Metabolomics annotation and metabolite reporting

- Annotation process
- Computational annotation
- Reporting standard

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Challenges, progress and promises of metabolite annotation for LC–MS-based metabolomics

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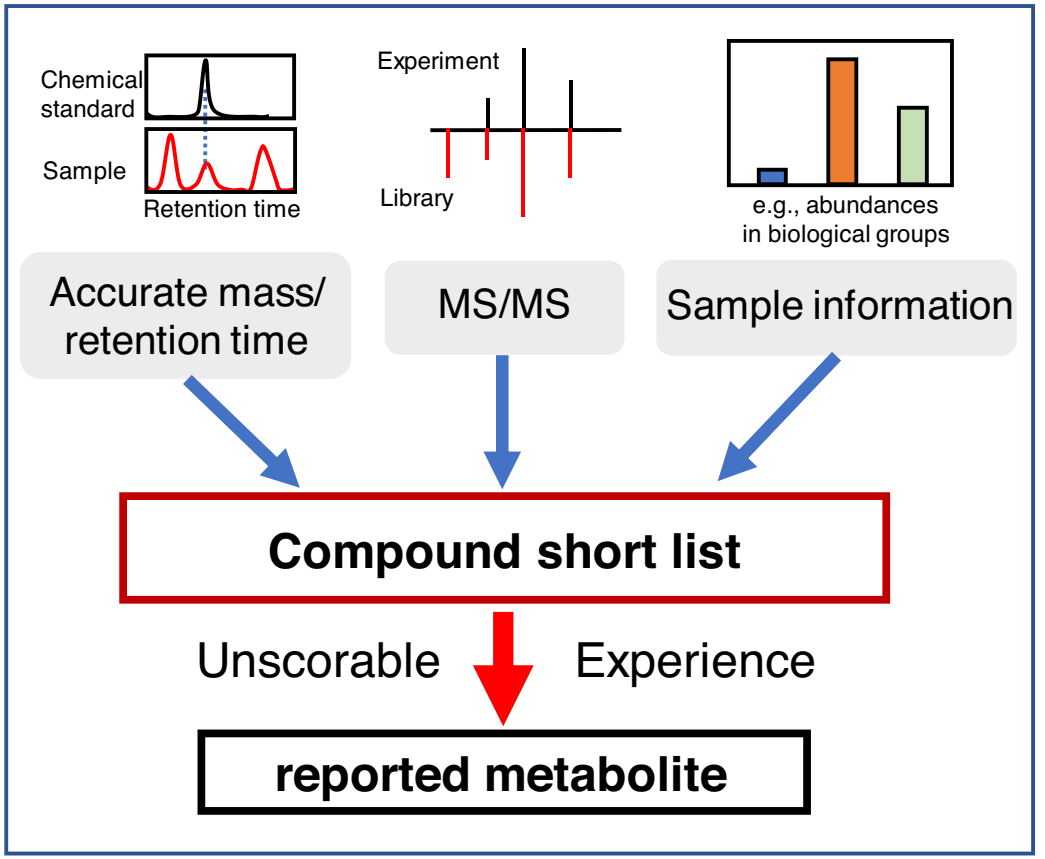
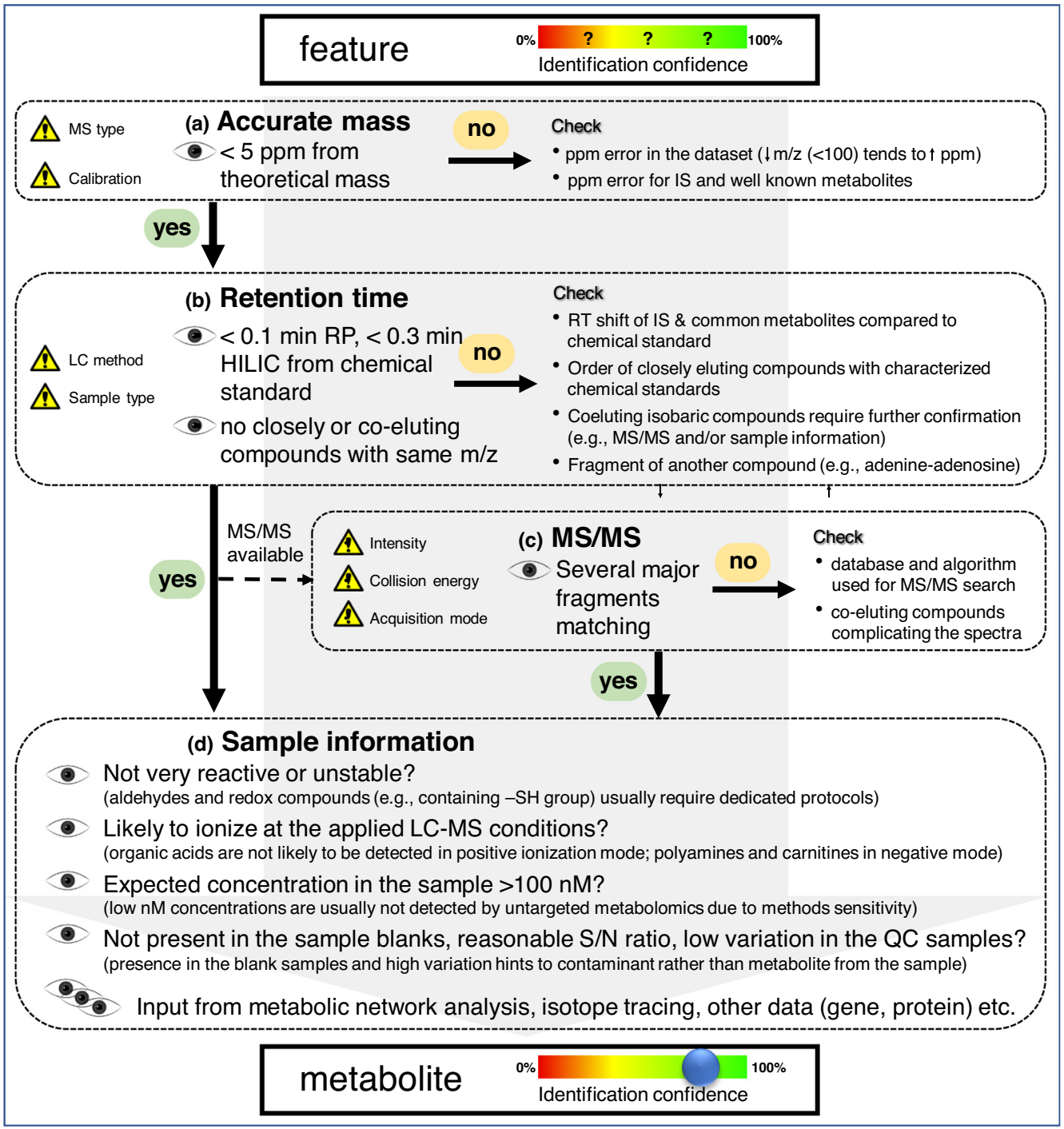


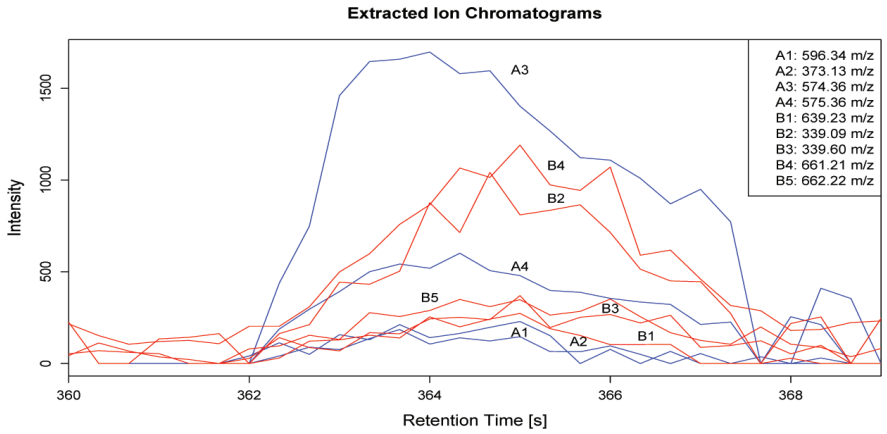


Chaleckis et al 2019

Computational annotation

id	m/z	rt [s]
1	339.09	369.1
2	339.59	369.1
3	373.13	368.6
4	574.36	368.7
5	575.36	368.7
6	596.34	368.4
7	639.23	368.7
8	661.21	369.1
9	662.22	369.1

Initial compound spectrum



	1	2	3	4	5	6	7	8
2	1.0							
3	0.34	0.36						
4	0.72	0.67	0.90					
5	0.68	0.47	0.68	1				
6	0.38	0.38	0.87	0.86	0.75			
7	0.76	0.72	0.73	0.82	0.88	0.70		
8	0.94	0.79	0.35	0.70	0.67	0.51	0.79	
9	0.88	0.84	0.46	0.62	0.70	0.62	0.81	1.0

Relationship scoring table

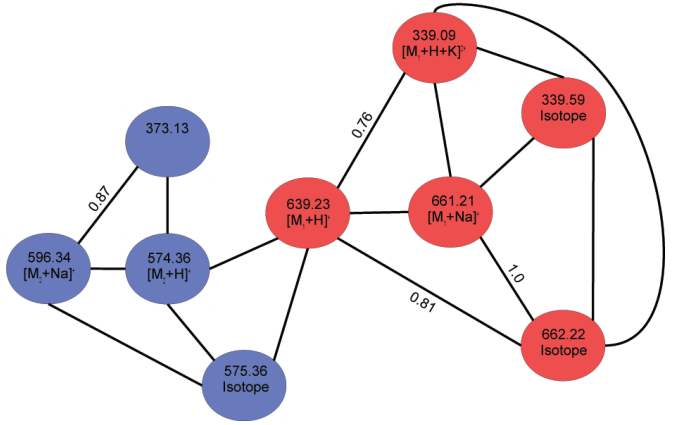
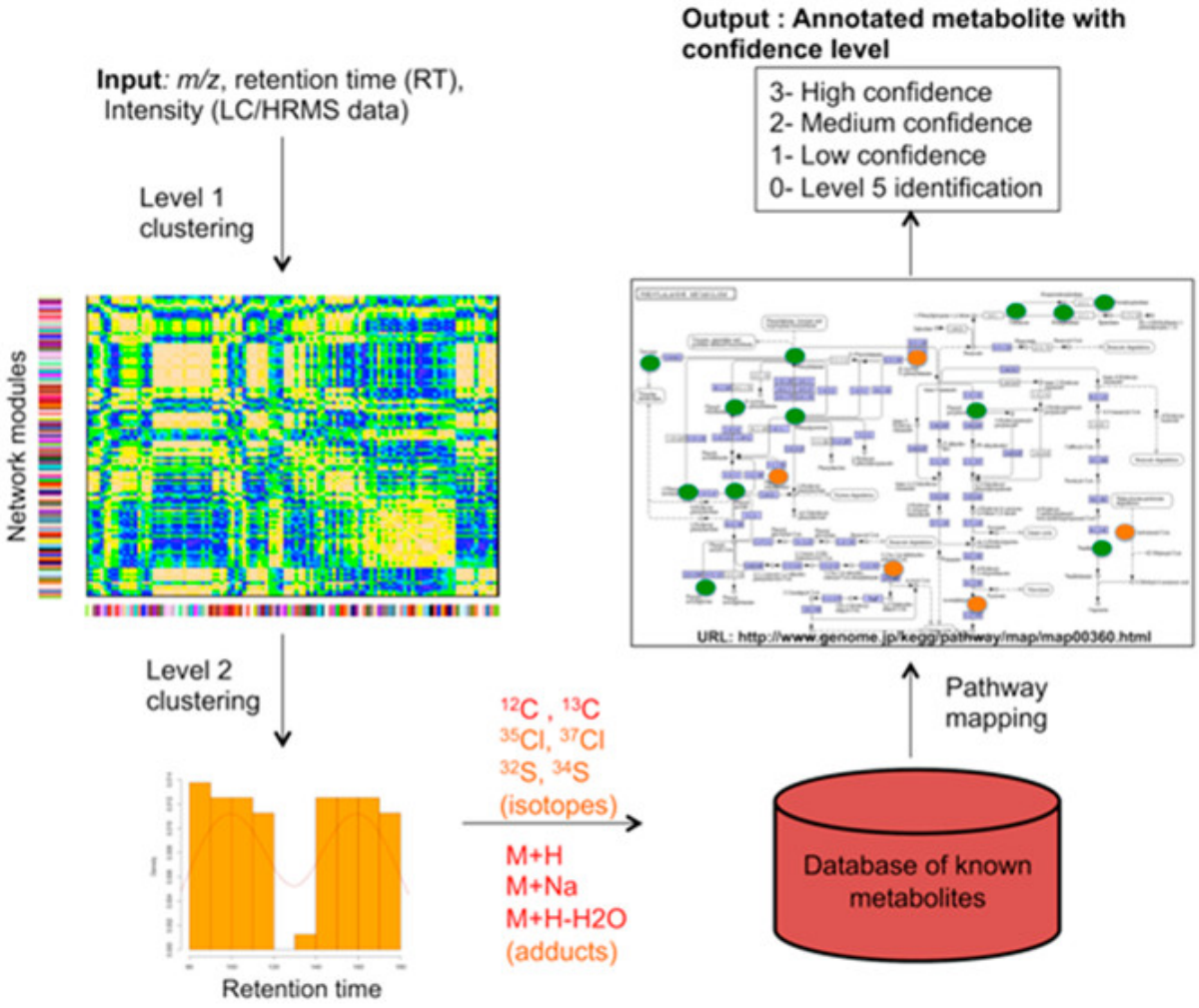


Figure 2. Schematic clustering of low-intensity features initially grouped by retention time into a single compound spectrum. Top left: the features, initially grouped by retention time. Top right: the EICs of all features. The labels A and B correspond to the result after graph clustering. Bottom left: the scoring matrix, used as edge weights in the graph. Bottom right: the relationship graph, where edges indicate an above-threshold score. The node labels include the ion species annotation, and the node color shows the graph separation after refinement with the LPC algorithm (A = blue, B = red).

CAMERA, Kuhl et al. 2012

Computational annotation



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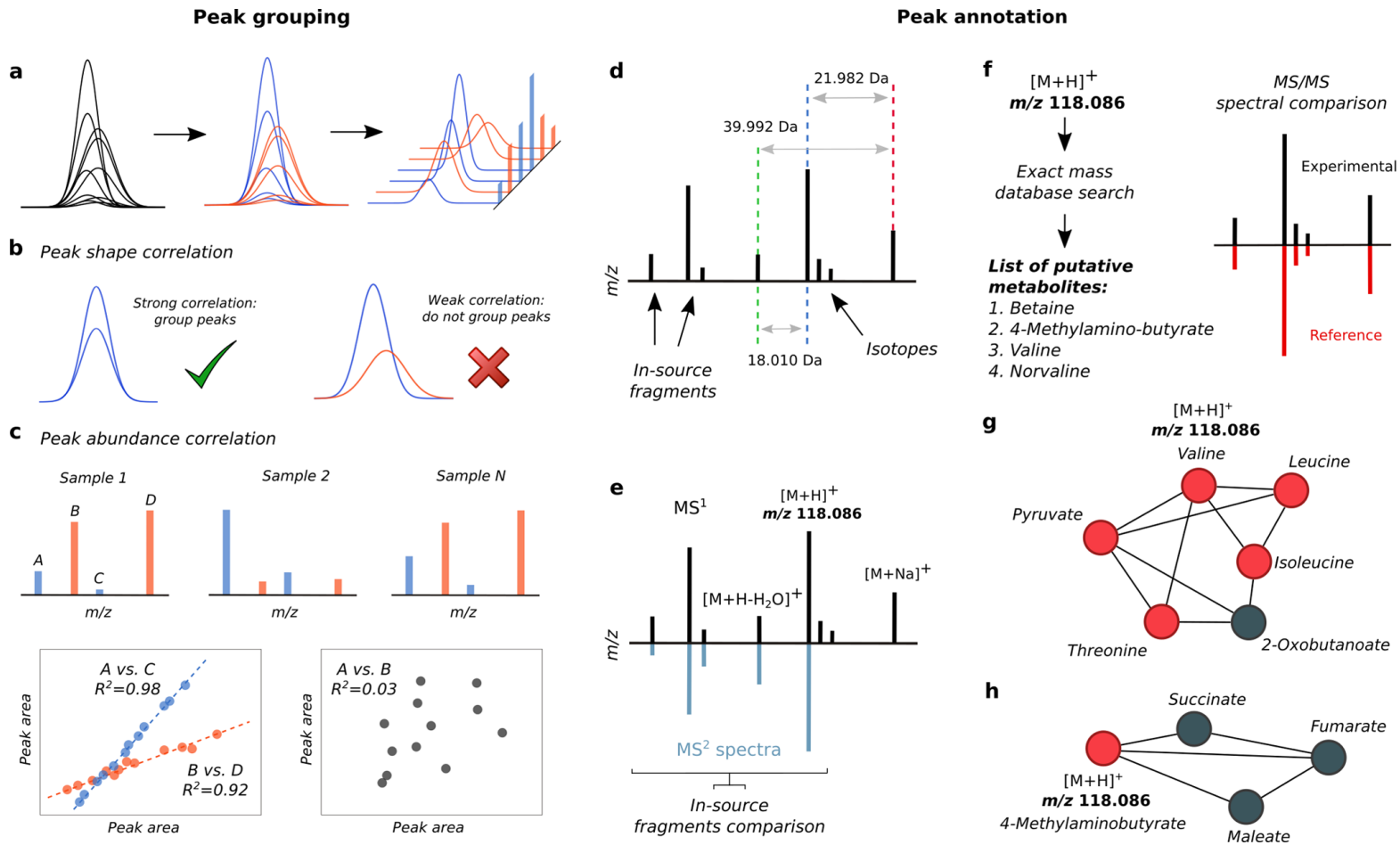
DOI: 10.1021/acs.analchem.6b01214

Computational annotation



Domingo-Almenara et al. 2018

Sumner et al 2007

1.Identified compounds. A minimum of two independent and orthogonal data relative to an authentic compound analyzed under identical experimental conditions are proposed as necessary to validate non-novel metabolite identifications

2.Putatively annotated compounds (e.g. without chemical reference standards, based upon physicochemical properties and/or spectral similarity with public/commercial spectral libraries).

3.Putatively characterized compound classes (e.g. based upon characteristic physicochemical properties of a chemical class of compounds, or by spectral similarity to known compounds of a chemical class).

4.Unknown compounds—although unidentified or unclassified these metabolites can still be differentiated and quantified based upon spectral data.

Sumner, L.W., Amberg, A., Barrett, D., Beale, M.H., Beger, R., Daykin, C.A.: Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI). Metabolomics **3**, 211–221 (2007)

Schymanski et al 2014

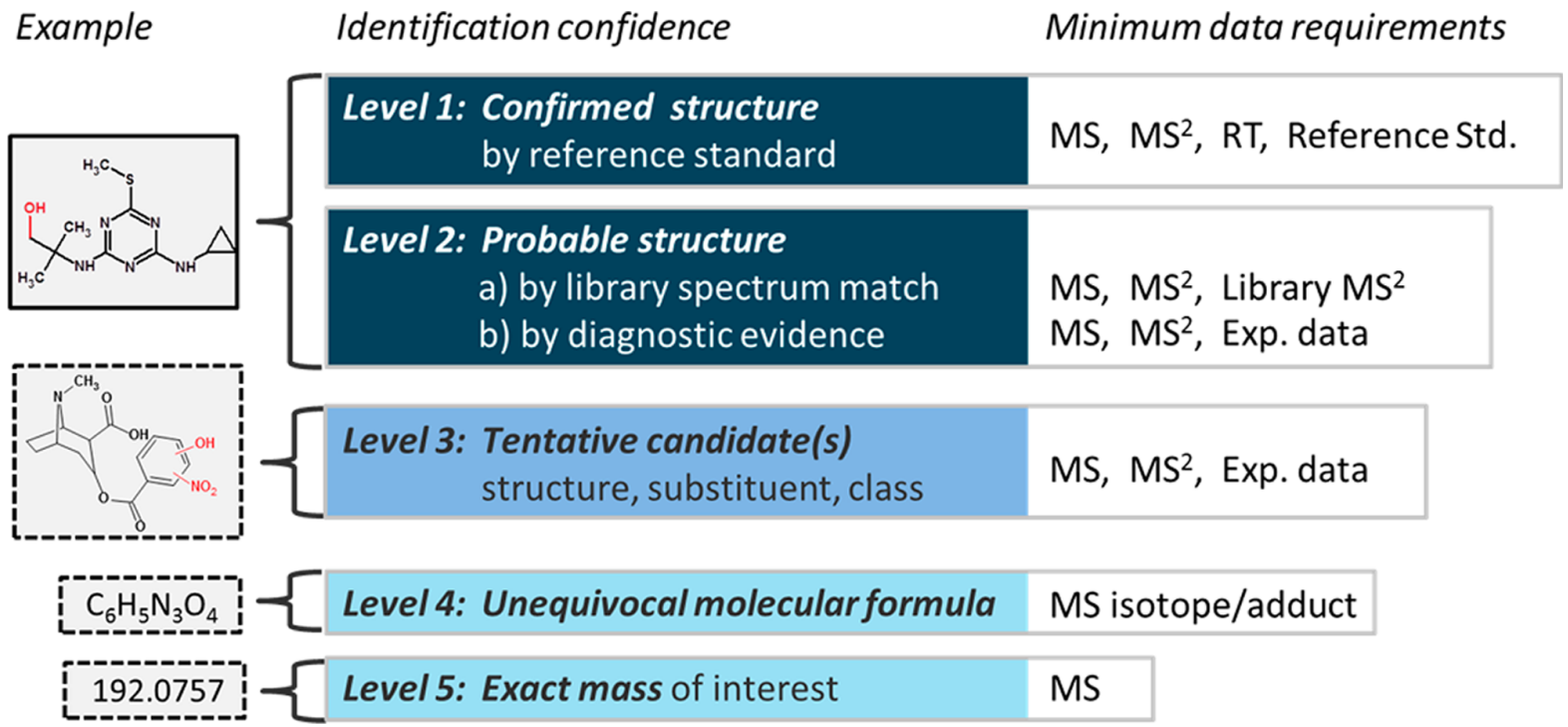


Figure 1. Proposed identification confidence levels in high resolution mass spectrometric analysis. Note: MS^2 is intended to also represent any form of MS fragmentation (e.g., MS^e, MS^n).

Schrimpe-Rutledge et al, 2016