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Unlocking the potential of High Throughput Purification with Advanced Automated Impurity Analysis

William Farrell

Senior Scientist, Virscidian LLC,

Dotmatics, A Siemens Company

Co-Authors:
Mark Bayliss, Joseph Simpkins, Stephane Murphy, Julie Wight, Mark Spears, Don Nguyen, Alyssa Cetin, Daniel Simpkins, David Snyderman

About Virscidian

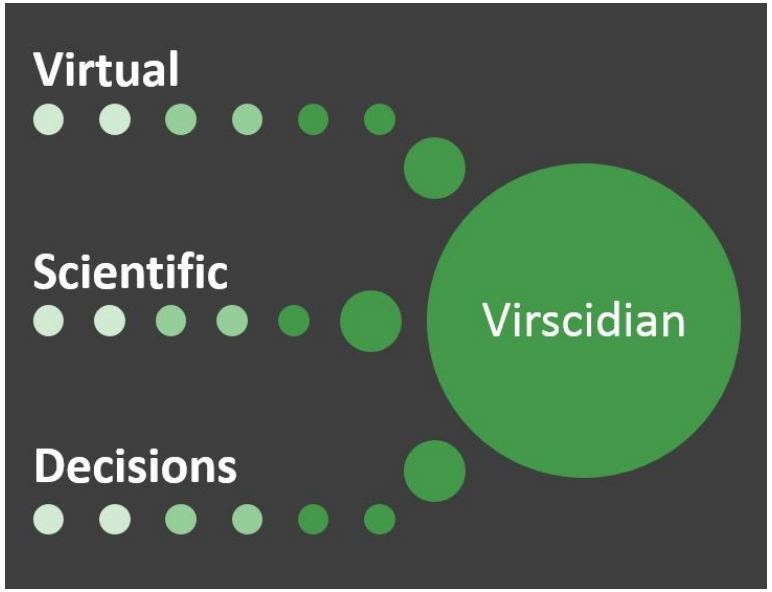
We are a software company that is on a mission to deliver:

Drug Discovery Software-enabled Synthesis to Registration & HTS Screening Workflows

End-to-end analytical software solutions that mimic and extend your natural laboratory workflows

Desktop and enterprise products developed for high to low sample throughput workflows

Best in class workflow driven LC/MS Automated data processing, results creation, review-by-exception



Acquired in Aug. 2024 by **Dotmatics**, which was subsequently acquired by **Siemens** in Apr. 2025, to accelerate scientific research and improve data-driven decision-making for our customers and partners, providing them with a broader range of innovative solutions.

Outline

- Evolution of Method Selection
- Advanced Automated Impurity Analysis

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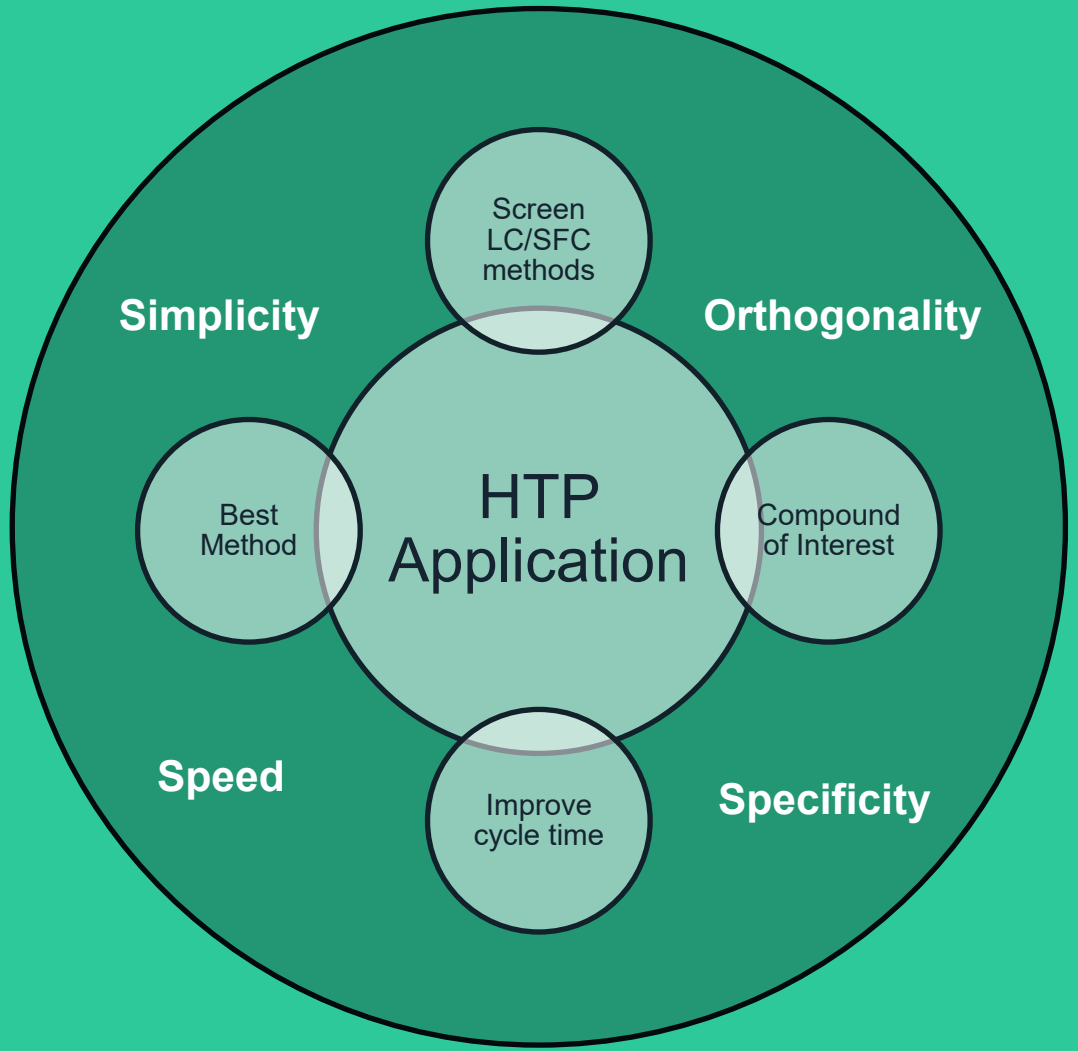
Initial Application & Approach Approach

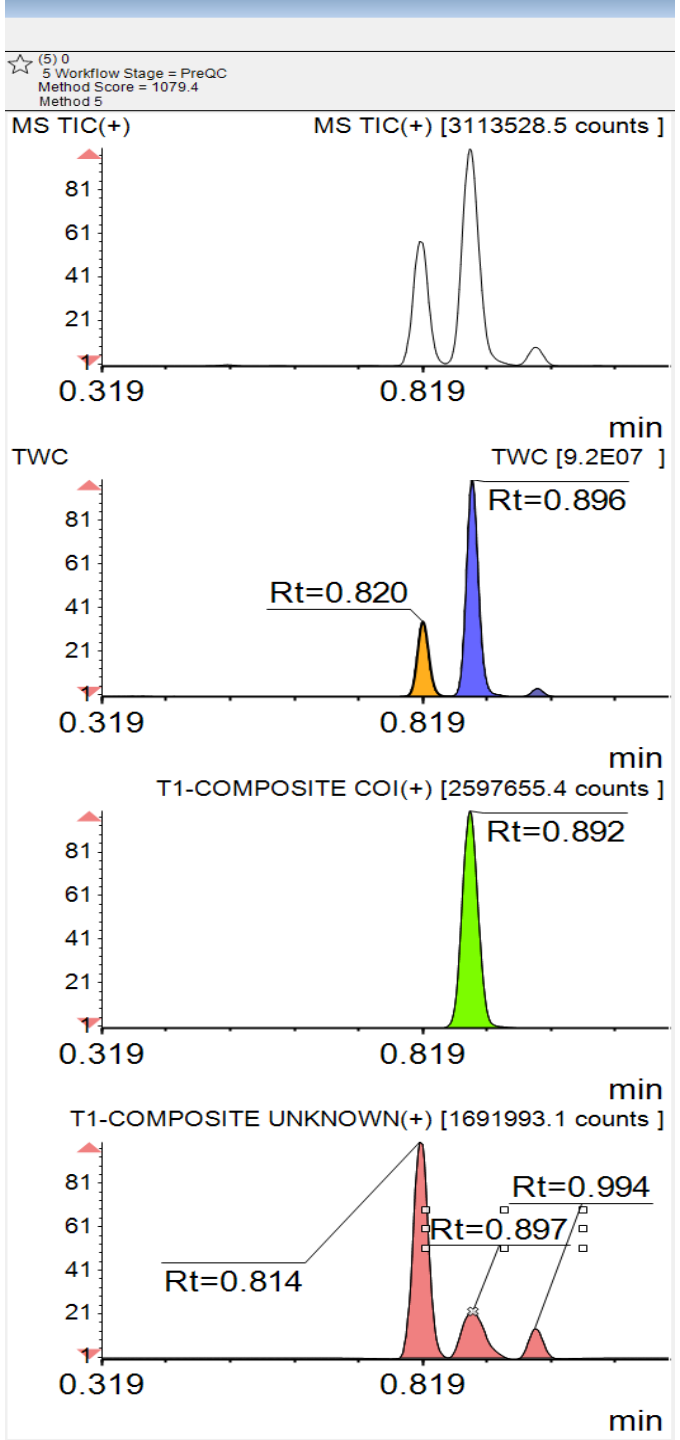


MS-TIC

UV-TWC

COI-EIC

Non-COI-EIC



[1] Aurigemma, C.M., et al, (2012) Journal of Chromatography A, 1229, pp. 260-267. https://doi.org/10.1016/j.chroma.2012.01.048

The goal of the Method Selection approach was to quickly identify conditions that could be used to obtain suitable purity

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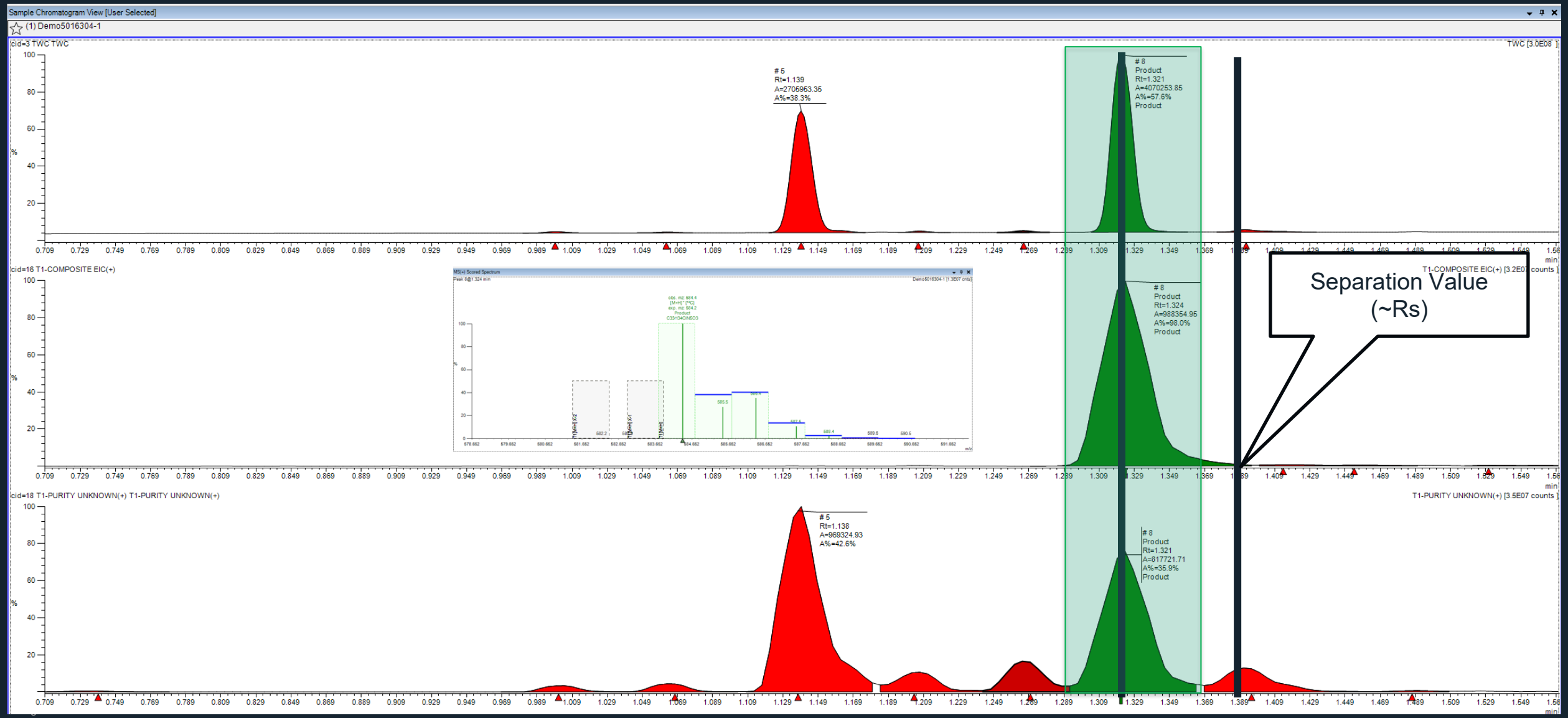

The resulting Method Scores were a best attempt to quantify the “best” method

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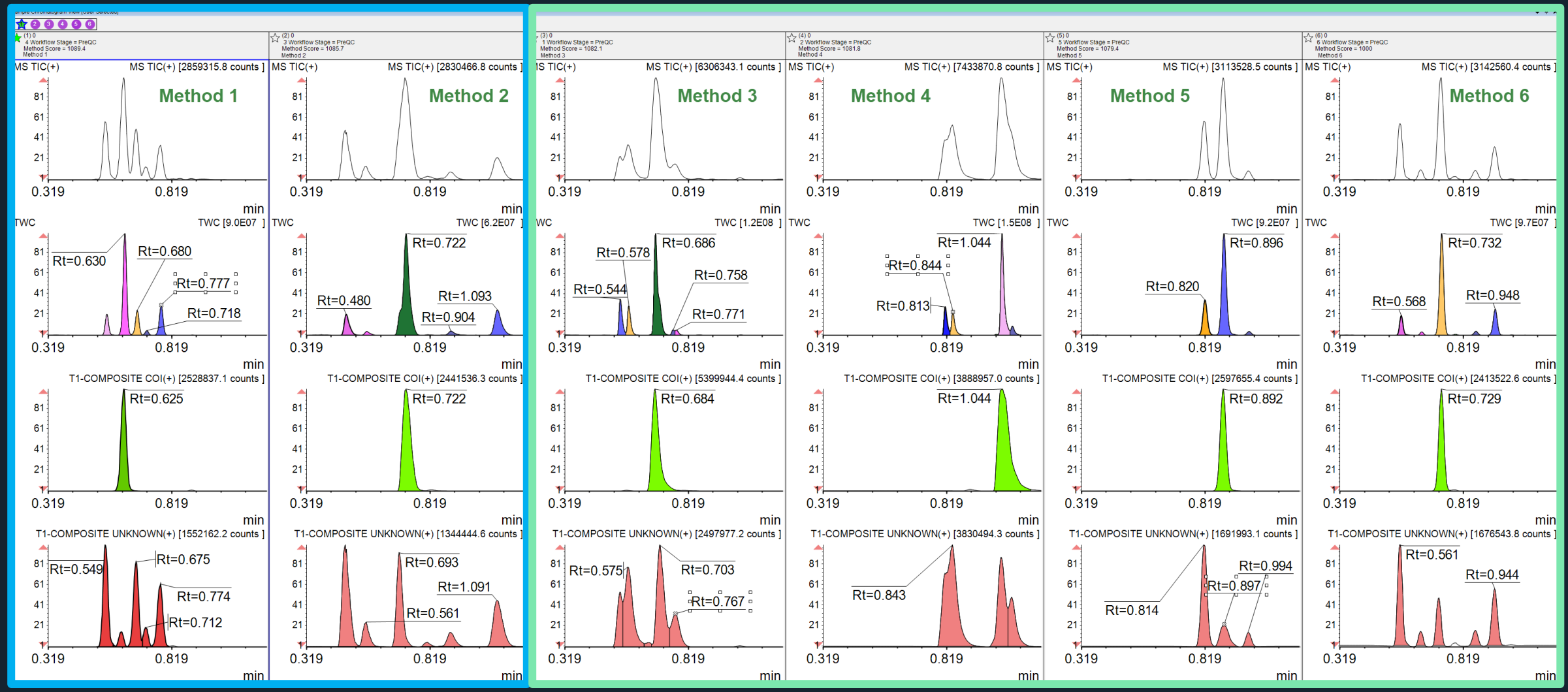
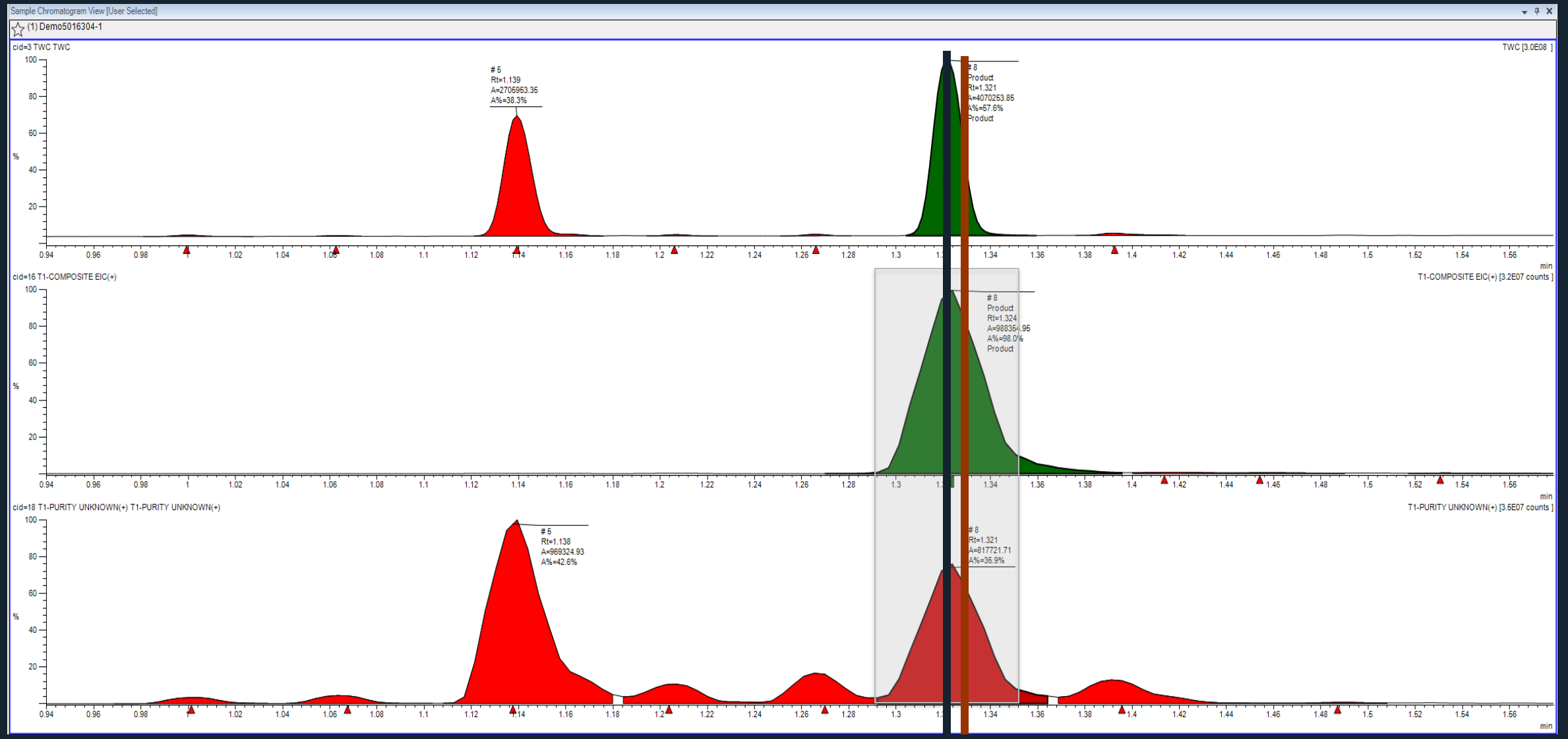
HPLC Methods

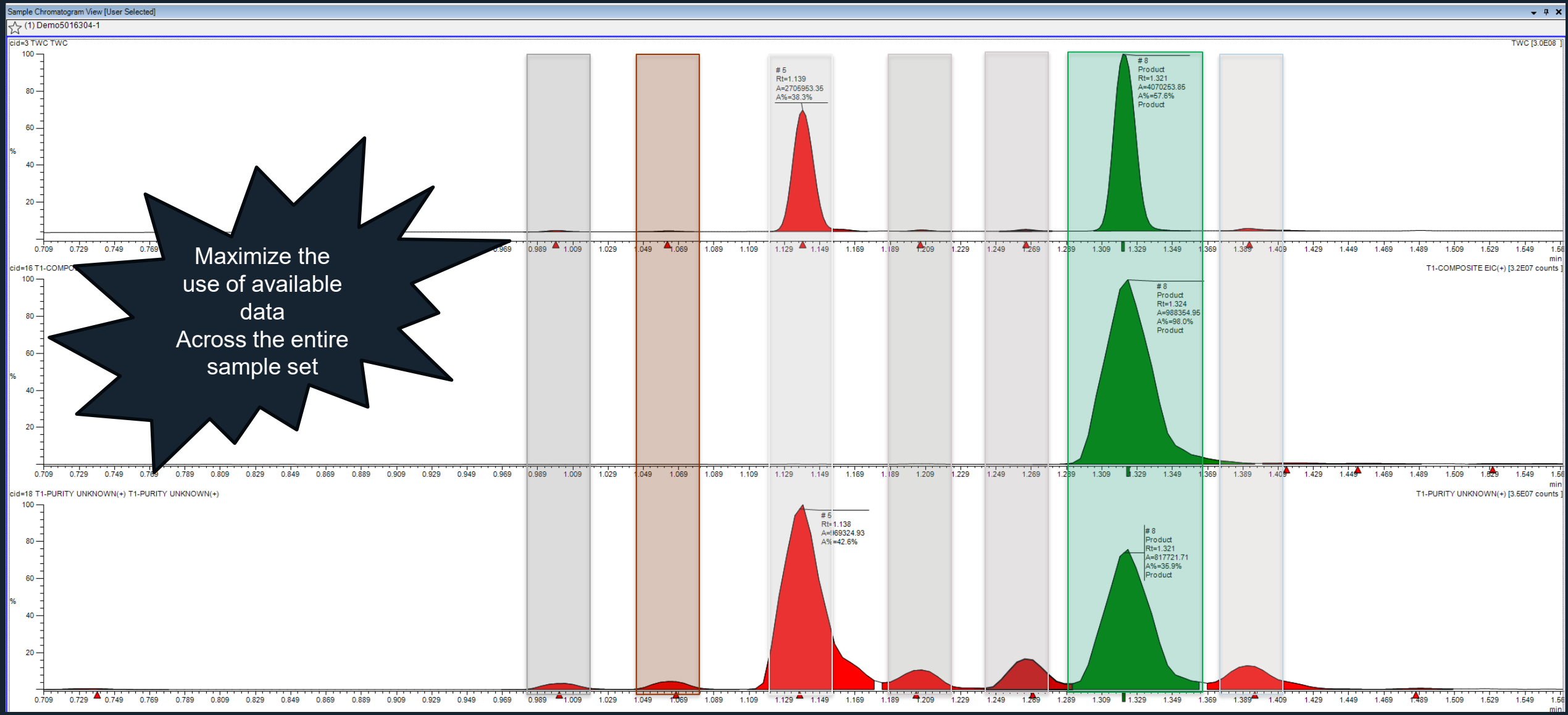
SFC Methods



Method Selection approach ignored the magnitude of any co-elution



Virscidian's latest Advanced Automated Impurity Analysis provides a more comprehensive analysis



Maximize the use of available data
Across the entire sample set

Analytical Studio enhancements select the best separation method from preliminary analysis and then…

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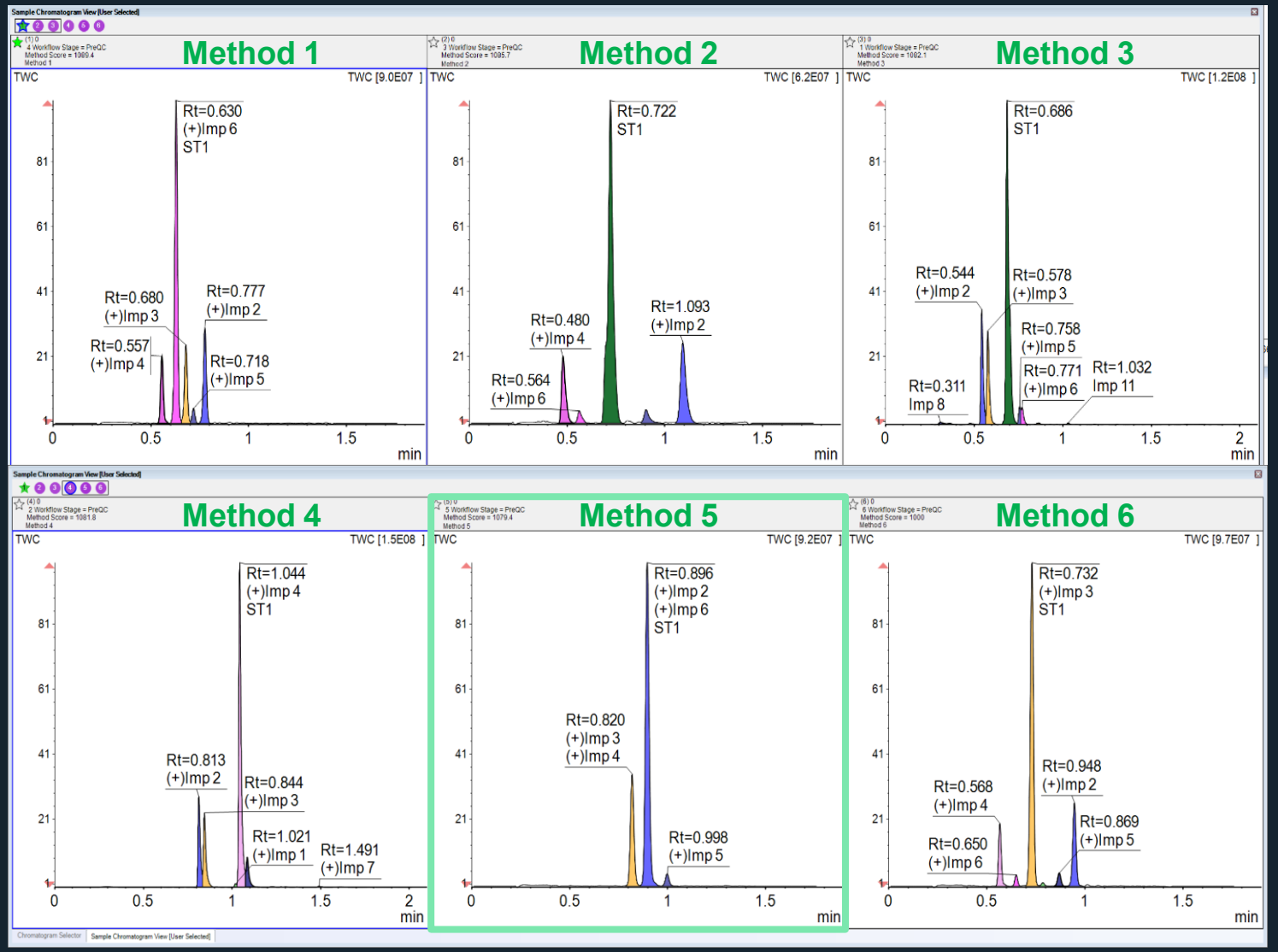
Uniquely identify impurities in any given sample

Automatically track impurities across the different methods

Quantitate impurities impact during co-elution



Advanced Automated Impurity Analysis translates MS learnings to UV data

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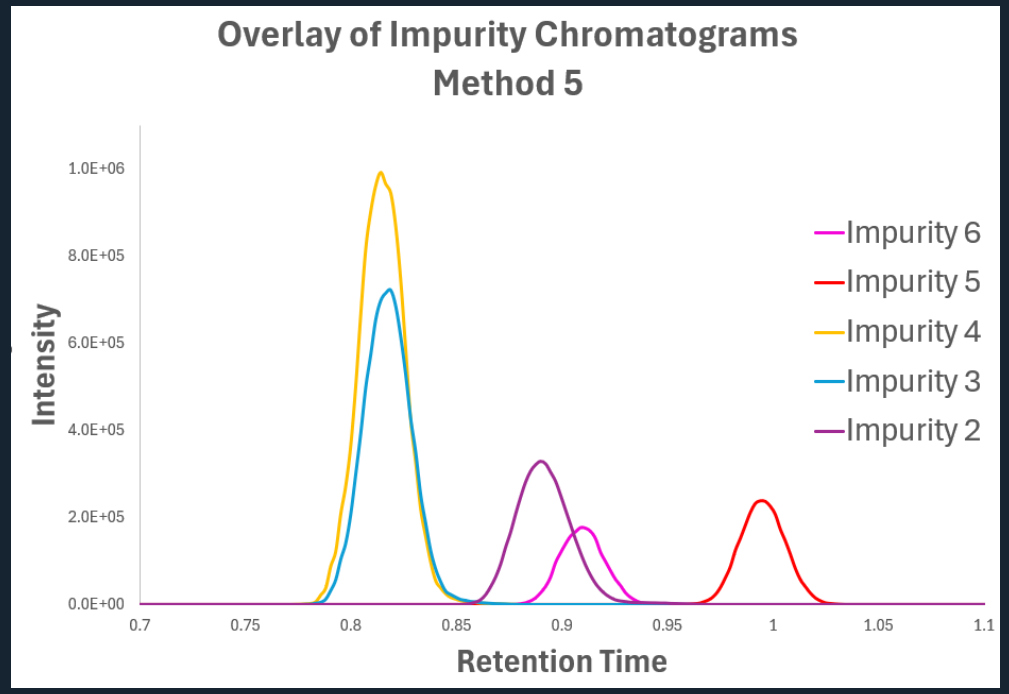

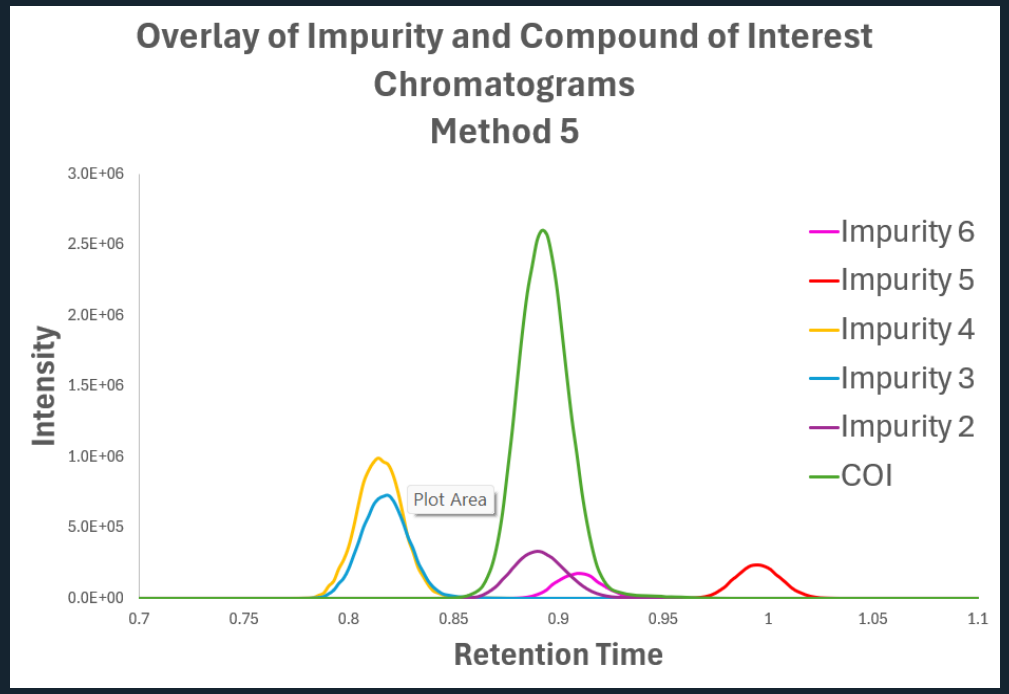

There are coeluting Impurities in **ALL** Methods – So which is the best one with the lowest Impurity Impact?

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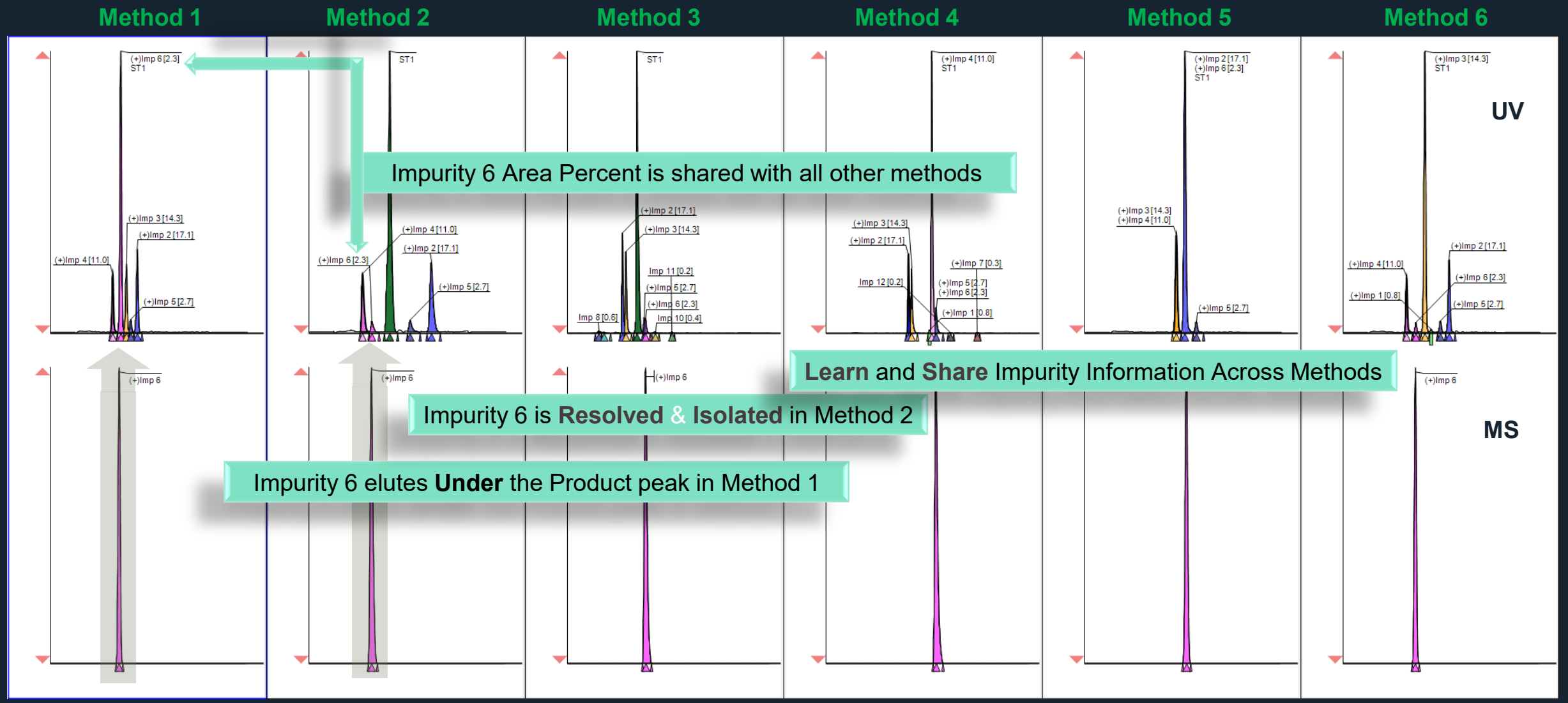

The new impurities are captured and applied across the dataset

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New substances are created in the Substance Editor…

Substance Editor

Options

Starts with / Contains

Populate identity signal list

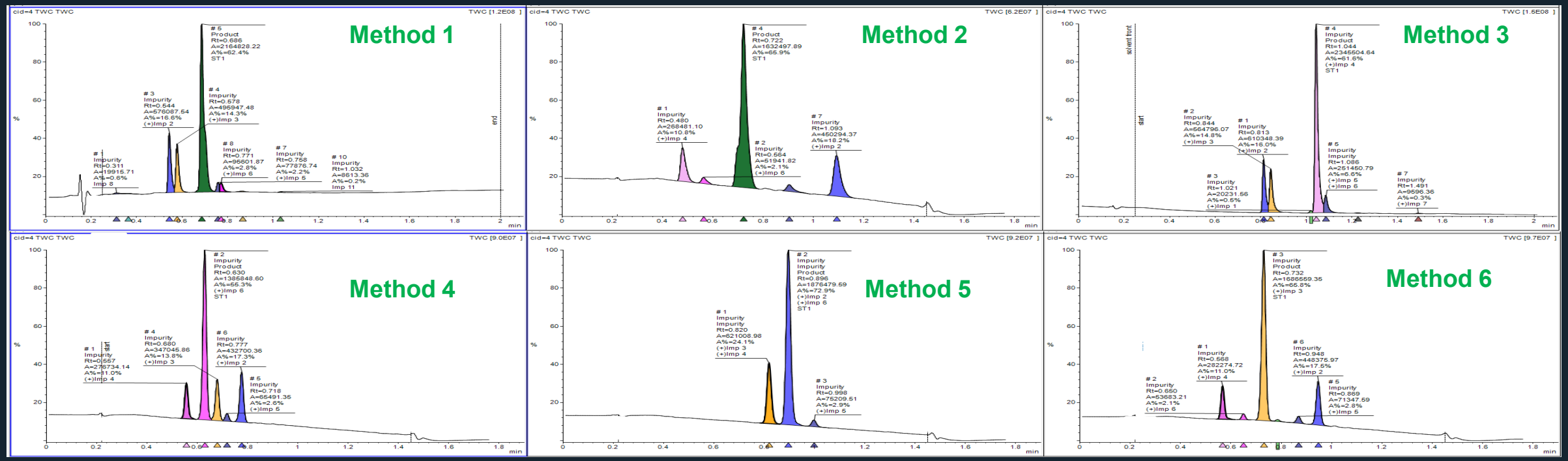
8 Substances

General					Target		Identity			Peak Selection		
Name	Color	Description	Class	Substance Type	Target	Formula	Confirmation Mode	Signal Assignment Mode	Identity Signal	Rt Criteria	Peak Selection	#Peaks
(+)Imp 1		319.2_333.0	Impurity	Impurity	2	319.2,92481	Rt Only	Identity and Non-MS	(+)Imp 1 EIC(+)	Full Time Range	Largest	2
(+)Imp 2		337.1_338.2	Impurity	Impurity	3	337.1,1069116	Rt Only	Identity and Non-MS	(+)Imp 2 EIC(+)	Full Time Range	Largest	2
(+)Imp 3		351.1_352.2	Impurity	Impurity	4	351.1,1377810	Rt Only	Identity and Non-MS	(+)Imp 3 EIC(+)	Full Time Range	Largest	2
(+)Imp 4		378.1_379.2_38...	Impurity	Impurity	5	378.1,57993	Rt Only	Identity and Non-MS	(+)Imp 4 EIC(+)	Full Time Range	Largest	2
(+)Imp 5		399.1_401.0	Impurity	Impurity	6	399.1,154179	Rt Only	Identity and Non-MS	(+)Imp 5 EIC(+)	Full Time Range	Largest	2
(+)Imp 6		413.1_415.0	Impurity	Impurity	7	413.1,187192	Rt Only	Identity and Non-MS	(+)Imp 6 EIC(+)	Full Time Range	Largest	2
(+)Imp 7		683.3	Impurity	Impurity	8	683.3,116625	Rt Only	Identity and Non-MS	(+)Imp 7 EIC(+)	Full Time Range	Largest	2
ST1			Analyte	Product	1		MS Only	MS Only and Other				

Current / Selected / All / Linked

Replace | Modify... | Rename... | Redefine... | Delete... | Append... | Load... | Save As...

… and peak annotations updated accordingly



Peak results can be displayed & customized to match preference

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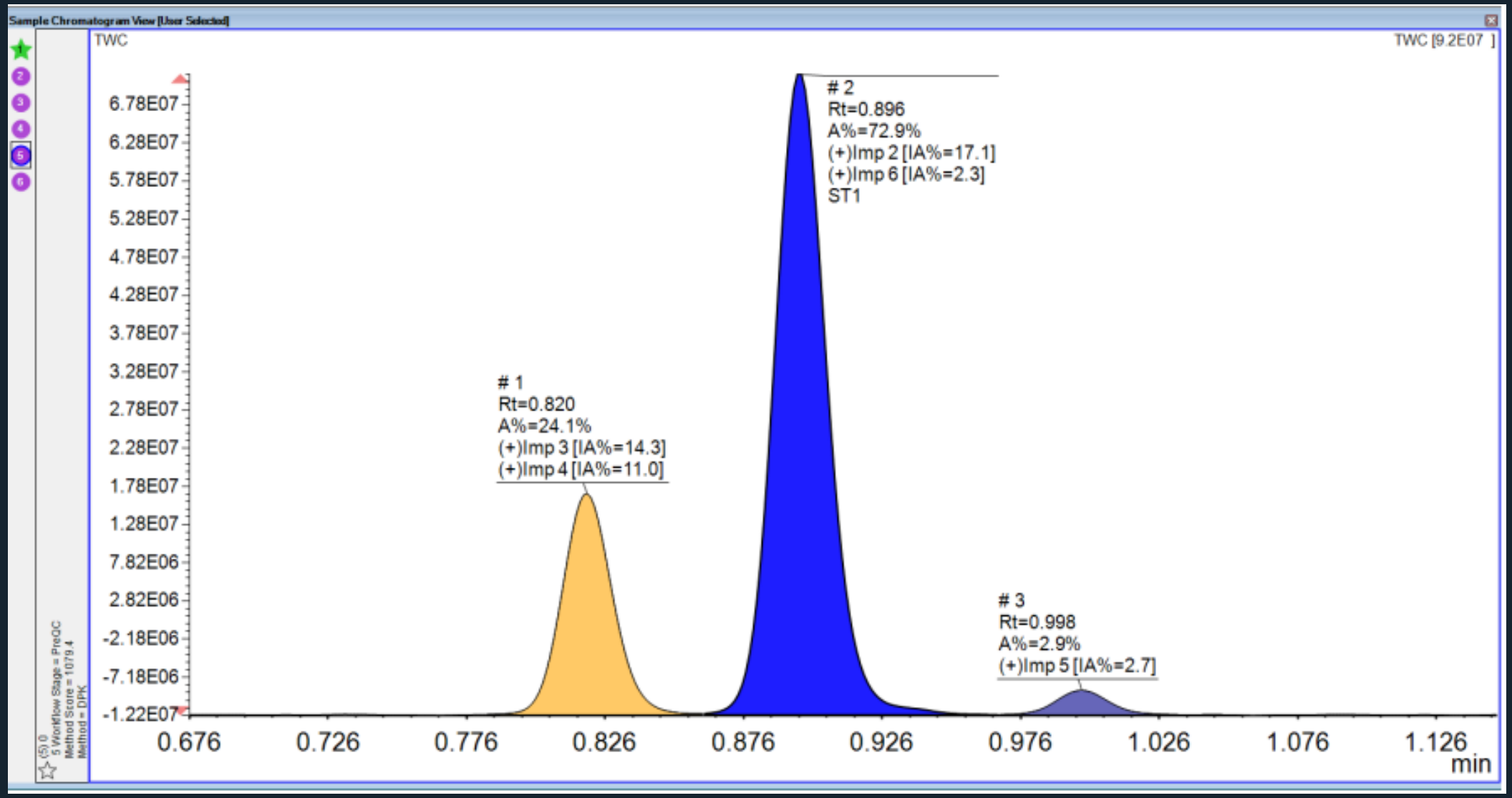

The new impurities are captured and applied across the dataset

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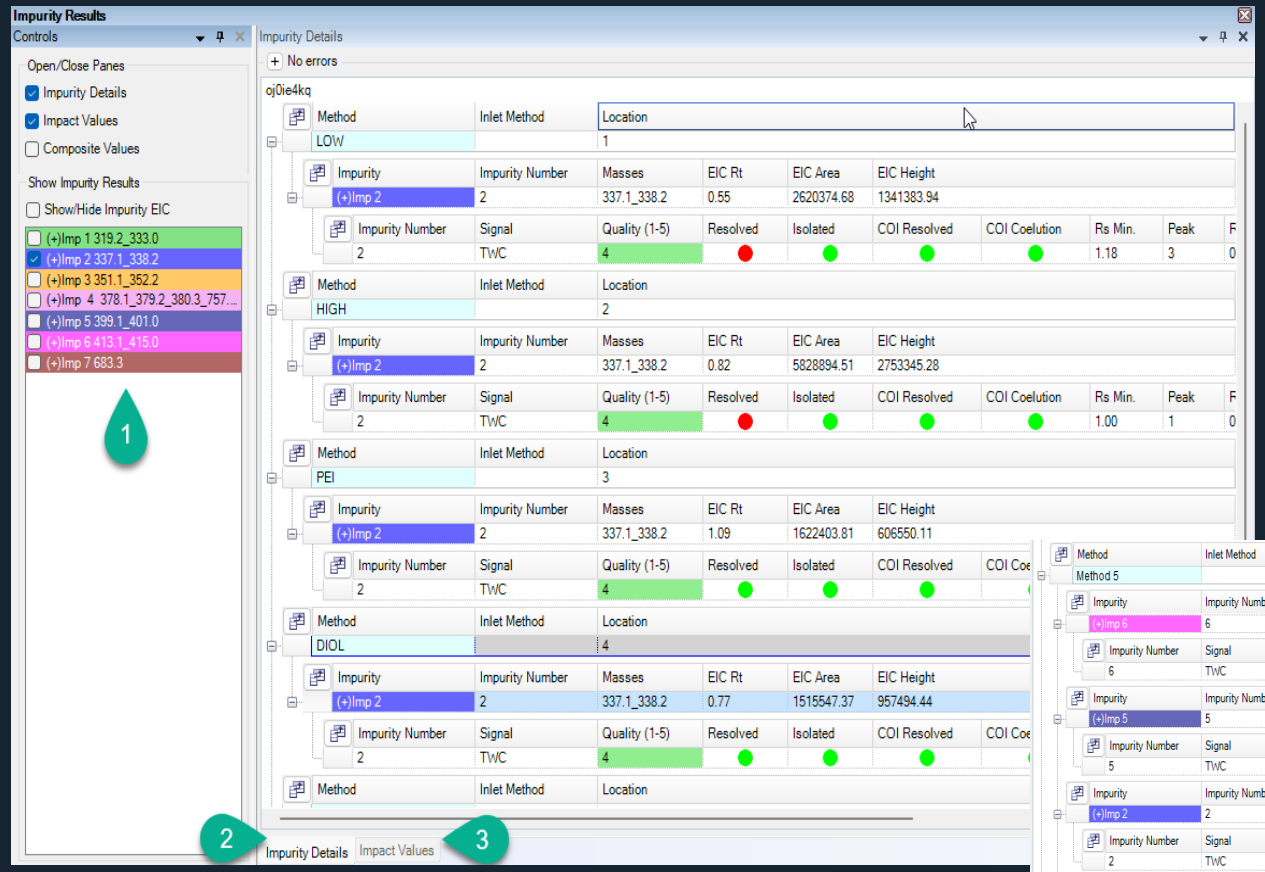
A new Impurity Results panel is introduced…



…that estimates the Impact Values for the impurities

Advanced Automated Impurity Analysis can be combined with existing Analytical Studio features

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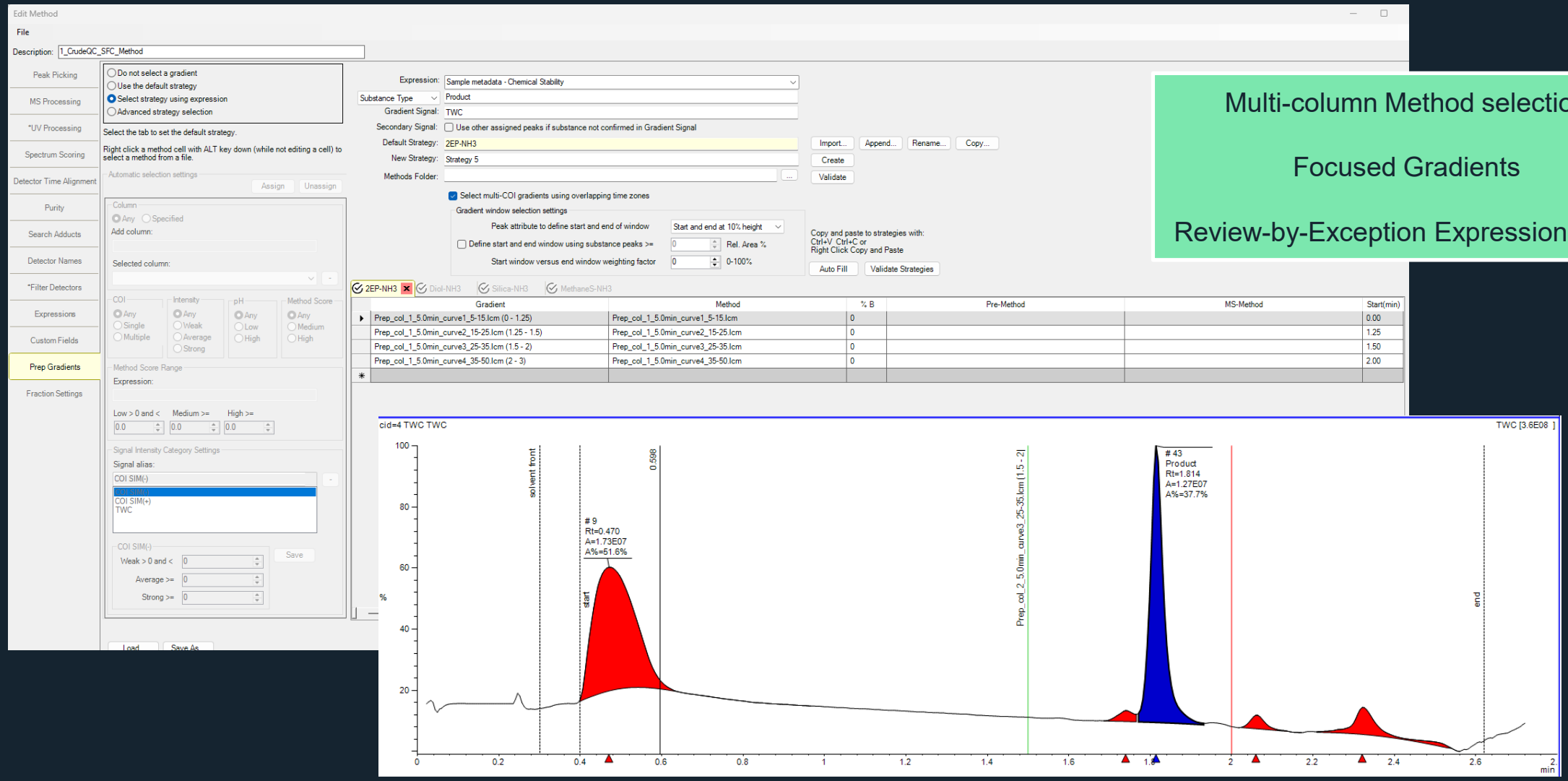

Multi-column Method selection

Focused Gradients

Review-by-Exception Expression Logic

Concluding Remarks

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Analytical Studio Professional method selection capabilities have evolved

- Moved from simplistic to comprehensive analysis
- Enable better informed decision making

Advanced Automated Impurity Analysis

- Utilizes all available data
- Assessments shared across samples to estimate impurity impacts
- Integrates seamlessly into HTP workflow

Virscidian continues to work to deliver cutting edge solutions

- Partner with customers and vendors
- Quickly move from idea to implementation

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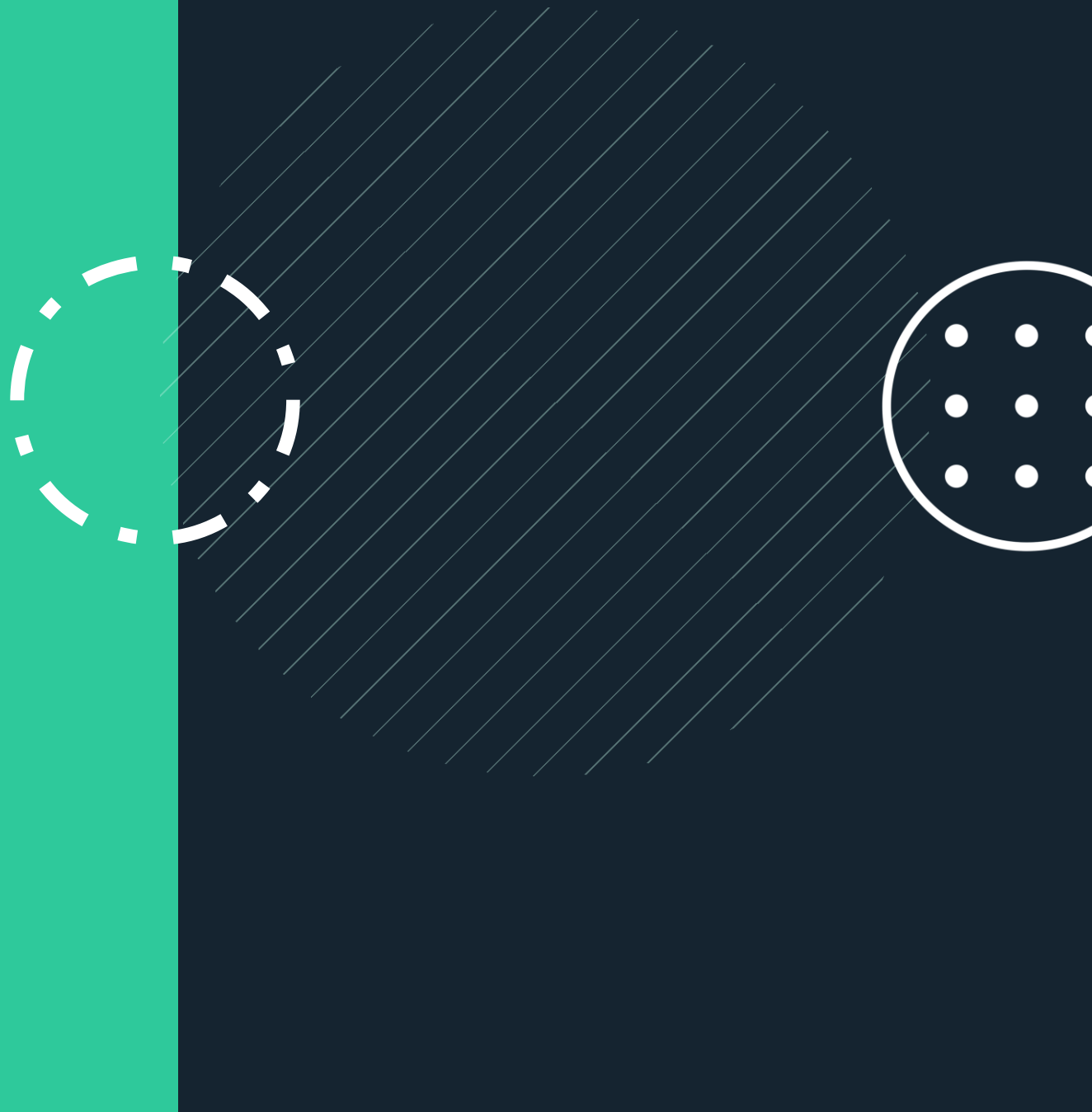
Get in touch:

bfarrell@virscidian.com

bill.farrell@dotmatics.com

Office: 858-304-8481

info@virscidian.com

https://www.virscidian.com/

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