Prediction of secondary metabolite encoding genes based on chemical structure analysis

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Prediction of secondary metabolite encoding genes based on chemical structure analysis

Dereplication of the secondary metabolite profile from the filamentous fungus *Aspergillus brasiliensis*, by High Performance Liquid Chromatography coupled with Diode Array Detection and High Resolution Mass Spectrometry lead to the discovery of a novel biomarker having a unique UV spectrum and elemental composition. Structural elucidation based on Nuclear Magnetic Resonance spectroscopy of the pure compound revealed an apolar polyketide or fatty acid derived secondary metabolite, possibly assembled from two entities, a C8 and a C12 chain, fused via a Claisen-like condensation and subsequent cyclisation to form a core lactone ring structure. Despite the apolar nature of the compound initial bioassay investigation have demonstrated antibacterial activity against methicillin-resistant *Staphylococcus aureus* MB5393. The metabolite was also identified in strains of *A. carbonarius* and *A. tubingensis*, setting the scene for comparative bioinformatics analysis of the three genomes. Four candidate gene clusters have been selected for construction of knock out mutants using CRISPR/Cas9 in *A. brasiliensis*. This poster will summarize our efforts towards characterization of the biosynthetic pathway of this new compound that we have named brasenol.