IX SYMPOSIUM OF MEDICINAL CHEMISTRY YOUNG RESEARCHERS

CSIC CHEMICAL LIBRARY (QCSIC): A NEW CHALLENGE AFTER THE COVID-19 OUTBREAK

CSIC IQM Consejo Superior de Investigaciones Científicas

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Introduction

The COVID-19 outbreak highlighted the necessity to access to a large collection of synthetic molecules as candidates for antiviral drug discovery. To achieve this objective the establishment of QCSIC, an Institutional Chemical Library of CSIC was decided. This involved the collection, organization, classification, and storage of chemical compounds synthesized by scientists from CSIC, initially focusing on three specific centers: IQM, IIQ, and IQAC. This chemical library includes the physical collection of substances in a format compatible with high-throughput screening (HTS) techniques, and their inventory in a virtual database, Lg-Chimio. The purpose of this chemical library is not limited to find antiviral drug candidates; the same logic applies to all type of biological targets.

The CSIC chemical library

1 **Substances are collected in vials and stored in boxes of 80 vials. Their structure, chemical properties and analytical data are registered in the database. The database must allow substructure query to find analogues in case a hit is confirmed.**

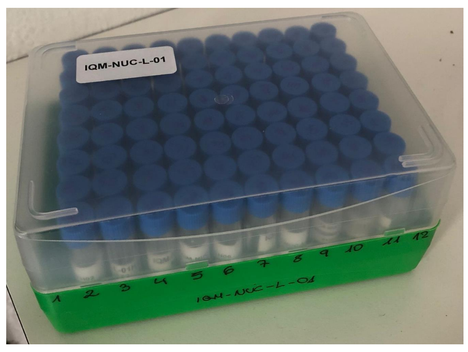

Figure 1. Vials in their storage box

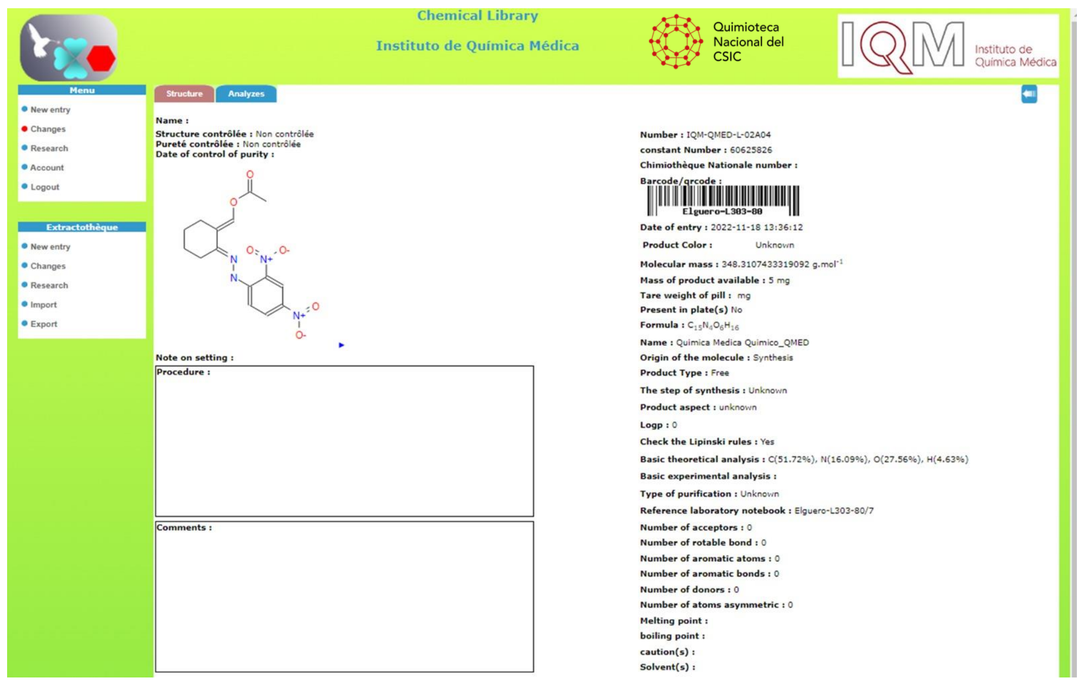

Figure 2. Substance description in the Lg-Chimio database

2 **Stock solutions of the collected substances are prepared in DMSO at 10 mM in 1 mL vials as a replica of the storage box. This replica is called the mother plate and stored at the chemical library.**

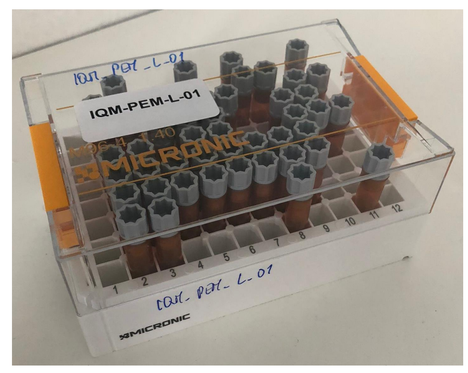

Figure 3. Stock solutions in a mother plate

3 **Replicas of the mother plate are prepared by collecting an aliquot of the mother plate. The library signs a MTA with the biologist, and then the plates are sent for screening.**

Figure 4. Greiner-type daughter plates

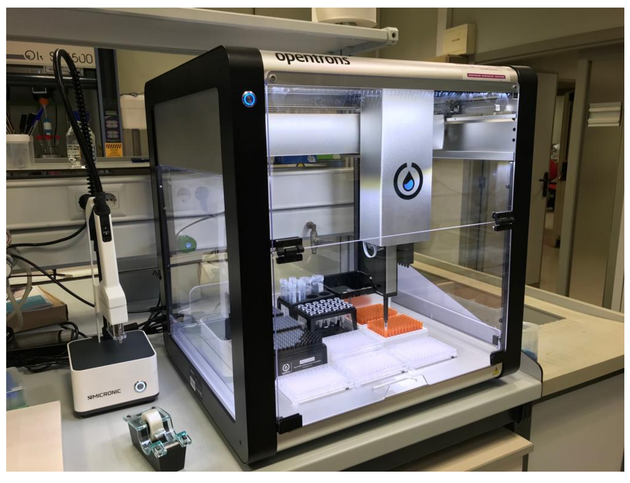

Figure 5. Illustration of the IQM robot. Automation improves the speed and precision of the process in comparison to manual pipetting

4 **The biologist blinds screens the compounds and sends a report to the chemical library.**

5 **If a hit is found, a secondary screening is operated to confirm the hit and establish dose-response results.**

6 **If the hit is confirmed, the chemical library connects the chemist and the biologist. Both partners decide if the project has potential for further developing**

7 **If both partners agree to carry on the project, the chemist reveals the structure and an MTA is signed by both parties.**

Research projects
Publications
Patents

Summary: benefits of a chemical library

- **For chemists:**
  - **A way to enhance their molecules beyond their primary purpose, by supplementing them with physico-chemical and biological data.**
  - **A way to preserve the heritage and know-how of the laboratory, the institute, and the institution.**
- **For biologists:**
  - **A way to provide a highly original and diverse collection of substances, without being limited to commercially available compounds.**
- **For both partners:**
  - **New research programs, due to the discovery of chemical probes or biologically active compounds. Managing the intellectual and industrial property issues**

Permanent and transversal initiative to stimulate scientific cooperation between chemists and biologists.

Data Uptade

- **To date, QCSIC contains 2184 compounds ready for testing.**
- **5 different biological screenings for the discovery of new antiviral and antibaterial hits are ongoing**

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Financiado por la Unión Europea NextGenerationEU
iQAC
Gobierno de España Ministerio de Ciencia e Innovación
PTI Salud Global CSIC Consejo Superior de Investigaciones Científicas
IQM
iiq Instituto de Investigaciones Químicas