

Metabolic Profiling of Green Tea and Coffee by UHPLC-MS/MS using a Novel C18-based Stationary Phase

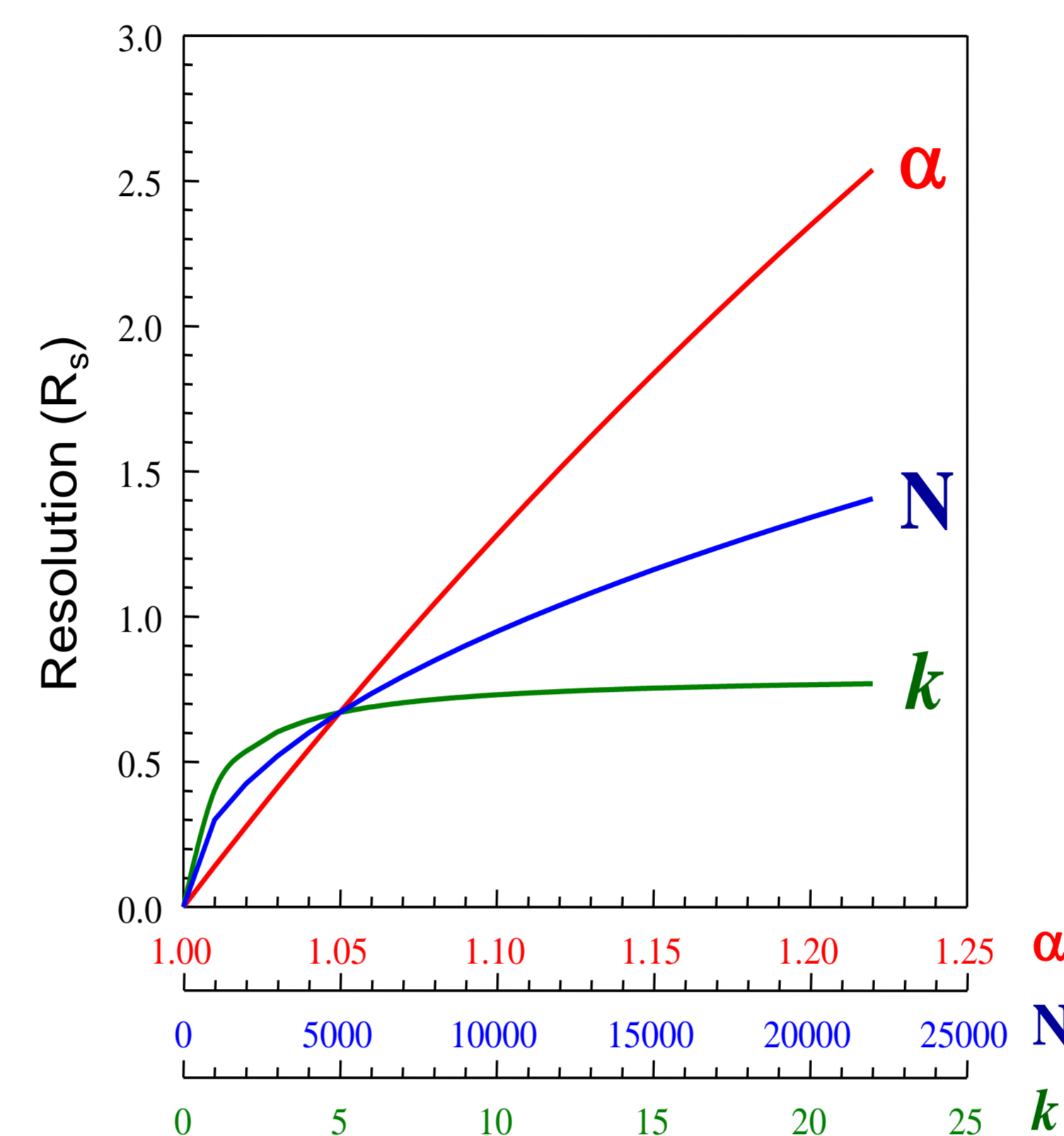
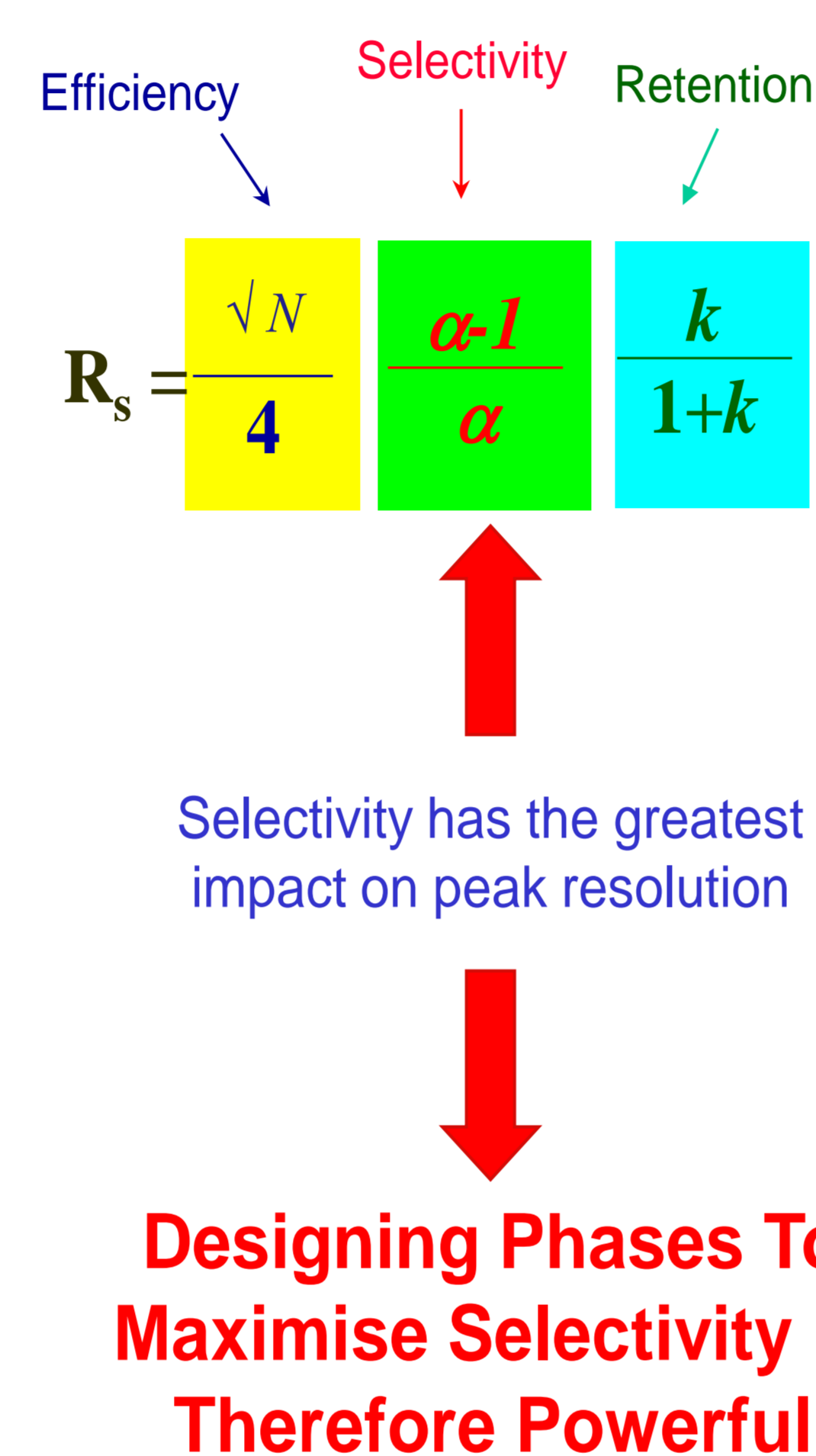
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1. BACKGROUND

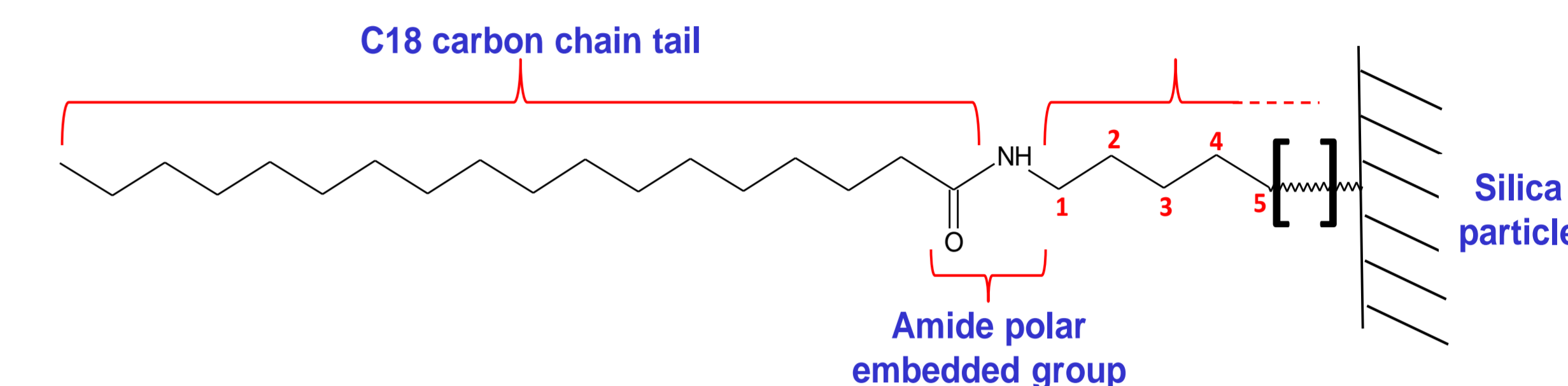
- Samples of **natural origin** tend to be **complex** with a range of **polar to non-polar analytes** present at **varying levels**.
- **Profiling natural products** is helpful for **quality** and **consistency** but can also be important for **safety** and **provenance**.
- **The components of teas and coffees** present an interesting **separation** and **detection** challenge with analytes varying from **small charged acids and bases** to **larger hydrophobic species**.
- This poster explores the use of a **1.7µm novel C18-based polar embedded** stationary phase suitable for the **retention and separation** of a wide range of **polar to non-polar analytes** in **teas and coffees**.

2. RESOLUTION, SELECTIVITY, EFFICIENCY & RETENTION



Zhao, J.H. and P.W. Carr. Analytical Chemistry, (1999) 71, 2623-2632

3. RATIONAL PHASE DESIGN TO MAXIMISE SELECTIVITY



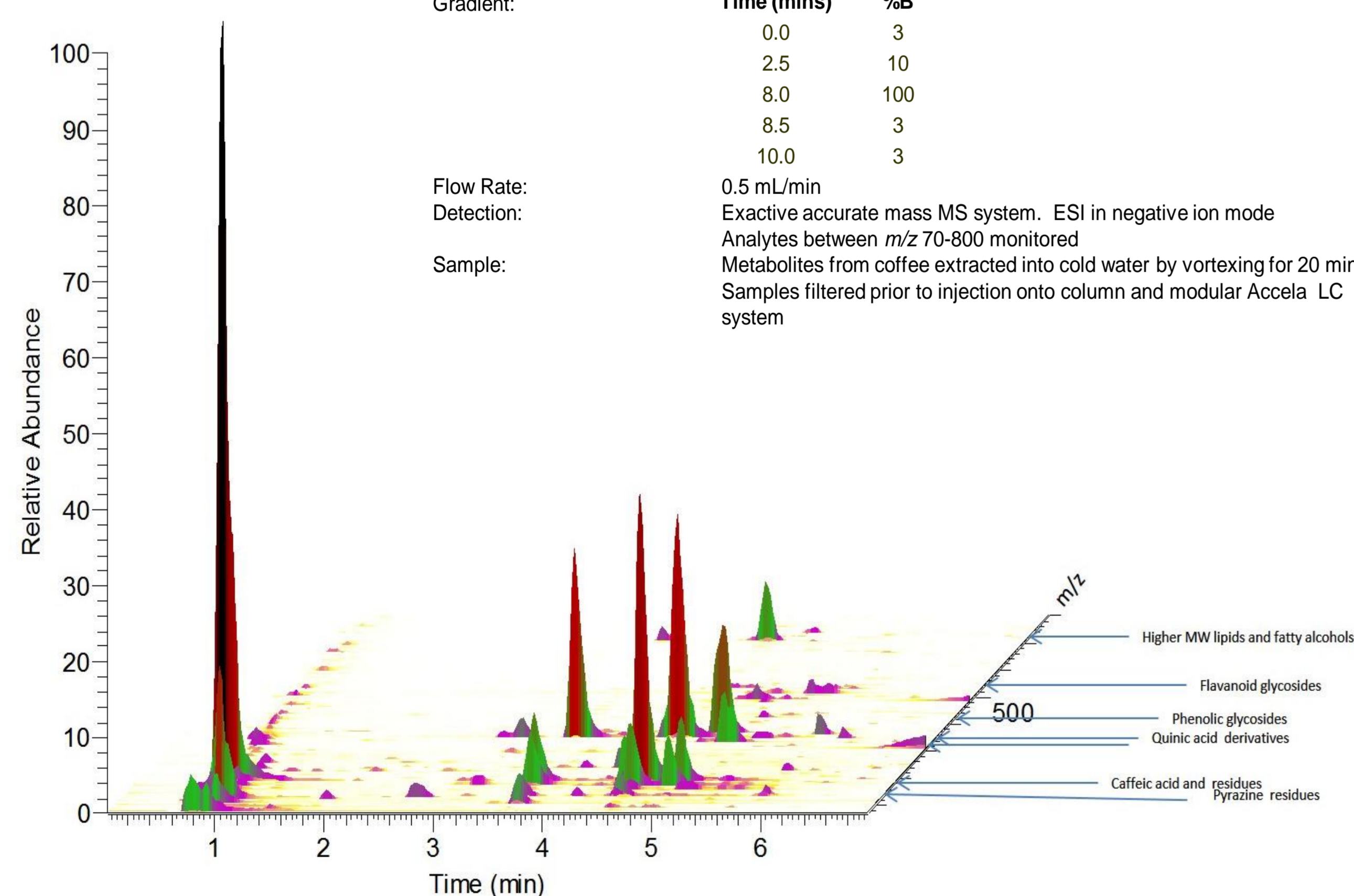
- Ligand contains an **embedded amide moiety**:
 - Designed to **retain polar and non-polar analytes** within a single run.
 - Ideal for **H-bond donor analytes**: **acids, phenolics, amines, amides** etc.
 - Suitable for **analysis of teas, beverages** etc.
- **Improved stability at low and mid pH** results from **extended carbon chain spacer**.
- **C18 terminology** comes from 18 carbon 'tail'.

4. COFFEA ARABICA METABOLITE PROFILING

Column: ACE Excel C18-Amide, 100 x 2.1 mm, 1.7µm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H₂O B: 0.01% formic acid in MeCN
Gradient:

Time (mins)	%B
0.0	3
2.5	10
8.0	100
8.5	3
10.0	3

Flow Rate: 0.5 mL/min
Detection: Exacte accurate mass MS system. ESI in negative ion mode
Analytes between m/z 70-800 monitored
Sample: Metabolites from coffee extracted into cold water by vortexing for 20 mins. Samples filtered prior to injection onto column and modular Accela LC system

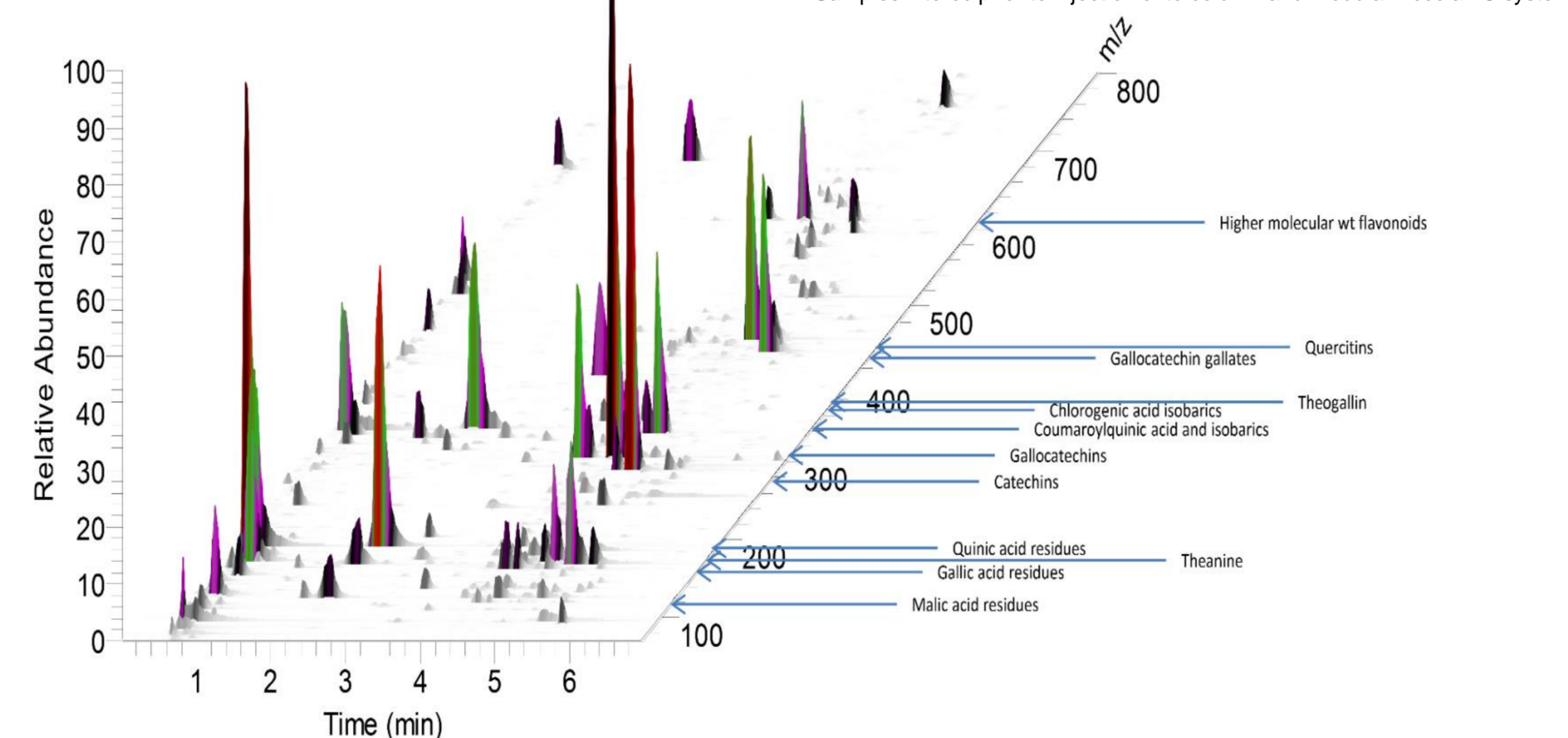


5. CAMELLIA SINENSIS GREEN TEA METABOLITE PROFILING

Column: ACE Excel C18-Amide, 100 x 2.1 mm, 1.7µm
Part Number: EXL-1712-1002U
Mobile Phase: A: 0.01% formic acid in H₂O B: 0.01% formic acid in MeCN
Gradient:

Time (mins)	%B
0.0	3
2.5	10
8.0	100
8.5	3
10.0	3

Flow Rate: 0.5 mL/min
Detection: Exacte accurate mass MS system. ESI in negative ion mode
Analytes between m/z 70-800 monitored
Sample: Metabolites from green tea extracted into cold water by vortexing for 20 mins. Samples filtered prior to injection onto column and modular Accela LC system



6. SUMMARY AND CONCLUSIONS

- A **rapid UHPLC** method using a novel **ACE Excel C18-Amide, 1.7µm** column with **high resolution MS** detection for **profiling natural product samples** has been established.
- The new method was used to **qualitatively explore the metabolite profile** of coffee and tea samples covering **polar to non-polar analytes**.
- The **novel ACE Excel C18-Amide** stationary phase demonstrated **excellent separation performance** for a range of analytes allowing **identification** of a variety of **small to medium sized** naturally occurring analytes.

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