Non-targeted analysis, interactive visualization, and online sharing of interactive LC-HRMS/MS data of polymers using a comprehensive software PolyMatch Suite

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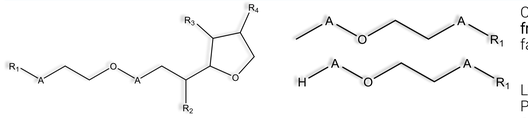
Introduction

Polymers and chemicals that form oligomeric series are essential in every day products including plastics, excipients, emulsifiers, lubricants, and detergents. They are also often found as a contaminant or mass spectral interference that needs to be identified before it can be removed. In this poster, we describe the application of PolyMatch, an open-source polymer discovery software used to identify components in Polysorbate 80.

The PolyMatch Database Covers over 775,000 Structures with Associated Fragmentation Rules



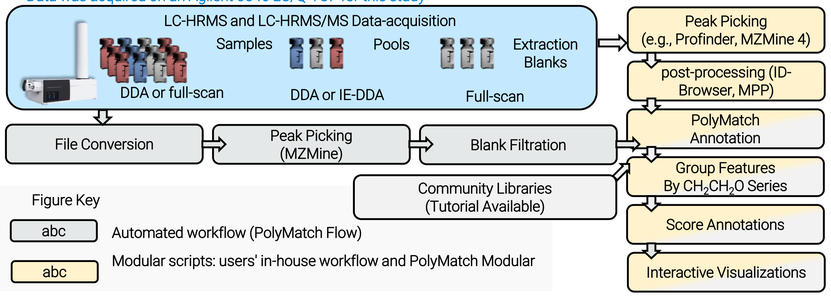
Class based libraries with fragmentation rules were generated for over **775,000+ species from 14 different components (polysorbate, polysorbide, and PEG)** including with/without fatty acid esters. Libraries have SMILES, Formula, Chemical Names, and Fragmentation:

$[C_3H_5O]^+$ $[C_4H_9O_2]^+$ $[C_6H_{13}O_3]^+$ $[C_8H_{17}O_4]^+$; $[FA+C_2H_3]^+$ and Adducts $[M+NH_4]^+$

Libraries were also generated for data that just contain MS/MS fragments corresponding to PEG fragments, forming over 64,450 PEG species. Below is an example of the naming conventions and identifications in PolySorbate 80.

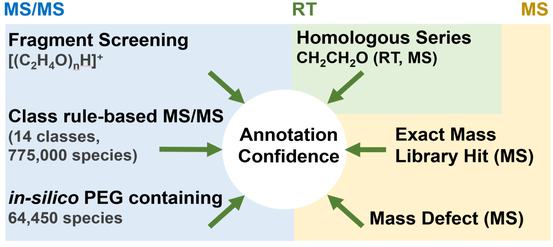
PolyMatch Covers the Entire Data-Processing Workflow, and Supports Various Acquisition Modes

Data was acquired on an Agilent 6546 LC/Q-TOF for this study



PolyMatch Flow and PolyMatch Modular (acquisition and data-processing workflow)

The PolyMatch software data analysis workflow starts by importing data collected using MS, DDA, or DIA data (with IonDecon), pooled and blank samples. PolyMatch algorithms cover file conversion, blank filtering, feature annotation, and visualization via PolyVI (visualization software). You can also generate your own libraries using the PolyMatch Generator from your own series of compounds. The software is extremely user friendly: just drag and drop vendor files onto the UI.



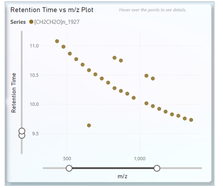
Annotation Evidence Compiled by PolyMatch

PolyMatch integrates a wide range of evidence to classify polymers: mass defect, retention time, and exact mass can be used alongside homologous series evidence to compile groups of chemicals that likely belong to the same class. MS/MS evidence can give structural information pertaining to class or species level assignments. Evidence used for annotation is shown bottom left and a homologous series retention time vs *m/z* is shown for Polysorbate-PEG bottom right.

Visualization Interface: All Mass Spectral Evidence Shown Simultaneously, Cross-Filtered, and Able to be Shared via Web Link

Filters (Left)

Various filters exist to home in on series, classes, and features of interest

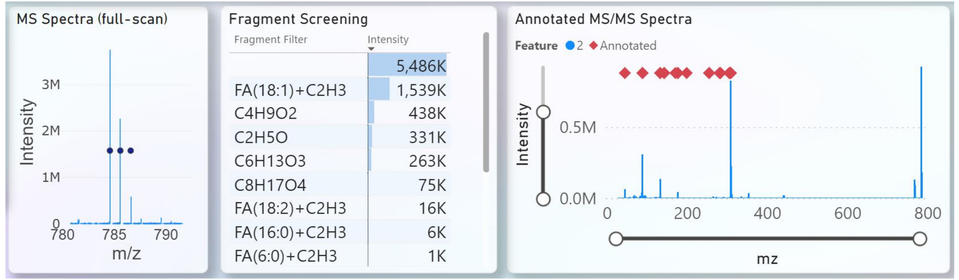


PolyMatch Visualizer: Visualizations show all the MS Evidence

A graphical interface (left) allows users to validate annotations and can be used to explore features using mass defect plots normalized to repeating units, retention time vs mass plots, annotated MS/MS spectra, annotated MS1 and EICs, fragment trace filters and numerous other filters, and tables providing all annotation evidence. All plots cross-filter and are dynamic, allowing users to see all evidence for a feature(s) simultaneously. Furthermore, interactive results can be shared via weblink without any software needed by the recipients.

Left: Visualizer Panes from PEG-8 to PEG-9 with all associated information; retention time and m/z plots are helpful for removing false positives.

Top Left: Automatically assigned series for Polysorbates
Top Right: Assigned series for Fatty Acid 18:1 containing PEGs



Above: **Automatically correctly assigned structure for PEG-11 FA 18:1 using PolyMatch fragmentation rules**

Conclusions

PolyMatch can be used to rapidly annotate polymers and oligomers in an automatic fashion, determine unknowns and expand annotation using an interactive visualizer

- Incorporates MS/MS, MS, EICs, homologous series, and retention time
- Has over 150,000 species with fragmentation in libraries; fragment screening and substructure assignment for unknowns
- Many previously unidentified species exist in datasets which can be discovered using the visual interface
- < 5% False Positive Rate

To install the software please visit: Innovativeomics.com/software
Questions? Trainings? Collaboration? Contact: jeremykoelmel@gmail.com

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