FOSSProF Final Report

Project Overview

- Project Title: **Advancing Biosensor Data Analysis Software SACMES**

- Project Summary: The objective of this study was to update and make more accessible a biosensor analysis script called SACMES, which our laboratory published as open access in 2019 (*Anal. Chem.* 2019, 91, 19, 12321–12328). SACMES allows the real-time data processing and visualization of electrochemical, aptamer-based sensor data. This technology is emerging as the future of continuous molecular sensing in the body. With support from FOSSProf, we updated all dated Python libraries and modules, and are in the process of further modularizing the code to make it easier to update in the future. Additionally, we uploaded the code to Pip, to facilitate its download and integration with Python environments. The software is already in use by tens of research groups around the globe. Our plan is to continue improving the code beyond the end of this project, to reach even more research groups across the globe and increase its impact.

- Target Audience: The primary users of this project are laboratories around the world working on aptamer-based biosensor development and implementation, as well as various commercial entities trying to take such biosensors to the medical industry.

- Code Repository: Please include links to publicly available code repositories.
    - https://pypi.org/project/SACMES-PYTHON-PACKAGE
    - https://github.com/netzlab/SACMES

Project Activities and Progress

- Work Completed: At the beginning of the project, the SACMES code was non-functional on the latest versions of Python due to deprecation of the necessary libraries called throughout the script. The team identified all deprecated libraries and commands, and updated the code to be fully functional with the latest Python implementations, while also maintaining backwards compatibility with older versions of Python. Finally, the code was uploaded to pip for easy distribution as we continue testing.

- Clearly outline the activities undertaken during the grant period. Did you achieve all your planned goals?

  To update deprecated libraries within the code, the hired student traced the entire codebase and generated a Miro workflow diagram: https://miro.com/app/board/uXjVNiUX7pI=/

Additionally, we created new helper.py and config.py scripts to call all necessary libraries and variables once, ensuring proper library updates and reducing code redundancy

A second goal was to modularize the code, further reducing redundancy in shared function and library calling. Unfortunately, this was not accomplished in full due to communication issues and lack of programming expertise of the student working on the project. However, we will continue pursuing this goal beyond the end of this funded project.

- Technical Milestones: Discuss any specific technical milestones achieved, such as code releases, documentation updates, or bug fixes. Quantify accomplishments with metrics where possible (e.g., user growth, code contributions).

  The code was updated and documented via pypi releases (https://pypi.org/project/SACMES-PYTHON-PACKAGE).

- Challenges and Solutions: Share any challenges encountered during the project and how you addressed them.

  The challenges we encountered during the project were inconsistencies with how the code would perform depending on the operating system of the user (either MacOS or WindowsOS). This was addressed by modifying the working pipeline to include troubleshooting in both systems prior to pushing system wide updates.

  Another challenge was maintaining communication and deadlines with the student in charge of the project. Future work will need to be completed by a software developer with more experience (already hired by PI Arroyo).

<u>Outcomes and Impact</u>

- Project Impact: SACMES is used daily in the Arroyo lab to support all new biosensor development efforts, including direct support of the research efforts of six graduate students, four postdoctoral scholars, one research associate, and various rotating undergraduates, furthering our research training mission. Addtionally, the code has been adopted by over a dozen groups around the globe, who had communicated to PI Arroyo concerns regarding library status and update needs. Direct citations to the code by the broad scientific community are listed below:

Sanduni W. Abeykoon, Ryan J. White. Single Voltammetric Sweep Calibration-Free Interrogation of Electrochemical Aptamer-Based Sensors Employing Continuous Square Wave Voltammetry. Analytical Chemistry 2024, 96 (18) , 6958-6967. https://doi.org/10.1021/acs.analchem.3c05920

Alexander Shaver, Kyle Mallires, Jonathan Harris, Jonathan Kavner, Bo Wang, Rebecca Gottlieb, Juan Lión-Villar, María Ángeles Herranz, Nazario Martín, Netzahualcóyotl Arroyo-Currás. Survey of Conductive

Polymers for the Fabrication of Conformation Switching Nucleic Acid-Based Electrochemical Biosensors. ACS Applied Polymer Materials 2024, 6 (1) , 541-551. https://doi.org/10.1021/acsapm.3c02206

Minh-Dat Nguyen, Khoa-Nam Nguyen, Samuel Malo, Indrani Banerjee, Donghui Wu, Laurence Du-Thumm, Philippe Dauphin-Ducharme. Electrochemical Aptamer-Based Biosensors for Measurements in Undiluted Human Saliva. ACS Sensors 2023, 8 (12) , 4625-4635. https://doi.org/10.1021/acssensors.3c01624

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Erfan Rahbarimehr, Hoi Pui Chao, Zachary R. Churcher, Sladjana Slavkovic, Yunus A. Kaiyum, Philip E. Johnson, Philippe Dauphin-Ducharme. Finding the Lost Dissociation Constant of Electrochemical Aptamer-Based Biosensors. Analytical Chemistry 2023, 95 (4) , 2229-2237. https://doi.org/10.1021/acs.analchem.2c03566

Alexander Shaver, J.D. Mahlum, Karen Scida, Melanie L. Johnston, Miguel Aller Pellitero, Yao Wu, Gregory V. Carr, Netzahualcóyotl Arroyo-Currás. Optimization of Vancomycin Aptamer Sequence Length Increases the Sensitivity of Electrochemical, Aptamer-Based Sensors In Vivo. ACS Sensors 2022, 7 (12) , 3895-3905. https://doi.org/10.1021/acssensors.2c01910

Yao Wu, Farshad Tehrani, Hazhir Teymourian, John Mack, Alexander Shaver, Maria Reynoso, Jonathan Kavner, Nickey Huang, Allison Furmidge, Andrés Duvvuri, Yuhang Nie, Lori M. Laffel, Francis J. Doyle III, Mary-Elizabeth Patti, Eyal Dassau, Joseph Wang, Netzahualcóyotl Arroyo-Currás. Microneedle Aptamer-Based Sensors for Continuous, Real-Time Therapeutic Drug Monitoring. Analytical Chemistry 2022, 94 (23) , 8335-8345. https://doi.org/10.1021/acs.analchem.2c00829

Alex M. Downs, Julian Gerson, M. Nur Hossain, Kyle Ploense, Michael Pham, Heinz-Bernhard Kraatz, Tod Kippin, Kevin W. Plaxco. Nanoporous Gold for the Miniaturization of In Vivo Electrochemical Aptamer-Based Sensors. ACS Sensors 2021, 6 (6) , 2299-2306. https://doi.org/10.1021/acssensors.1c00354

Zhi-min Chen, Yi Wang, Xing-yuan Du, Jian-Jun Sun, Sen Yang. Temperature-Alternated Electrochemical Aptamer-Based Biosensor for Calibration-Free and Sensitive Molecular Measurements in an Unprocessed Actual Sample. Analytical Chemistry 2021, 93 (22) , 7843-7850. https://doi.org/10.1021/acs.analchem.1c00289

Alexander Shaver, Nandini Kundu, Brian E. Young, Philip A. Vieira, Jonathan T. Sczepanski, Netzahualcóyotl Arroyo-Currás. Nuclease Hydrolysis Does Not Drive the Rapid Signaling Decay of DNA Aptamer-Based Electrochemical Sensors in Biological Fluids. Langmuir 2021, 37 (17) , 5213-5221. https://doi.org/10.1021/acs.langmuir.1c00166

Miguel Aller Pellitero, Samuel D. Curtis, Netzahualcóyotl Arroyo-Currás. Interrogation of Electrochemical Aptamer-Based Sensors via Peak-to-Peak Separation in Cyclic Voltammetry Improves the Temporal Stability and Batch-to-Batch Variability in Biological Fluids. ACS Sensors 2021, 6 (3) , 1199-1207. https://doi.org/10.1021/acssensors.0c02455

Andrea Idili, Julian Gerson, Tod Kippin, Kevin W. Plaxco. Seconds-Resolved, In Situ Measurements of Plasma Phenylalanine Disposition Kinetics in Living Rats. Analytical Chemistry 2021, 93 (8) , 4023-4032. https://doi.org/10.1021/acs.analchem.0c05024

Shao Su, Jianfeng Ma, Yongqiang Xu, Hemeng Pan, Dan Zhu, Jie Chao, Lixing Weng, Lianhui Wang. Electrochemical Analysis of Target-Induced Hairpin-Mediated Aptamer Sensors. ACS Applied Materials & Interfaces 2020, 12 (42) , 48133-48139. https://doi.org/10.1021/acsami.0c12897

Claudio Parolo, Andrea Idili, Gabriel Ortega, Andrew Csordas, Alex Hsu, Netzahualcóyotl Arroyo-Currás, Qin Yang, Brian Scott Ferguson, Jinpeng Wang, Kevin W. Plaxco. Real-Time Monitoring of a Protein Biomarker. ACS Sensors 2020, 5 (7) , 1877-1881. https://doi.org/10.1021/acssensors.0c01085

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Jaume Béjar-Grimalt, Francesc A. Esteve-Turrillas, Sergio Armenta, Salvador Garrigues, David Pérez Guaita. DrogoFinder: An open-source graphical user interface for the identification of illicit drugs using infrared spectroscopy. Microchemical Journal 2024, 199 , 109801. https://doi.org/10.1016/j.microc.2023.109801

Maria Reynoso, An-Yi Chang, Yao Wu, Raygan Murray, Smrithi Suresh, Yuma Dugas, Joseph Wang, Netzahualcóyotl Arroyo-Currás. 3D-printed, aptamer-based microneedle sensor arrays using magnetic placement on live rats for pharmacokinetic measurements in interstitial fluid. Biosensors and Bioelectronics 2024, 244 , 115802. https://doi.org/10.1016/j.bios.2023.115802

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Netzahualcoyotl Arroyo-Currás, Philippe Dauphin-Ducharme, Karen Scida, Jorge L. Chávez. From the beaker to the body: translational challenges for electrochemical, aptamer-based sensors. Analytical Methods 2020, 12 (10) , 1288-1310. https://doi.org/10.1039/D0AY00026D

- Community Engagement: Did you actively engage with the open source community through contributions, conferences, or workshops? Share details and metrics of participation.

  We did not actively engage with the open-source community.

- Sustainability / Future Plans: Explain how the project will be sustained beyond the grant period. Are there plans for future development, funding, or community support? Is there potential for further impact?

PI Arroyo has hired a new software developer to continue our efforts towards modularizing the code and making it more efficient for (a) data processing and (b) customization. Additionally, the code will be further developed to include new data processing and actuation functions, such as closed-loop features as well as novel noise removal methods.

- Lessons Learned: Share key takeaways and insights gained from the project.

The main lesson learned is that adequate software development necessarily requires dedicated, experienced personnel. Although we appreciated the computer sciences student working with us for this project, the student was not up to the level that was needed to accomplish more ambitious goals. Additionally, we learned about different platform options and updates to make the code more streamlined and accessible to future developers.

- Attachments: The screenshot below shows the visual output of SACMES (now working under new Python implementations), which transforms raw biosensor data (the gaussian curves seen at the left) to in-vivo, real-time pharmacokinetic measurements (the red data shown at the right).