

Grouping Natural Complex Substances (NCS) for Safety Assessment through Multi-component SPR Analysis.

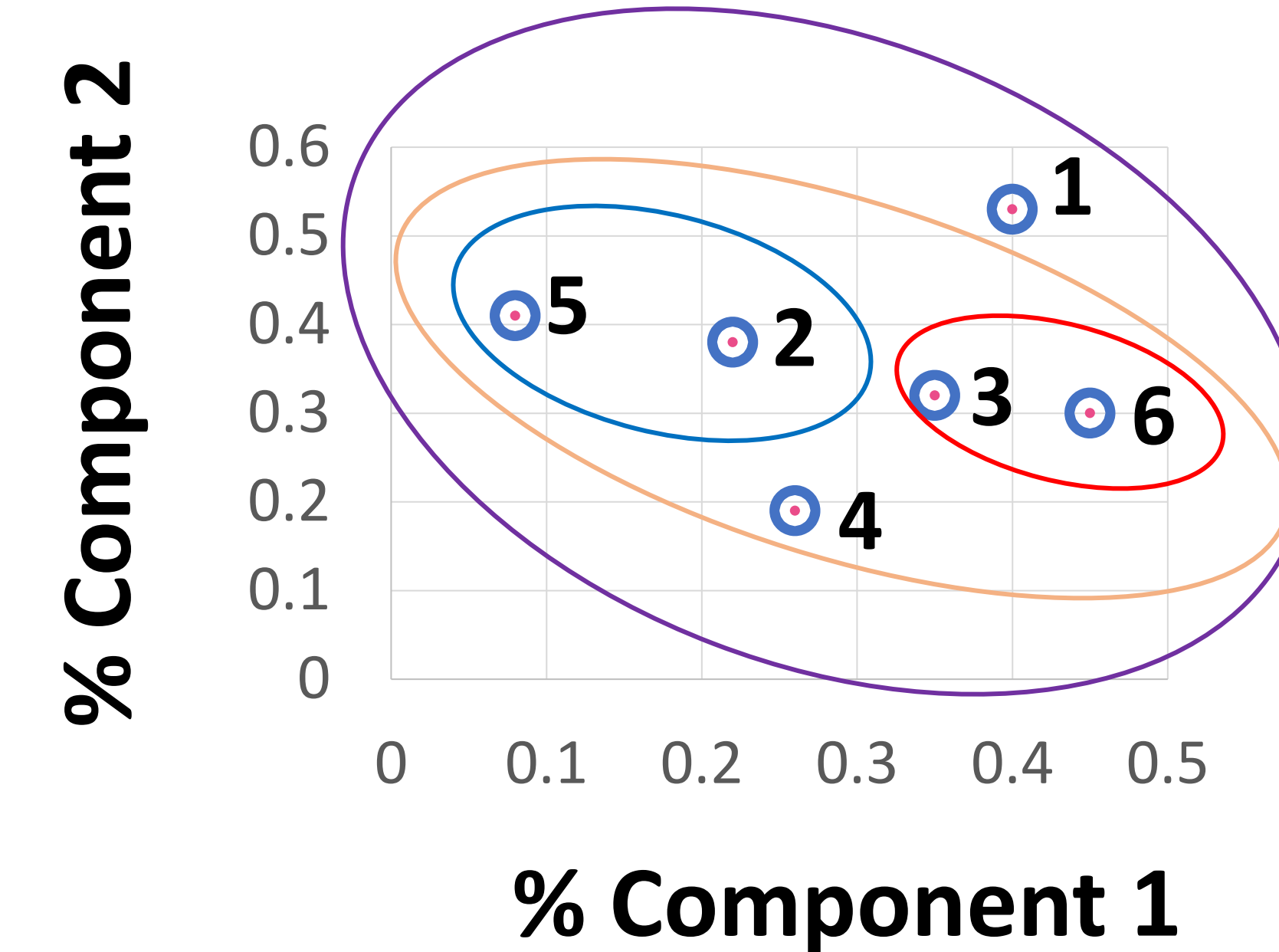
The chemical similarity between Natural Complex Substances (NCS) is driven predominantly by the sources (plant parts) from which the substances are derived.

(Plant taxonomy, geographical origin, and processing for extraction of an oil all play a secondary role in the final composition of the NCS.)

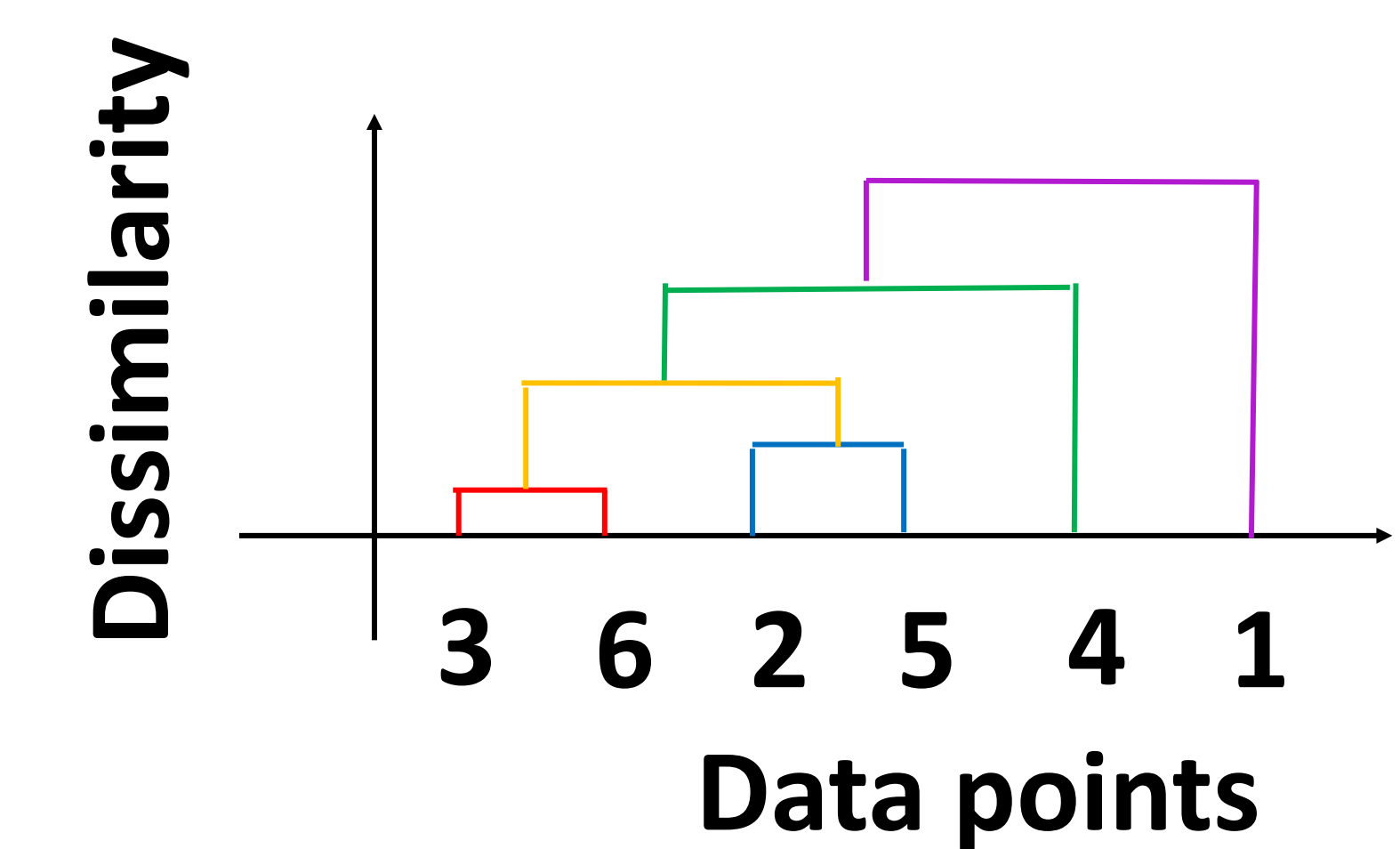
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An example below explains agglomerative hierarchical clustering

1. Data



2. Dendrogram



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INTRODUCTION:

- Knowing the "similarity" between complex substances is crucial for the safety assessment program.
- Clustering NCS based on similarity in composition helps prioritize the substances for high throughput evaluation by performing data analysis, searching for read-across analogs, or device testing strategies for data generation.

METHODS

- Multicomponent SAR is applied over NCS matrix.
- IFRA/IOFI matrix is first divided according to family and genus.
- Rutaceae* family and *Citrus* genus was selected for a pilot study as, collectively, this family represents the highest usage NCS.
- Rutaceae* NCS were clustered using the Agglomerative Hierarchical Clustering (AHC) method.
- AHC yields a dendrogram that shows the linkages within and between clusters.
- [IRFM discrete fragrances clustering and read-across search criteria](#) is applied over AHC groups to further refine the clusters.

