Supplementary Information:

Multi-Modal Structure Characterization of Synthetic Batch Impurities with Liquid Chromatography Coupled to Infrared Ion Spectroscopy

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Content:

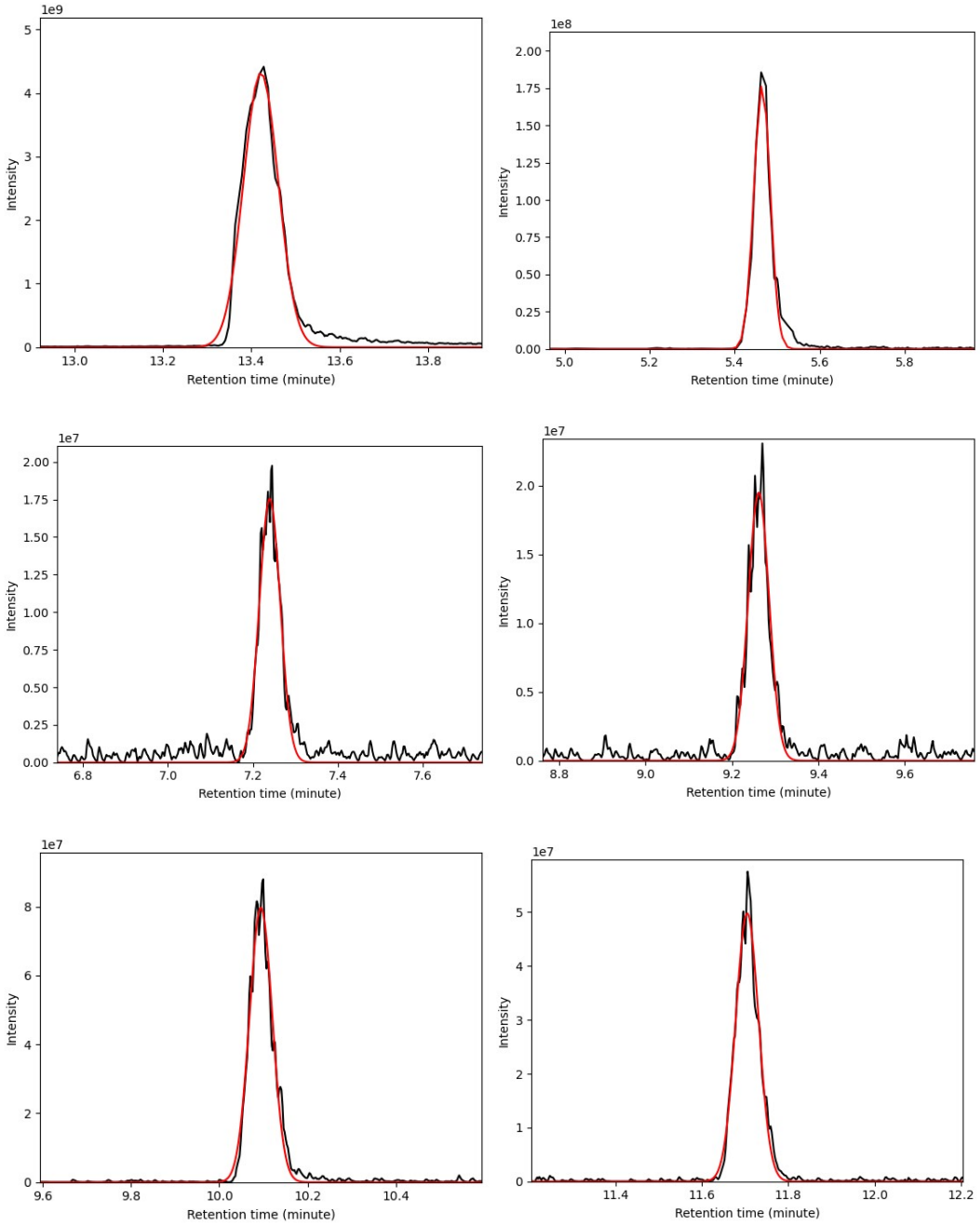
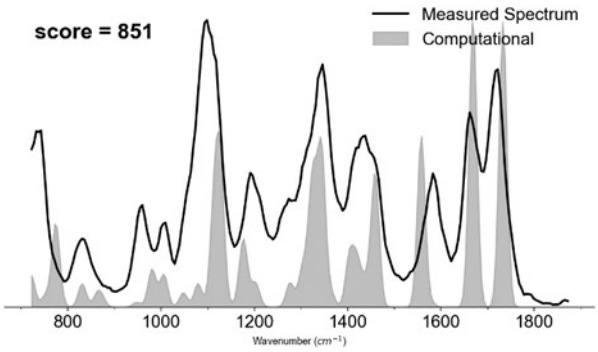
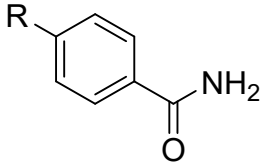


Figure S1. Extracted ion chromatograms of the protonated ions of main product and impurities **1- 5** (black traces, from left to right and top to bottom). Red traces are fitted Gaussians used for integration.

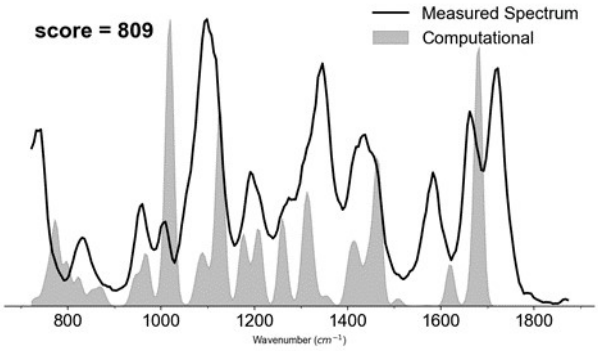
Table S1. Similarity scores for the comparison of the IRIS spectra of the impurities with the reference materials. For impurity **1**, **2** and **3**, the highest score is found to the corresponding reference standard, indicated in green.

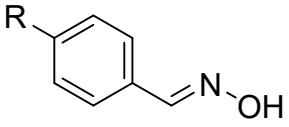
	reference 1	reference 3	active ingredient
impurity **1**	**985**	889	822
impurity **2**	906	925	836
impurity **3**	887	**985**	912
impurity **4**: reconverted to m/z 360	859	937	**974**
impurity **4**	877	930	921
impurity **5**	902	952	913





Assigned structure impurity





Alternative aldoxime

Figure S2. Comparison of the measured IRIS spectrum of impurity **2** with different candidates. We assign the impurity structure as the top candidate.

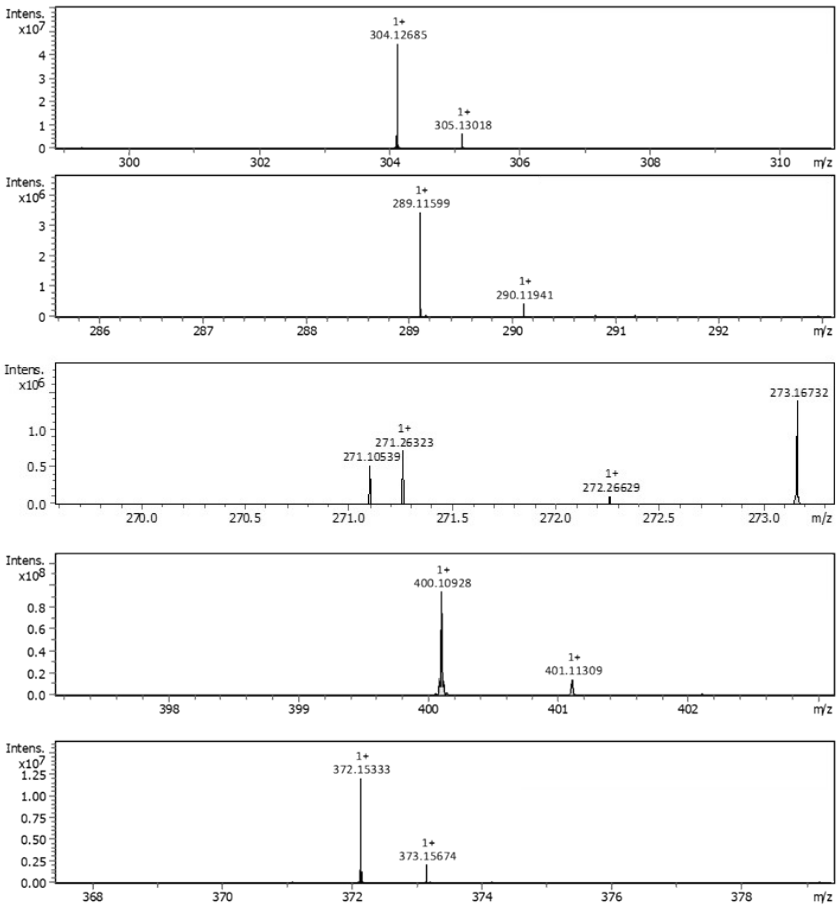
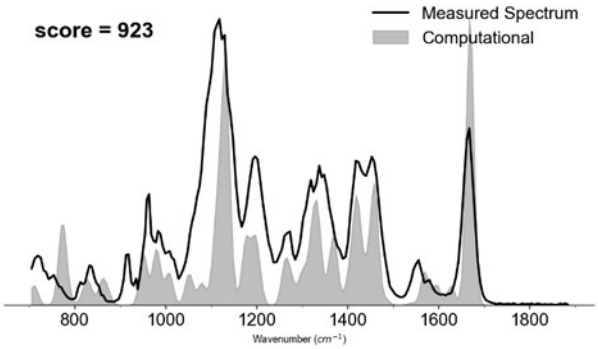
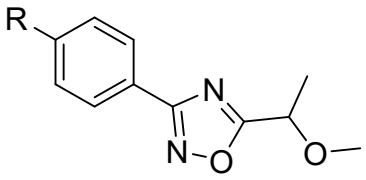
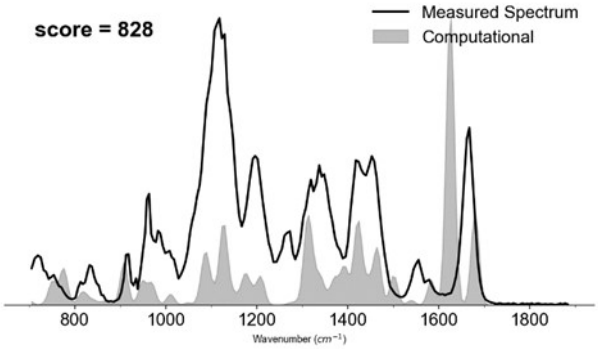


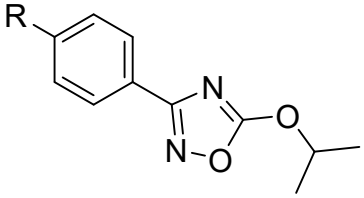
Figure S3. High resolution mass spectra of the sodium adducts of Impurity **1-5** (from top to bottom). The observed masses deviate from the theoretical accurate masses by 0.24, 0.39, 0.28, 0.51, and 0.91 ppm, respectively.





Assigned structure impurity





Alternative isopropanoxy candidate

Figure S4. Comparison of the measured IRIS spectrum of impurity **5** with different candidates. We assign the impurity structure as the top candidate.

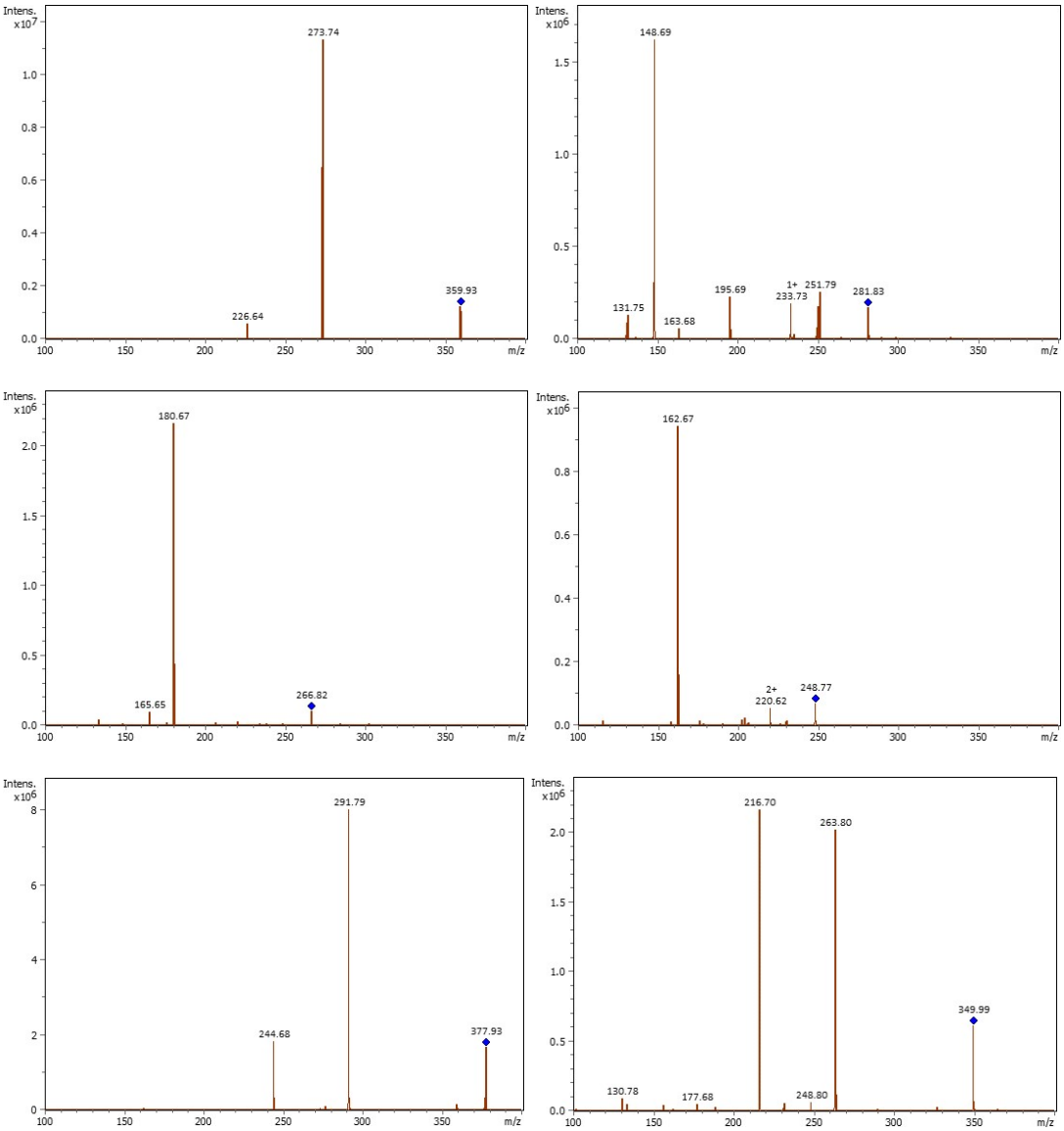


Figure S5. CID MS/MS spectra of the protonated ions of main product and impurities **1-5** (from left to right and top to bottom).