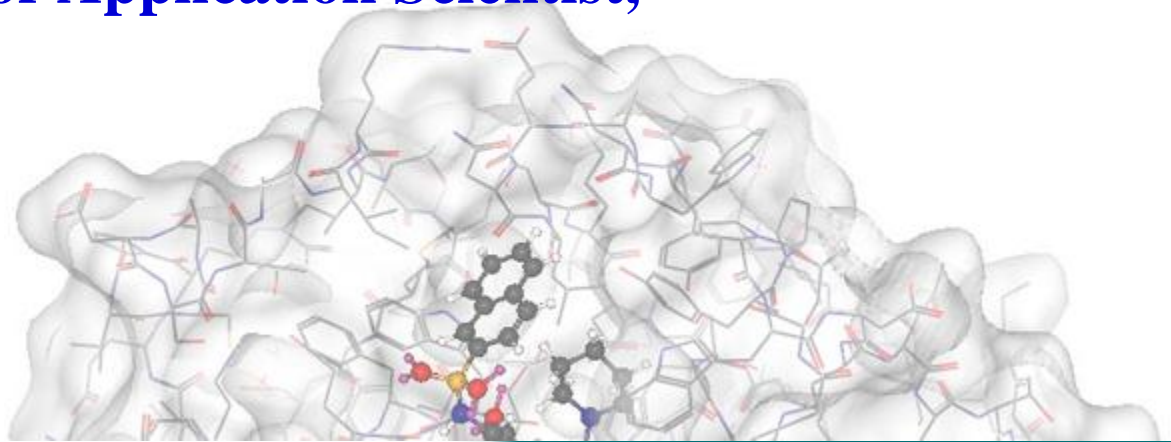




ChemAxon

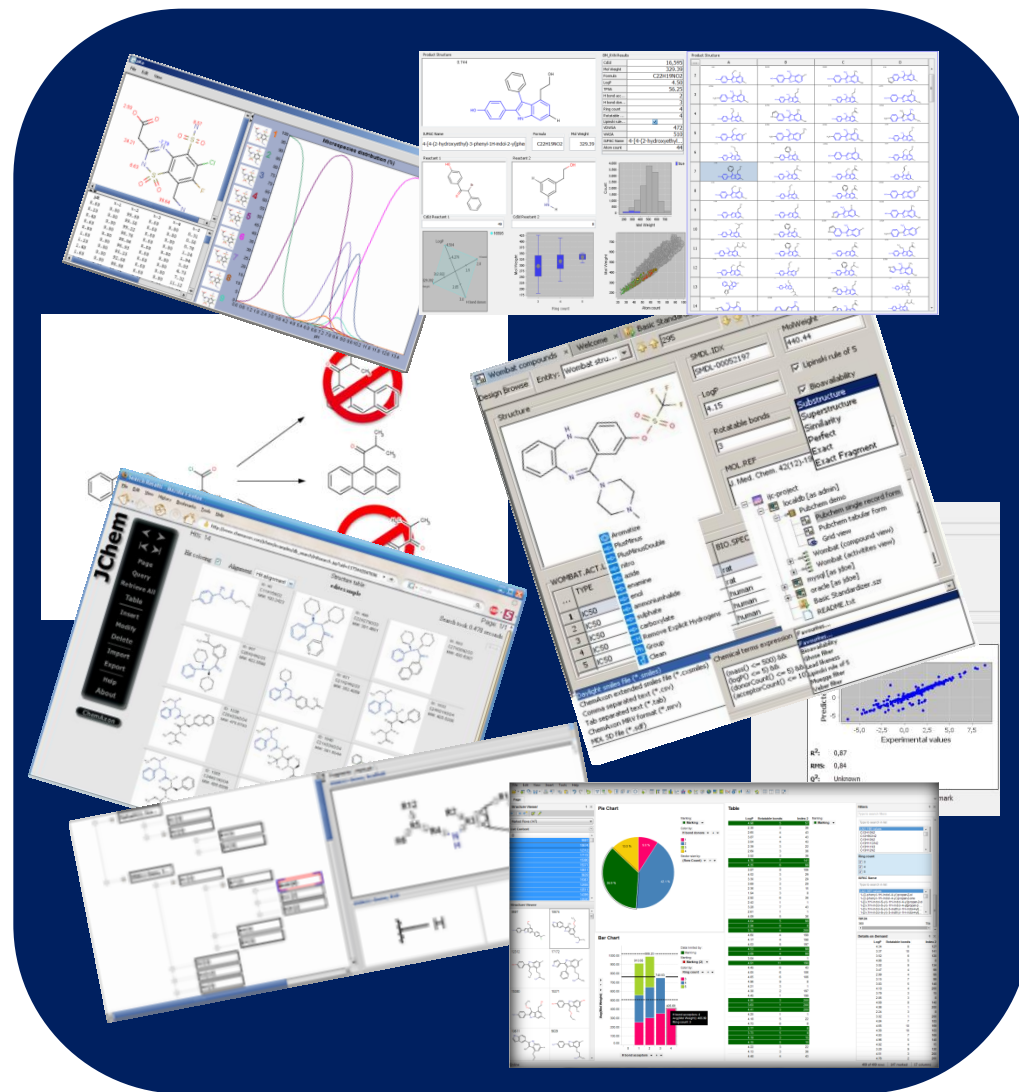
Speeding and Refining Chemical Analysis and Visualization in Drug Discovery Processes: a Powerful Combination of Instant JChem and Spotfire

**Krisztian Niesz, Senior Application Scientist,
Group leader**



What is this integration all about?

- IJC is an “out of the box” desktop application designed for biologists and chemists.
- IJC is a fast and scalable database application for chemistry, a tool with powerful search + rich chemistry functionalities.
- Spotfire is a powerful data discovery & visualization tool.
- Together they form an integrated solution for visualization, analysis & exploration!





PerkinElmer

The place for **Spotfire®** in Science
TIBCO Software

PerkinElmer and TIBCO Form Strategic Alliance

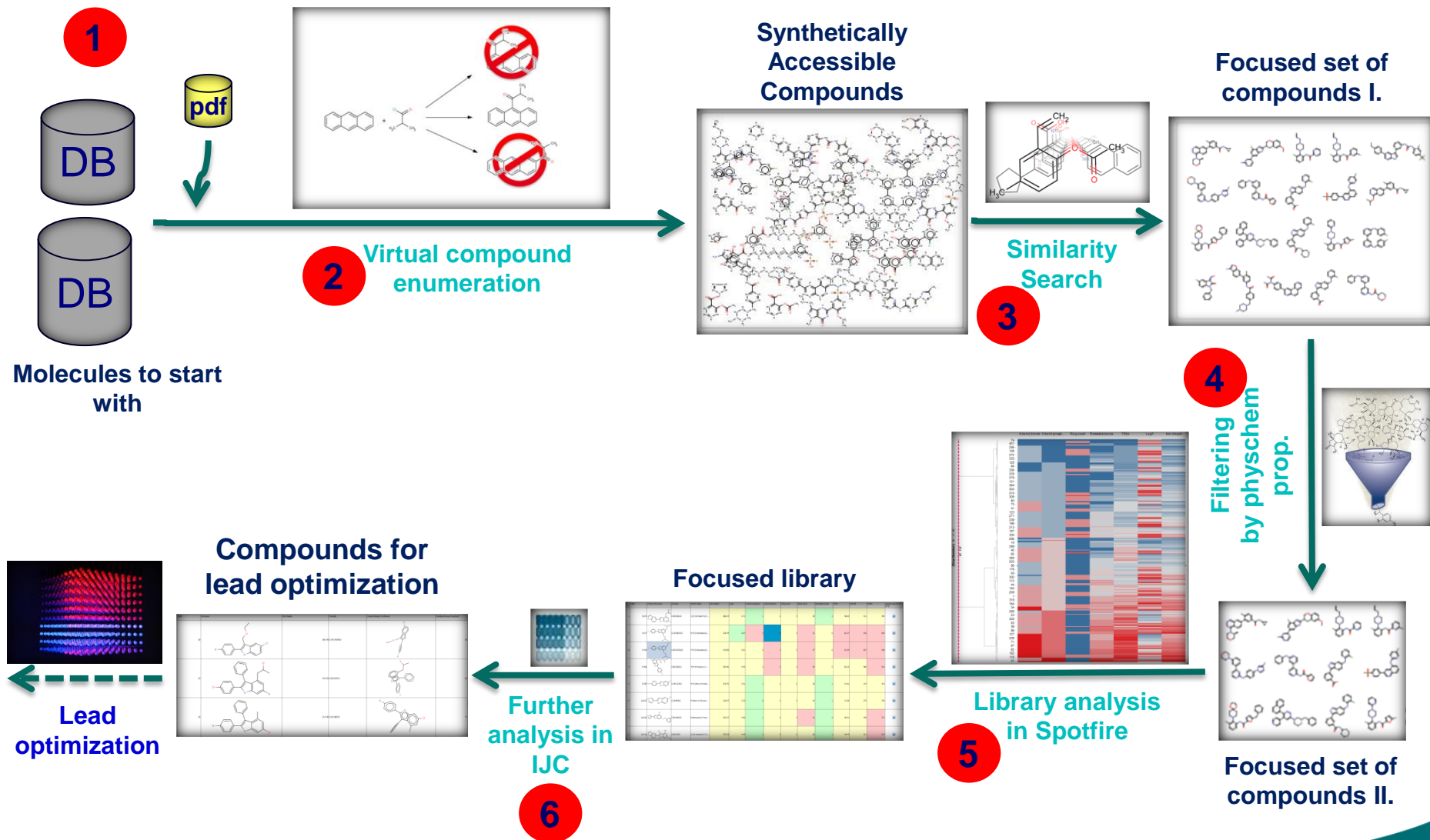
September 11, 2012 – PerkinElmer, Inc. and TIBCO Software Inc. announced today that they have entered into a decisive strategic relationship. Under the terms of this new agreement, PerkinElmer has licensed the exclusive, worldwide rights to the TIBCO Spotfire® software platform in certain scientific research and development applications markets including basic and preclinical development in life sciences; research and development in chemical, petrochemical, food and beverage, consumer products and academia; as well as quality assurance and quality control in manufacturing.

[Press Release](#) >

[More Information](#) >

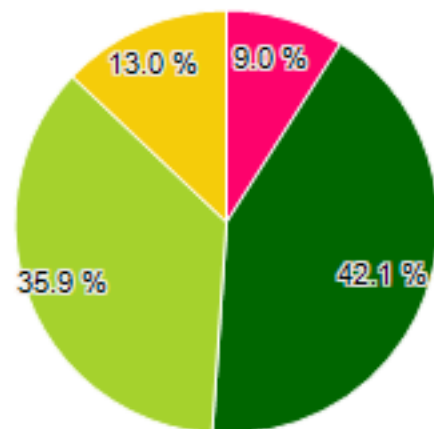
„PerkinElmer’s intention is to continue to provide an open chemistry platform that works with a range of different cheminformatics systems.”

Performing a simple lead discovery workflow with Instant JChem & Spotfire



DEMONSTRATION

Pie Chart



Marking:

■ Marking

Color by
H bond donors

■ 1

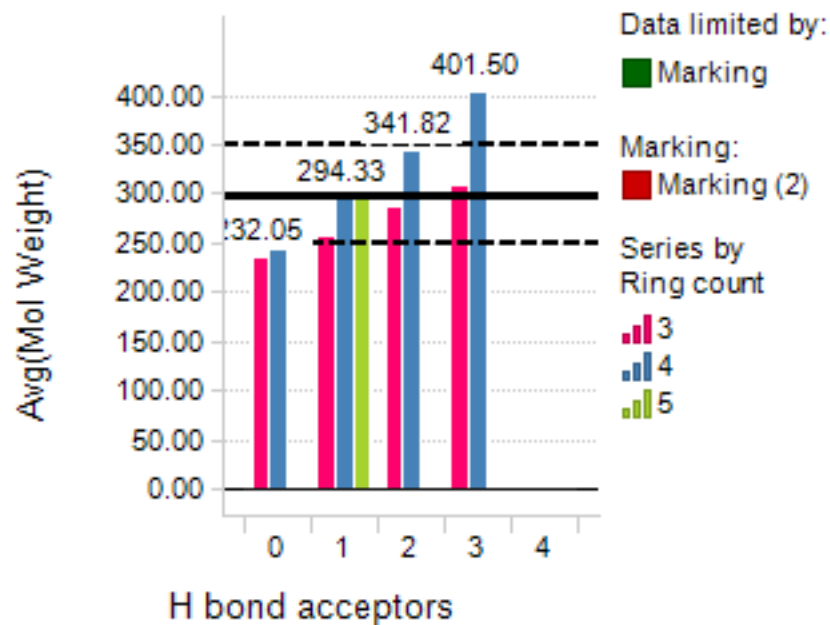
■ 2

■ 3

■ 4

Sector size by
(Row Count)

Combination Chart



Data limited by:

■ Marking

Marking:

■ Marking (2)

Series by
Ring count

■ 3

■ 4

■ 5

Table

	LogP	Rotat...	Marking:
	4.98	5	■ Marking
	2.30	3	
	2.65	4	
	3.87	4	
	3.04	4	
	2.39	3	
	2.69	3	
	3.52	3	
	4.76	7	
	4.35	6	
	3.87	8	
	4.52	3	
	3.30	3	
	3.69	3	
	2.36	3	
	1.94	3	
	2.92	6	
	2.42	1	
	3.28	7	
	2.61	1	
	4.09	5	
	4.64	5	
	2.56	6	
	3.78	4	
	4.60	4	



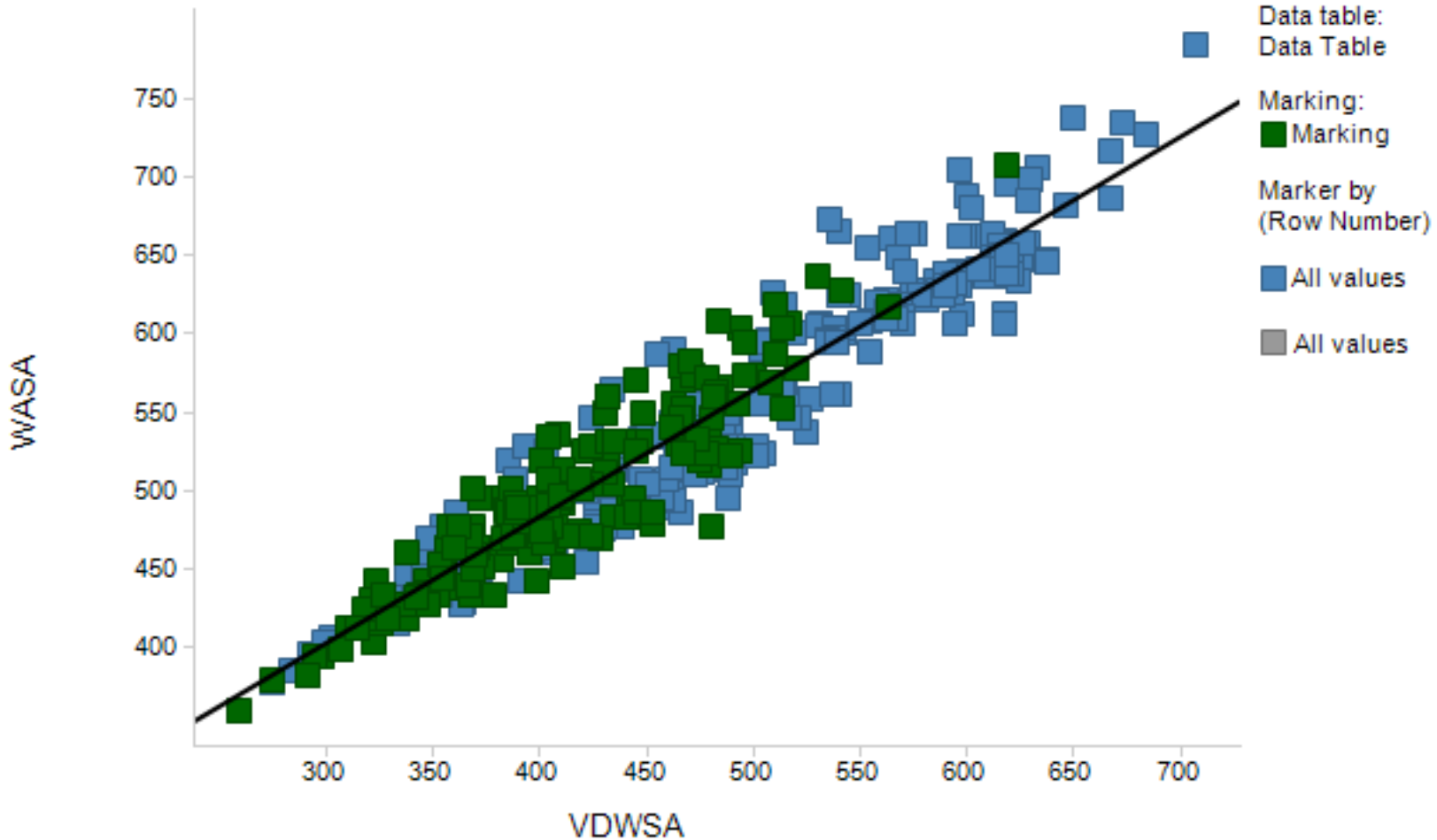
Data Relationships

Data Relationships (Linear Regression)

Y (numerical)	X (numerical)	p-value	F Stat	RSq	R	Data table:
WASA	VDWSA	2.63E-214	4083.94	0.91	0.95	Data Relationships

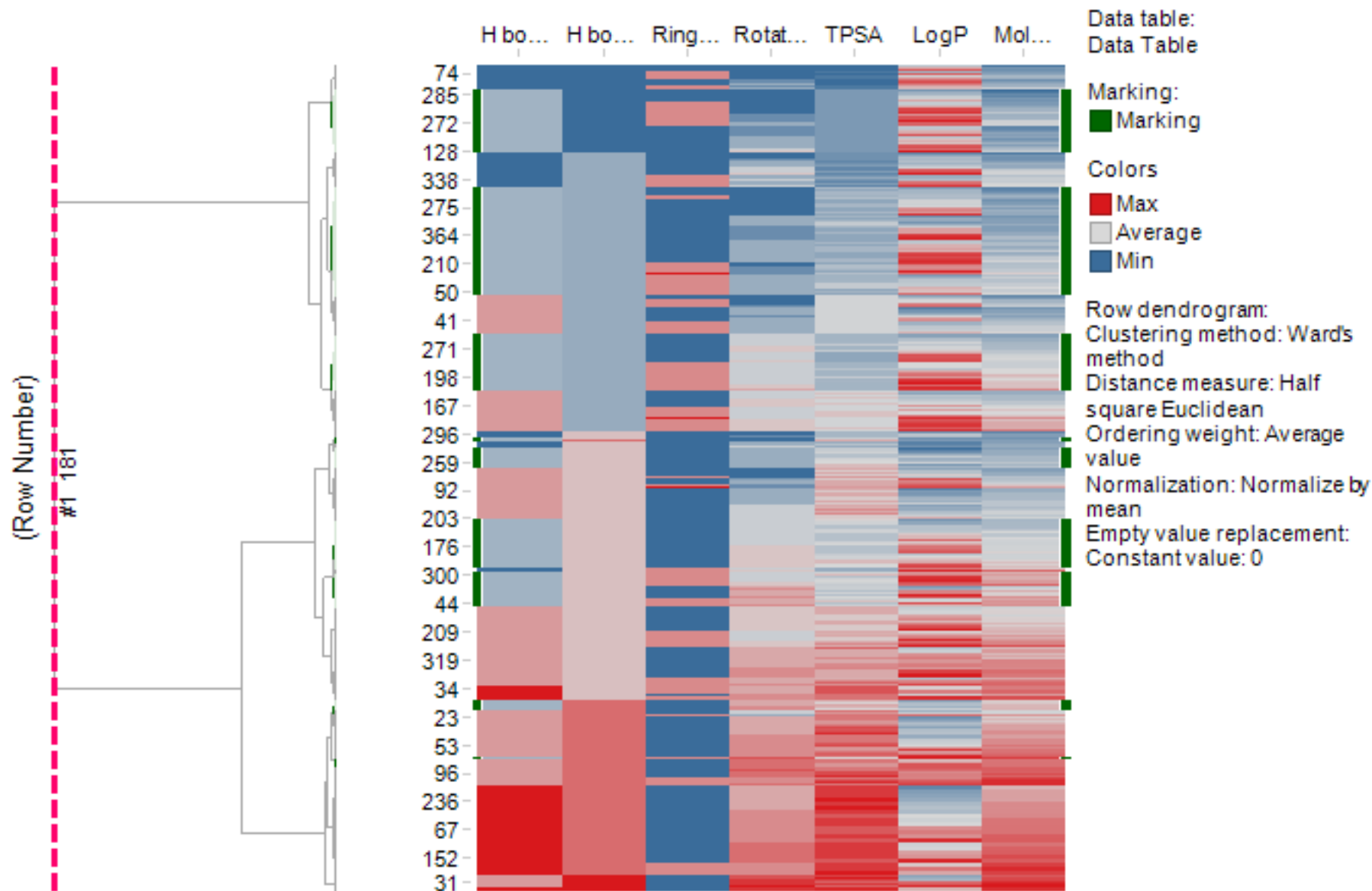
Marking:
■ Marking

Data Relationships (Details)



Clustering

Heat Map



Thank you for your attention!

