MS Dereplication for Rapid Discovery of Structurally New or Novel Natural Products

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In order to accelerate the isolation and characterisation of structurally new or novel natural products, it is crucial to develop e_cient strategies that prioritise samples with greatest promise early in the workflow so that resources can be utilised in a more e_cient and cost-e_ective manner. Two complementary approaches have been developed: One is based on targeted identification of known compounds held in a database based on high resolution MS and predicted LC retention time data [1]. The second is an MS metrics-based approach where the software algorithm calculates metrics for sample novelty, complexity, and diversity after interrogating databases of known compounds, and contaminants. These metrics are then used to prioritise samples for isolation and structure elucidation work [2]. Both dereplication approaches have been validated using natural product extracts resulting in the isolation and characterization of new or novel natural products.

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References

1. Chervin, J.; Stierhof, M.; Tong, M.H.; Peace, D.; Hansen, K.Ø.; Urgast, D.S.; Andersen, J.H.; Yu, Y.; Ebel, R.; Kyeremeh, K.; et al. Targeted Dereplication of Microbial Natural Products by High-Resolution MS and Predicted LC Retention Time. J. Nat. Prod. **2017**, 80, 1370–1377, doi:10.1021/acs.jnatprod.6b01035.
2. Tabudravu, J.N.; Pellissier, L.; Smith, A.J.; Subko, K.; Autréau, C.; Feussner, K.; Hardy, D.; Butler, D.; Kidd, R.; Milton, E.J.; et al. LC-HRMS-Database Screening Metrics for Rapid Prioritization of Samples to Accelerate the Discovery of Structurally New Natural Products. J. Nat. Prod. **2019**, 82, 211–220, doi:10.1021/acs.jnatprod.8b00575.