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Title: Calculation of Retention Time Tolerance Windows with Absolute Confidence from Shared Liquid Chromatographic Retention Data

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1 **Calculation of Retention Time Tolerance Windows with Absolute**
2 **Confidence from Shared Liquid Chromatographic Retention Data**

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21
22 **Abstract**

23 Compound identification by liquid chromatography-mass spectrometry (LC-MS) is a tedious
24 process, mainly because authentic standards must be run on a user's system to be able to
25 confidently reject a potential identity from its retention time and mass spectral properties.
26 Instead, it would be preferable to use *shared* retention time/index data to narrow down the
27 identity, but shared data cannot be used to reject candidates with an absolute level of confidence
28 because the data are strongly affected by differences between HPLC systems and experimental
29 conditions. However, a technique called "retention projection" was recently shown to account for
30 many of the differences. In this manuscript, we discuss an approach to calculate appropriate

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