

Research in the Christmann Group

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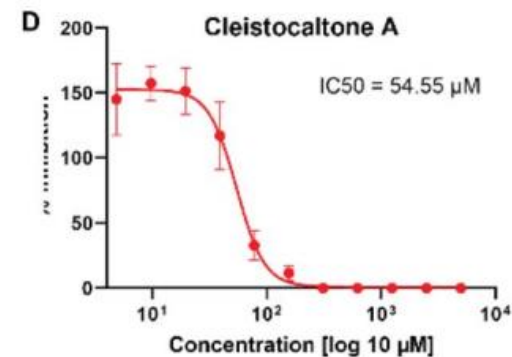
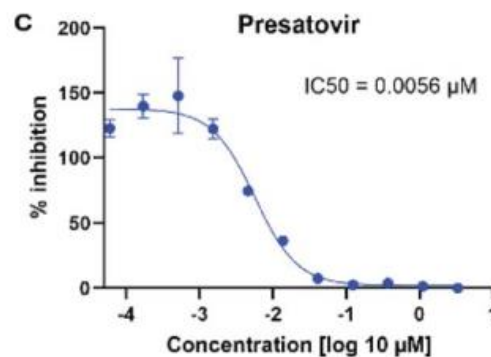
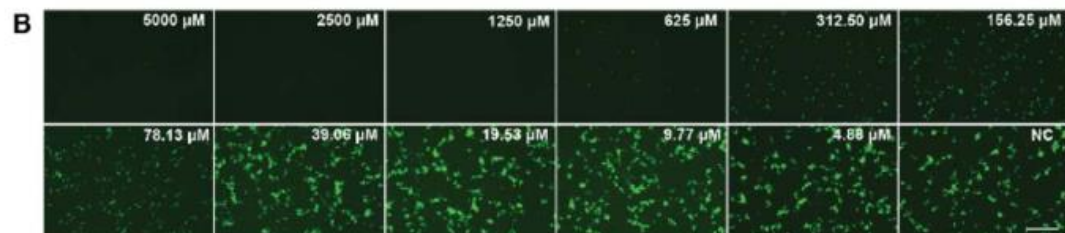
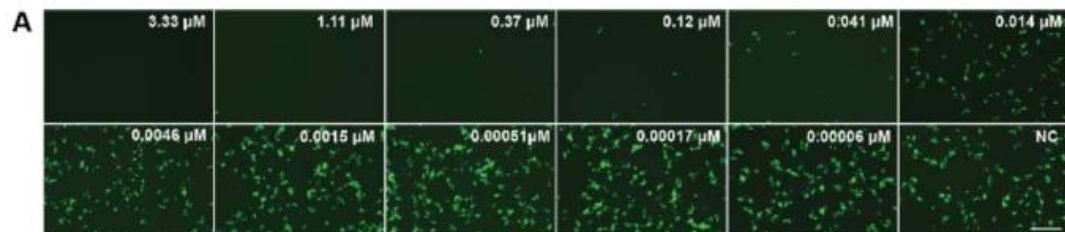
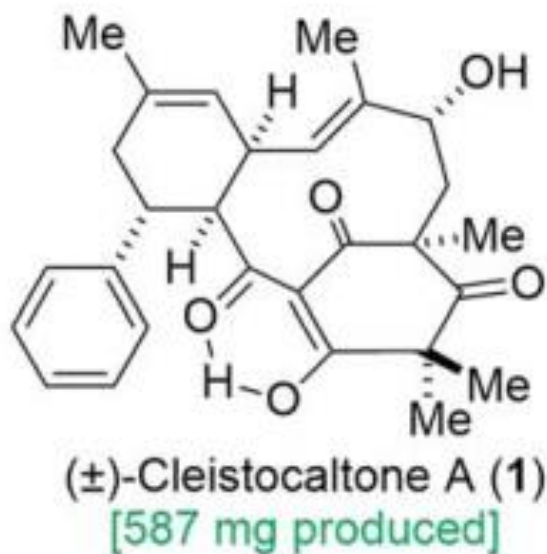
Introduction

Program Objectives

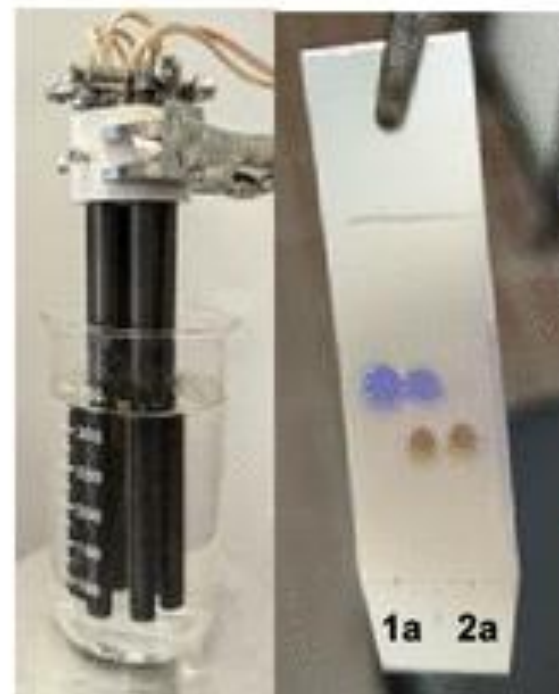
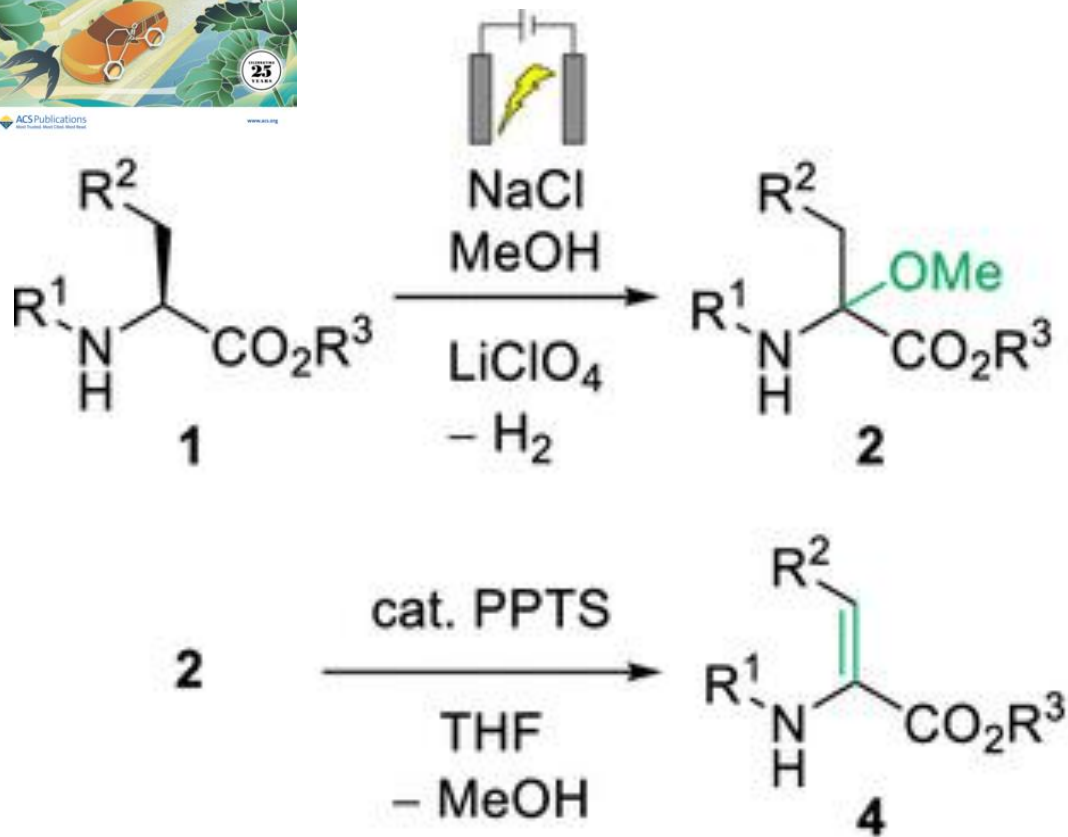
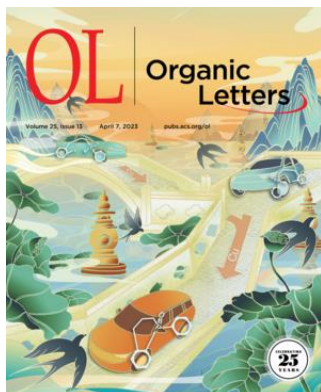
- modulation of biological processes
- development of synthetic methods and strategies
- training of students

General Approach

- highly selective natural products
- development of short, flexible and scalable syntheses
- address the chemical space beyond derivatizations
- tools for chemical biology

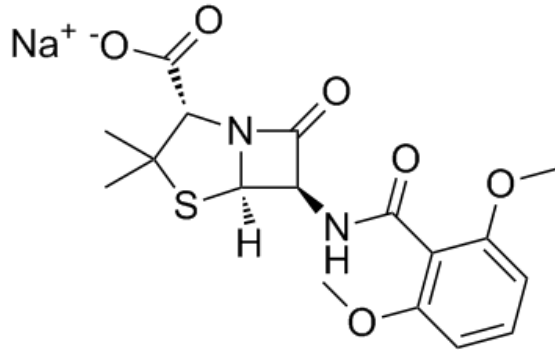


Chem. Sci., 2024,15, 10121-10125



Org. Lett. **2023**, *25*, 2228–2232

Bacteria can evolve resistance against any antibiotic



Methicillin



picture: Uwe Gille

MRSA is short for Methicillin-resistant Staphylococcus aureus

“A lot of people don’t get to the Antarctic, so there are a lot of things that have not been explored there,” said Renee Fleeman, who was the lead microbiology student at the University of South Florida (USF) on the project. “There’s a lot of diversity that has been undiscovered, and there’s a lot of things that we can find from the natural products in Antarctica.”



Photo: Jim McClintock



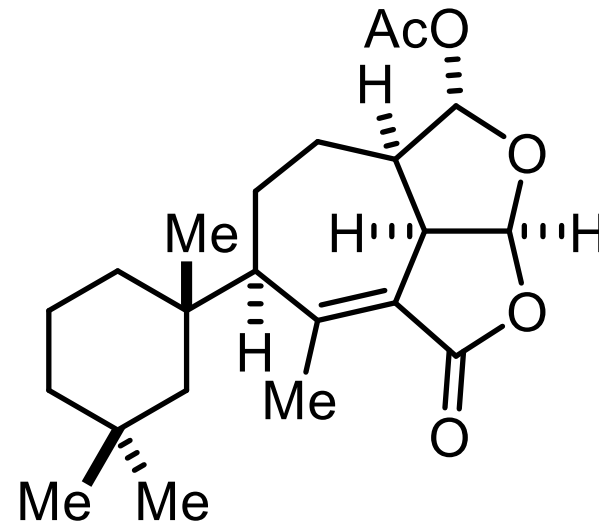
Photo: Joanna Hubbard

“Darwinolide fights off one of the hardest barriers in MRSA to fight, which is the biofilm,” said Jaqueline Fries, a postdoctoral research fellow at Simon Fraser University and lead author of the team’s recent paper. “It’s pretty selective towards that, which is important for any kind of antibiotic research.”

Darwinolide – a Biofilm-Selective Antibiotic against MRSA from the Antarctic Sponge *Dendrilla membranosa*



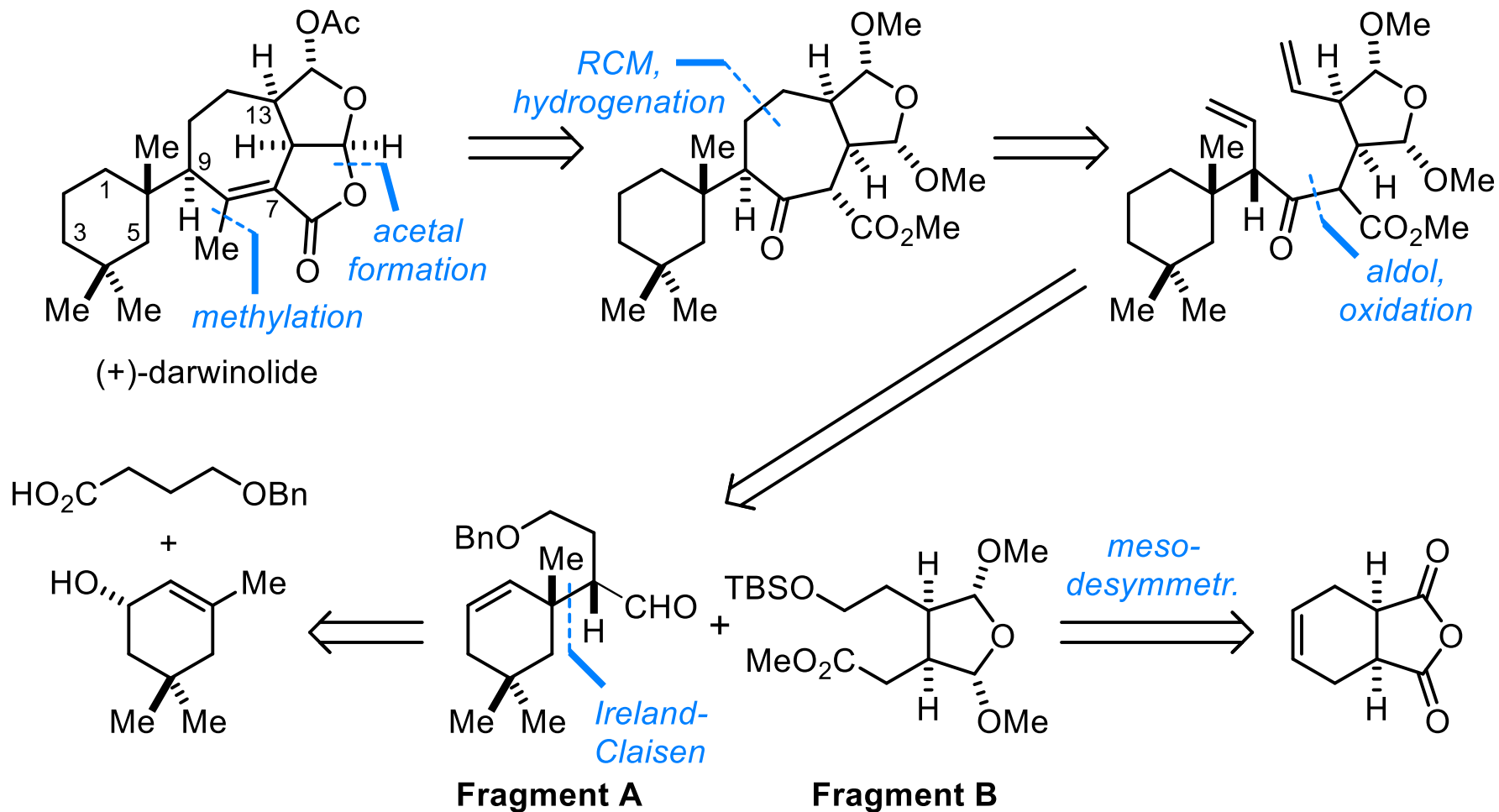
Foto: Bill Baker



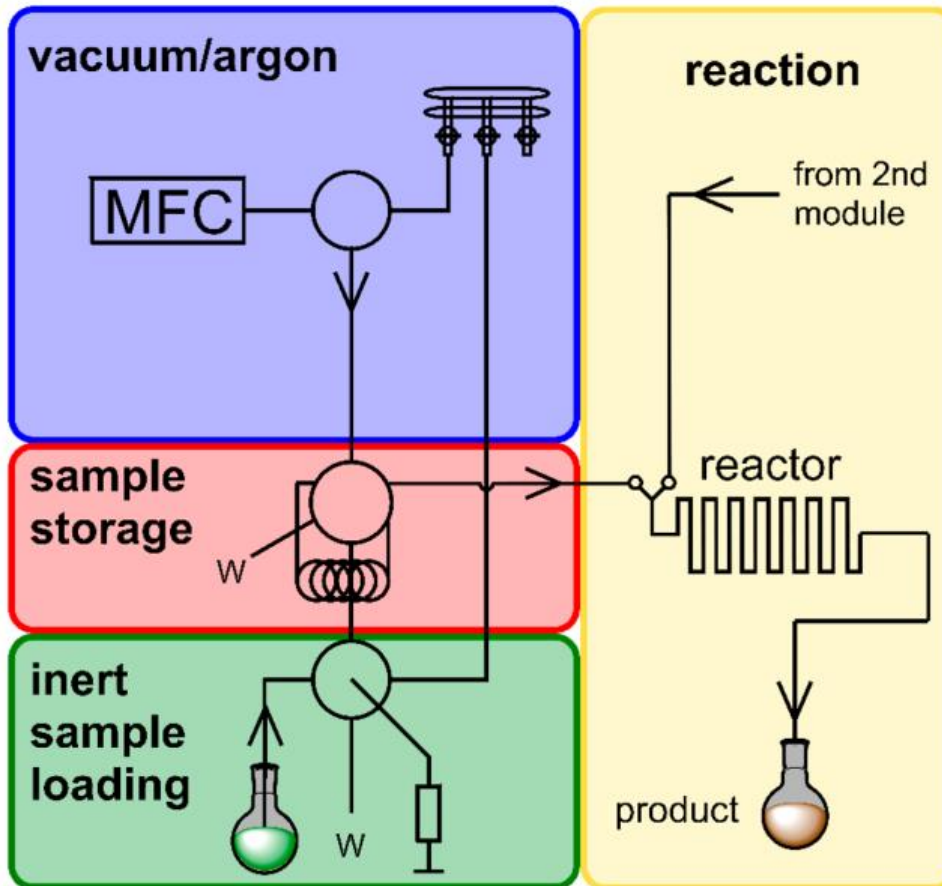
Darwinolide

- exhibits cytotoxicity against methicillin-resistant *Staphylococcus aureus* (MRSA) biofilms ($IC_{50} = 33.2 \mu M$)
- 4-fold selectivity towards MRSA biofilms over planktonic cell

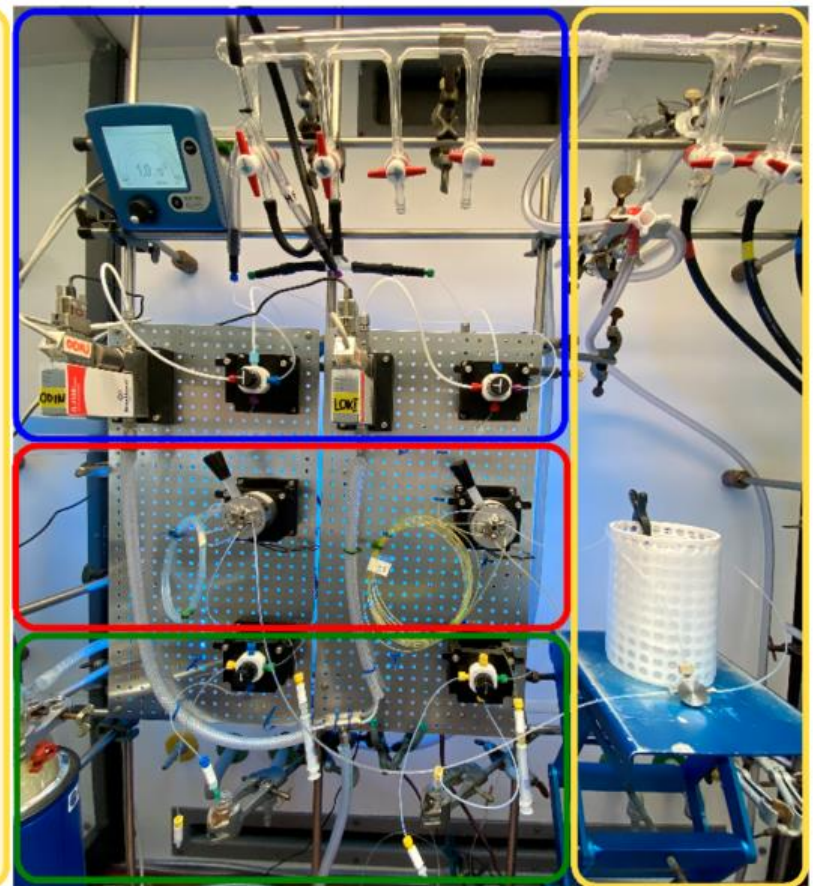
B. J. Baker et al. *Org. Lett.* **2016**, *18*, 2596.



A) concept sketch



B) prototype



How it started

Taking a 3-hours Python crash course with my son, an opportunity offered itself to validate anecdotal experience from reviewing against a much bigger data sample



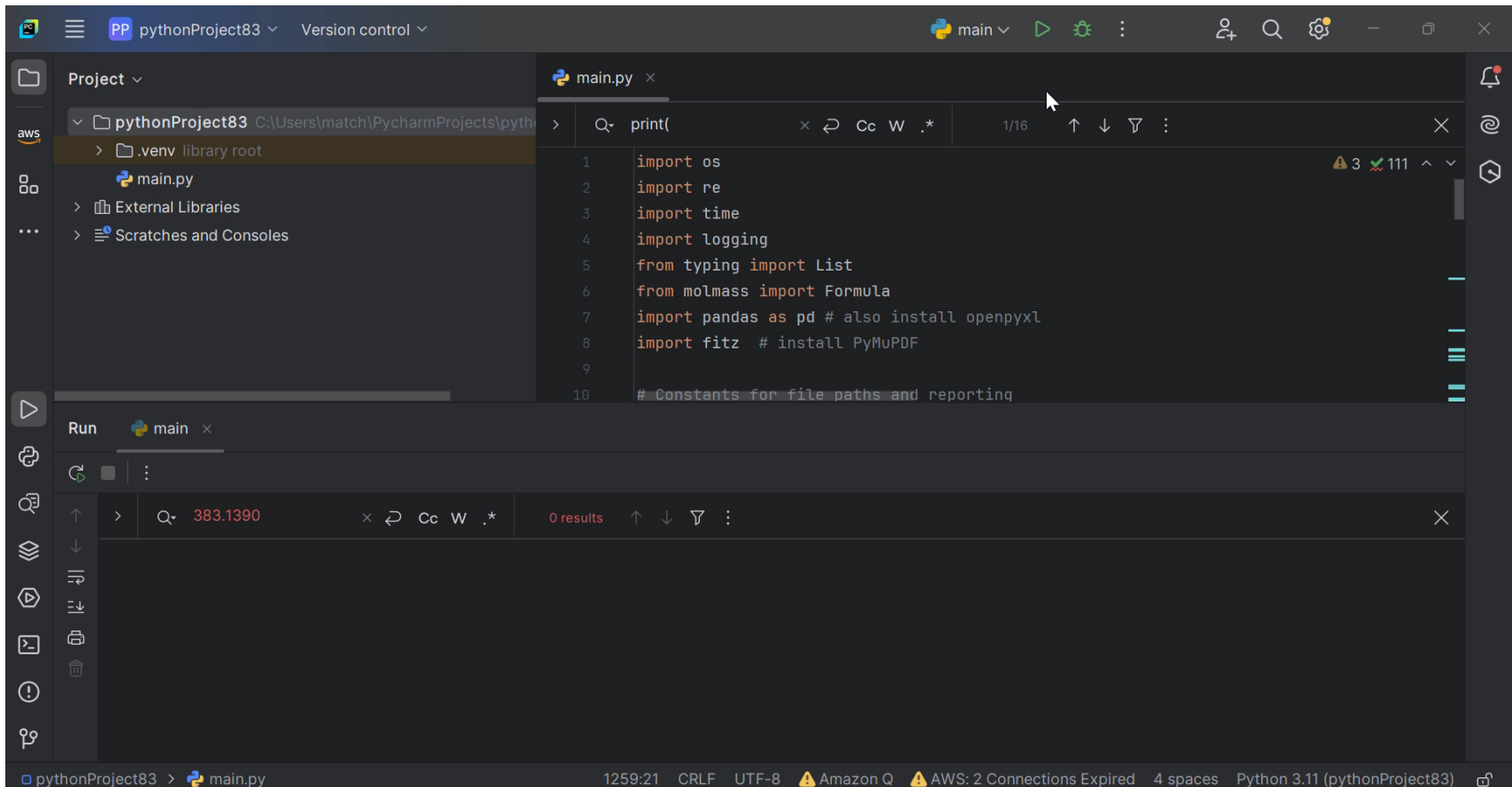
Python Tutorial Deutsch (Komplettkurs) - Python lernen in unter 4 Stunden



<https://www.youtube.com/watch?v=RBpK8C3N-Y8>

The Approach

Generate a Python script that reads SI PDFs from a folder into a string, extracts HRMS data, recalculates HR masses, and comments potential deviations



The screenshot shows the PyCharm IDE interface. The main editor window displays the following Python code in `main.py`:

```

1  import os
2  import re
3  import time
4  import logging
5  from typing import List
6  from molmass import Formula
7  import pandas as pd # also install openpyxl
8  import fitz # install PyMuPDF
9
10 # Constants for file paths and reporting

```

Below the editor, the Run console is visible, showing a search for `383.1390` with `0 results`. The status bar at the bottom indicates the project is `pythonProject83`, the file is `main.py`, and the Python version is `Python 3.11 (pythonProject83)`. There are also system notifications for `Amazon Q` and `AWS: 2 Connections Expired`.

