The Great ESKAPE: Reisolating Natural Products From Fungal Extracts

Megan Tran, Benjamin Smith, Bill Baker University of South Florida, Department of Chemistry

Figure 2. Bioassay of CQ10- 20A-4 Against ESKAPE Pathogens

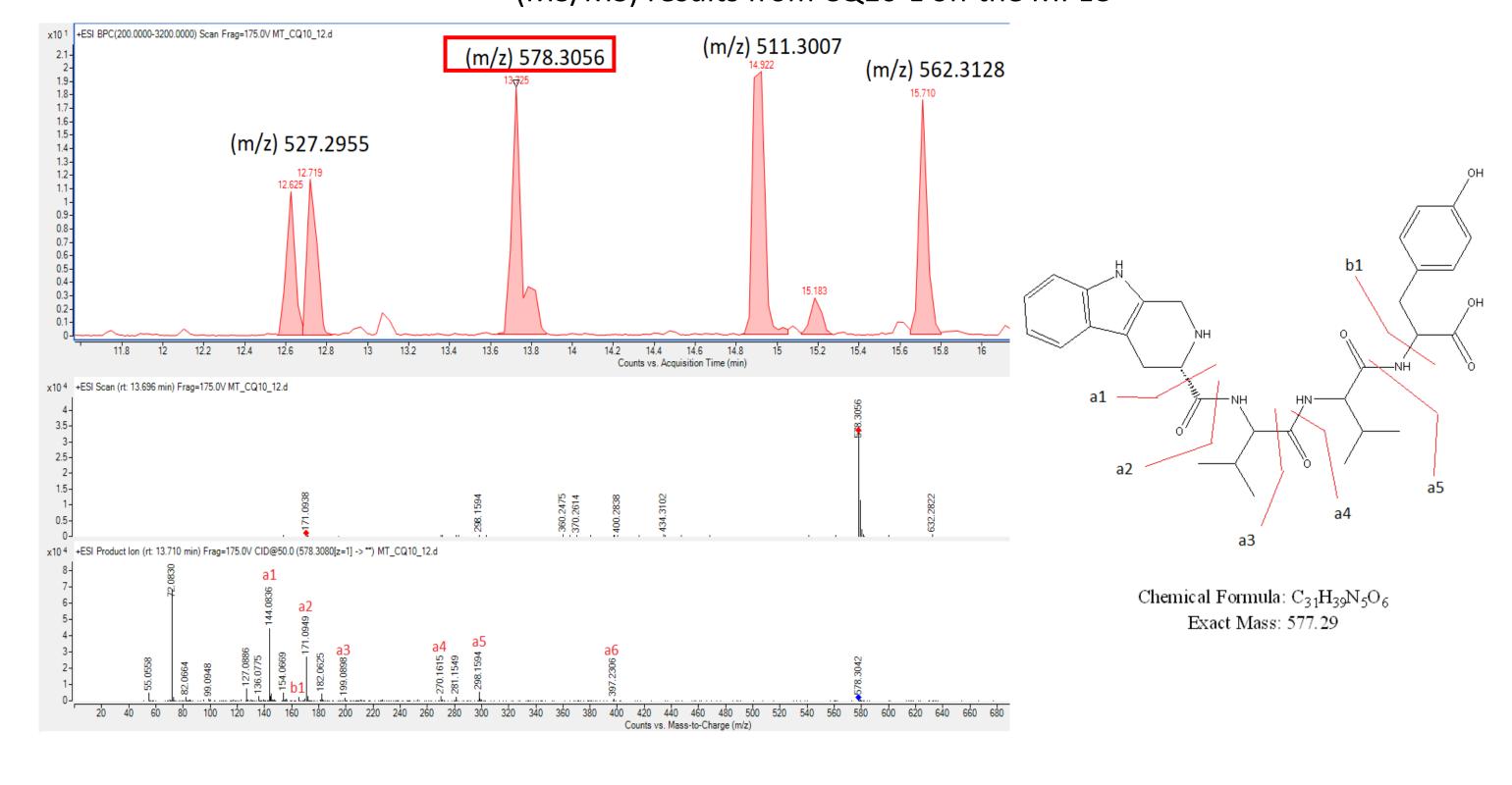
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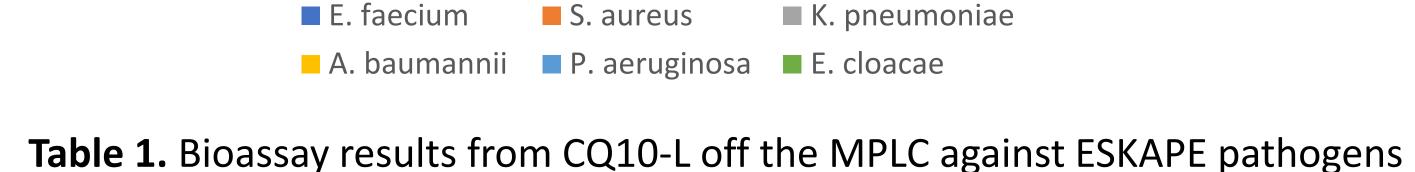
Introduction

- ESKAPE pathogens are a group of drug-resistant infection causing agents common in hospital settings, responsible for causing treatment resistant pneumonia, sepsis, and bloodstream infections.¹
- Natural products (NPs) are secondary metabolites produced by fungus during normal life functions that are not necessary for survival.²
- When submitted to Antimicrobial Bioassay (AMBA), samples of an epiphytic fungi (*unnamed*) collected from mangrove forests in Tampa, FL, had hits for ESKAPE and Naegleria (amoeba) pathogens.
- NPs from this fungi may potentially be used for the treatment of these pathogens, especially in antibiotic resistant cases³.

Results

Figure 3. Liquid Chromatography Mass Spectrometry (LCMS) and Tandem Mass Spectrometry (MS/MS) results from CQ10-L off the MPLC





CQ10-L

Methods

Figure 1. Research workflow **Partitioning** Extraction **Fungal Growth** 1st Partition: 1:1 Hexane:MeOH 🖿 2nd Partition 1:1 EtOAc:H2O 21 Days EtOAc layer of interest MPLC Bioassay Day 1: 1:3 MeOH:EtOAc Use loop tool to Day 2: 100% EtOAc inoculate fungi in CG10-20A-4 Day 3: 100% EtOAC bag of rice, tightly seal bag HPLC **Further** Against ESKAPE **Analysis** pathogens Collected 10 Metabolomics fractions; time-based

Purification of

desired NP

Structure elucidation

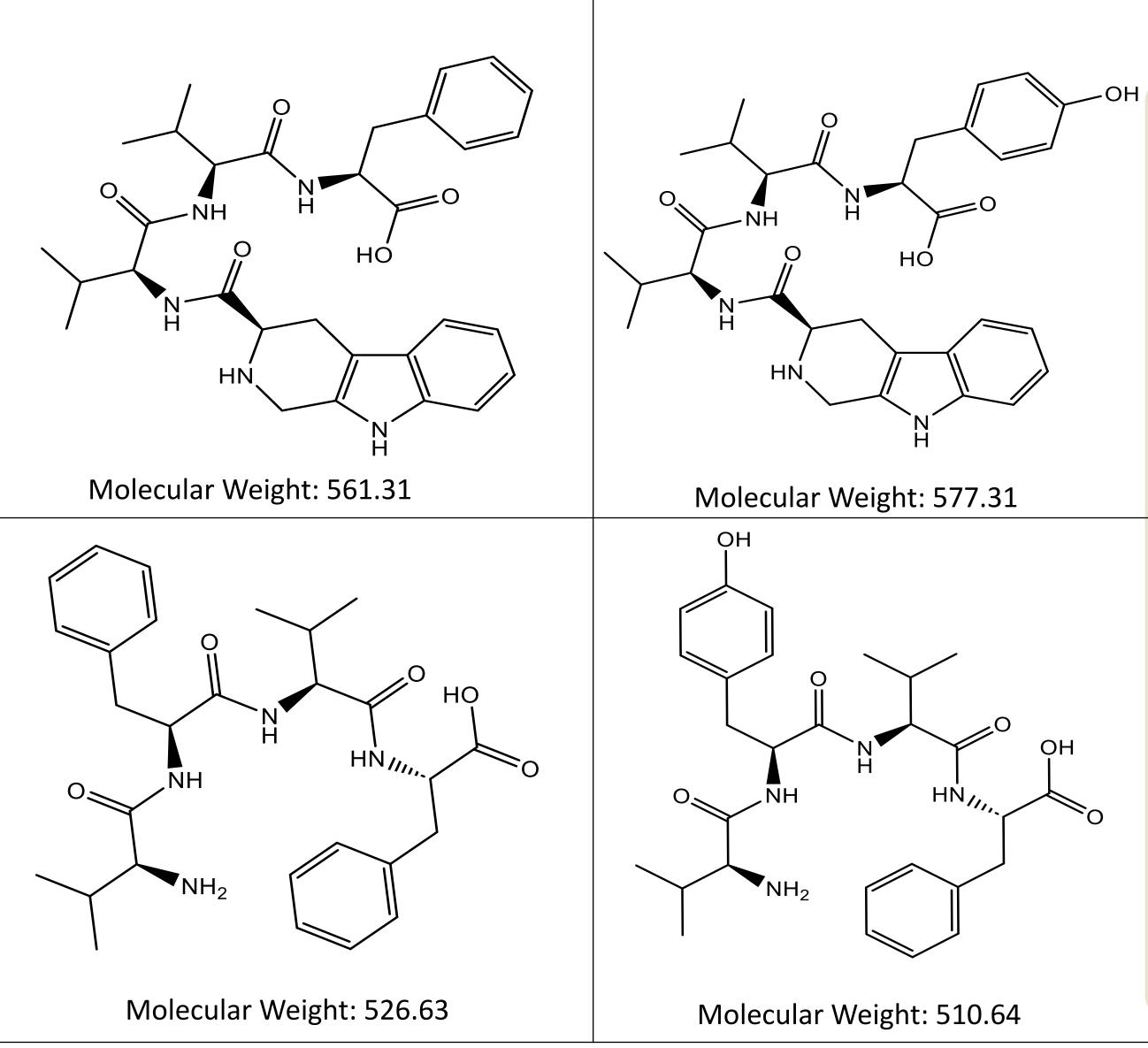


Figure 4. Nuclear Magnetic Resonance (NMR) results from CQ10-L subfraction 2

Discussion

Bioassay results (Table 1) show that this Fraction CQ10-L is active against the ESKAPE pathogen $E.\ faecium$. LCMS, MS/MS, (Figure 3) and NMR (Figure 4) analysis indicates the four NPs present in fraction CQ10-L present have the following masses: 510.30 \pm .10 amu, 526.29 \pm .01 amu, 577.31 \pm .01 amu, and 561.31 \pm .01 amu. The fragmentation masses shown in the collected MS/MS data matches with the structures made.

How these functional groups contribute to antimicrobial activity against ESKAPE pathogens, and *E. faecium* in particular is still unclear. However, Alpha-ergocryptinine with similar functional groups is also known to have antimicrobial effects⁴. This provides ample opportunity to explore structural and functional comparisons.

Future Works

- The NP present in CQ10-L requires advanced purification better isolate and identify the compound.
- Refer to Global Natural Product Social Molecular Networking database to verify identity compound.
- Compare functional groups with other existing NPs.
- Consider how identified functional groups interact with prokaryotic cell function.

Contact

¹H NMR, LCMS-QTOF,

HSQC → SMART NMR

Megan Tran megantran@usf.edu

References

Selve we well paper

Provides compounds'

structure info from each

fraction

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- 2. Capecchi, Alice, and Jean-Louis Reymond. "Classifying natural products from plants, fungi or bacteria using the COCONUT database and machine learning." Journal of cheminformatics 13.1 (2021): 1-11.
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