6, previously reported by Stanek at al. 201 ametry data - it refers to the preprint: https://doi.org/10.26	<ol> <li>This dataset and its description is published as a first draft 434/chemnxiv-2023-95s19.</li> </ol>	Herrmann, David (2024): Analytical data: cyclic voltammetry - Version v Karlsruhe Institute of Technology. D0I: 10.22000/jSiYquBfZcUmVY.Jx		
words:	Cyclic voltammetry Open Science Electrochemistry Research data management Digitalization					
iguage:	English					
lishers:	Karlsruhe Institute of Technology					
luction year:	2024					
ject areas:	Chemistry Materials Science					
ource type:	(Dataset) Collection					
ware used:	Resource production		G			
ware:	Chemotion ELN-1.0 RAD/					
lication year:	2024			4Chem (•)		
its holders:	Herrmann, David					
ting:	German research foundation - (National Research Data Infr	astructure for Chemistry (NFDI4Chem))(441958208)				

RADAR Metadata	Content	Statistics		Technical Metadata	
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Name		Storage	Metadata	Upload	Action
🖹 c45c6be7-82ba-4c76-9065-7c4d0286f	d5b.zip	1.7 MB			
metadata_CV_including ferrocene.xlsx		15.8 kB			
metadata_CV_without ferrocene.xlsx		15.7 kB			
Showing 1 to 3 of 3 entries					< 1 >

**Figure S13:** Representation of the same dataset in three different repositories: CV dataset in RADAR4Chem (https://dx.doi.org/10.22000/jSIYquBfZcUmVYJx). The logo was arranged.

**Table 2.** List of the DOI-Links for the different Chemotion repository entries published by the diverse research facilities for the same compound. Following the links for the sample leads to the same molecule page in the Chemotion repository but on the right spot, while following the link for

an analysis shows an extra page only showing the wanted analysis together with the sample's structure (see Figure S14).

Side	DOI for sample	DOI for analysis
Institute of Biological and Chemical Systems – Functional Molecular Systems (IBCS-FMS), KIT, Germany	https://dx.doi.org/10.14272/UVL HGRADYISRGZ- UHFFFAOYSA-N.10	https://dx.doi.org/10.14272/UVLHGR ADYISRGZ-UHFFFAOYSA- N/CHMO0000025.17
Institute for Applied Materials – Electrochemical Technologies (IAM-ET), KIT, Germany	https://dx.doi.org/10.14272/UVL HGRADYISRGZ- UHFFFAOYSA-N.8	https://dx.doi.org/10.14272/UVLHGR ADYISRGZ-UHFFFAOYSA- N/CHMO0000025.14
Institute of Organic Chemistry (IOC), KIT, Germany	https://dx.doi.org/10.14272/UVL HGRADYISRGZ- UHFFFAOYSA-N.7	https://dx.doi.org/10.14272/UVLHGR ADYISRGZ-UHFFFAOYSA- N/CHMO0000025.11
University - Institute of Organic Chemistry & Institute of Plant Biochemistry - Bioinformatics & Scientific Data, Leipzig, Germany	https://dx.doi.org/10.14272/UVL HGRADYISRGZ- UHFFFAOYSA-N.11	https://dx.doi.org/10.14272/UVLHGR ADYISRGZ-UHFFFAOYSA- N/CHMO0000025.18 (*)
Chair of Bioinorganic Chemistry and Institute of Inorganic Chemistry (IAC), RWTH Aachen University, Germany	https://dx.doi.org/10.14272/UVL HGRADYISRGZ- UHFFFAOYSA-N.14	https://dx.doi.org/10.14272/UVLHGR ADYISRGZ-UHFFFAOYSA- N/CHMO0000025.21 (**)

(\*) The PSSESSION format of the PalmSens device used by the group in Leipzig University is able to hold data of more than one measurement, so they are able to submit one analysis datafile containing a measurement with Ferrocene added and a measurement without Ferrocene. (\*\*) The group from Aaachen only submitted the measurement containing the compound only.

The submission of the alternative compound could also be found in the Chemotion repository using this DOI: https://dx.doi.org/10.14272/PHXDKLQHLVWUNE-UHFFFAOYSA-N.3



This information is based on the molecular structure shown on the left side. For a decoupled sample, please refer to its individual details.

Formula: C28H36CuF6N8P

Canonical SMILES: F[P-](F)(F)(F)(F)(F)F.CN(C(=Nc1cccc2c1nccc2)N(C)C)C.CN(C(=Nc1cccc2c1nccc2)N(C)C)C.[Cu+] InChI: InChI=1S/2C14H18N4.Cu.F6P/c2\*1-17(2)14(18(3)4)16-12-9-5-7-11-8-6-10-15-13(11)12;;1-7(2,3,4,5)6/h2\*5-10H,1 -4H3;;/q;;+1;-1 InChIKey: UVLHGRADYISRGZ-UHFFFAOYSA-N

Exact Mass:







Published on 2024-03-08	
cyclic voltammetry (CV)	0
Author: <sup>1</sup> Claudia Bizzarri <sup>1</sup>	
1. Karlsruhe Institute of Technology, Deutschland	
Analysis DOI:       10.14272/UVLHGRADYISRGZ-UHFFFAOYSA-N/CHM00000025.11       Image: Son-LD         Analysis ID:       CRD-39102       Image: CRD-39102       Image: CRD-39102         Content:       CV (1 mM in MeCN vs. Ref (Fc+/Fc) = 0 V, v = 0.1 V/s, to neg.): E1/2 ([Cu(TMGqu)2]2+/[Cu(TMGqu)2]+, ΔEp) = -0.43 V (78 mV).	
Datasets CBz_20230907_ACN_Cu(TMGqu)2PF6_100 mVs-1_Fc	

Published on 2024-03-12	
cyclic voltammetry (CV) Authors: ②Alrik Dorn <sup>1</sup> - ③Tillmann G. Fischer <sup>2</sup> - ③Kirsten Zeitler <sup>1</sup> 1. Institute of Organic Chemistry, Leipzig University, Germany 2. Bioinformatics & Scientific Data. Leibniz Institute of Plant Biochemistry, Germany	0
Analysis DOI:       10.14272/UVLHGRADYISRGZ-UHFFFAOYSA-N/CHM00000025.18       Image: Son-LD         Analysis ID:       CRD-39581       CRD-39581         Content:       CV (1 mM in MeCN vs. Ref (Fc+/Fc) = 0.38 V, v = 0.1 V/s, to pos.): E1/2 ([Cu(TMGqu)2]2+/[Cu(TMGqu)2]+, ΔEp) = -0.04 V (80 mV).	
Datasets ADO-1_CuTMGqu2PF6	L 2 8

Published on 2024-07-29	
cyclic voltammetry (CV)	0
Authors: 😳 Alexander Hoffmann <sup>1</sup> - 💿 Sonja Herres-Pawlis <sup>2</sup>	
1. Institute of Inorganic Chemistry, RWTH Aachen University, Germany	
2. Fachgruppe Chemie, Rheinisch Westfälische Technische Hochschule Aachen, Germany	
Analysis DOI:       10.14272/UVLHGRADYISRGZ-UHFFFAOYSA-N/CHM00000025.21       Image: Son-LD         Analysis ID:       CRD-43416       Image: CRD-43416       Image: CRD-43416         Content:       CV (1 mM in MeCN vs. Ref (Fc+/Fc) = 0 V, v = 0.1 V/s, to neg.): E1/2 ([Cu(TMGqu)2]2+/[Cu(TMGqu)2]+, ΔEp) = -0.46 V (73 mV).	
Datasets	
CV of [Cu(TMGqu)2] by 100mV/s	1

**Figure S14:** Representation of an analysis in Chemotion Repository when following the associated DOI-Link. The upper part, which shows the structural formula of the molecule, is identical for all analyses and is therefore only shown once.

A comparison of Figures S11 to S14 shows that the Chemotion repository has a clear advantage in the representation of the relationship between the analysis data set and the assigned sample due to its architecture.

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