DTU Library

Prediction of secondary metabolite encoding genes based on chemical structure analysis

Petersen, Thomas Isbrandt; Nielsen, Maria Lund; Hoeck, Casper; Frandsen, Rasmus John Normand; Larsen, Thomas Ostenfeld

[Link back to DTU Orbit](#)

POSTER SESSION ABSTRACTS
Session CS5 Applied genomics and biotechnology
CS5T73

Tuesday 5th April
14:00 - 16:00

ISBRANDT Thomas *(1), LUND NIELSEN Maria (1), HOECK Casper (3), J. N. FRANDSEN Rasmus (2), O. LARSEN Thomas (1)*
(1) Natural Product Discovery, Department of Systems Biology, Technical University of Denmark, Søltofts Plads, Lyngby, Denmark
(2) Eucaryotic Molecular Cell Biology, Department of Systems Biology, Technical University of Denmark, Lyngby, Denmark (3) Department of Chemistry, Technical University of Denmark, Kemitorvet, Lyngby, Denmark

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.