Visualizing chemical data

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DataViz Forum

The University Of Sheffield.

Visualizing chemical data
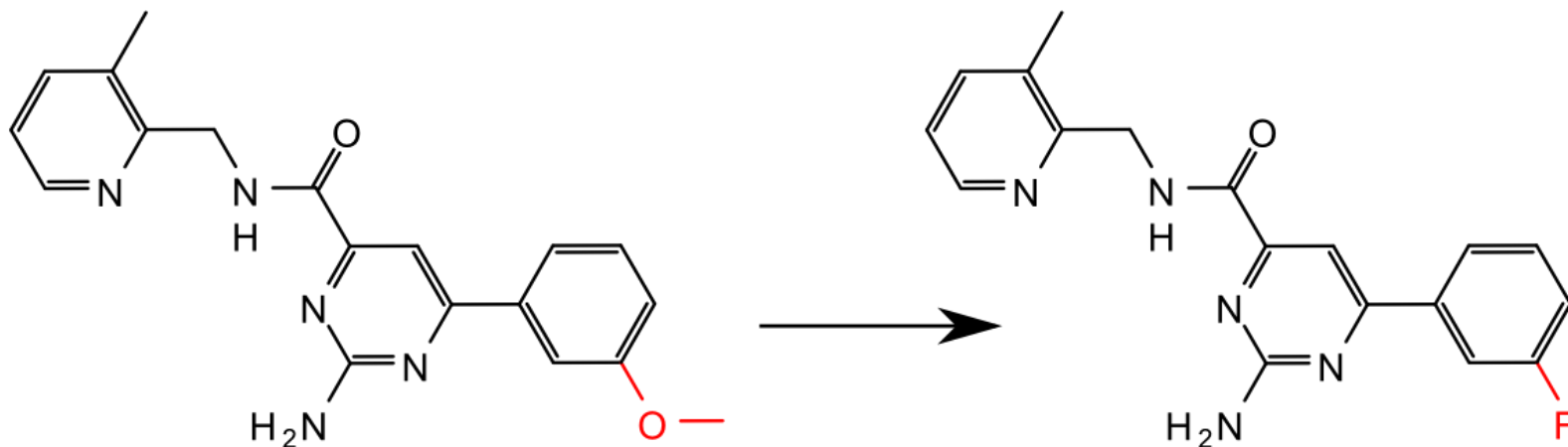
Property changes?

Structure space

Property space

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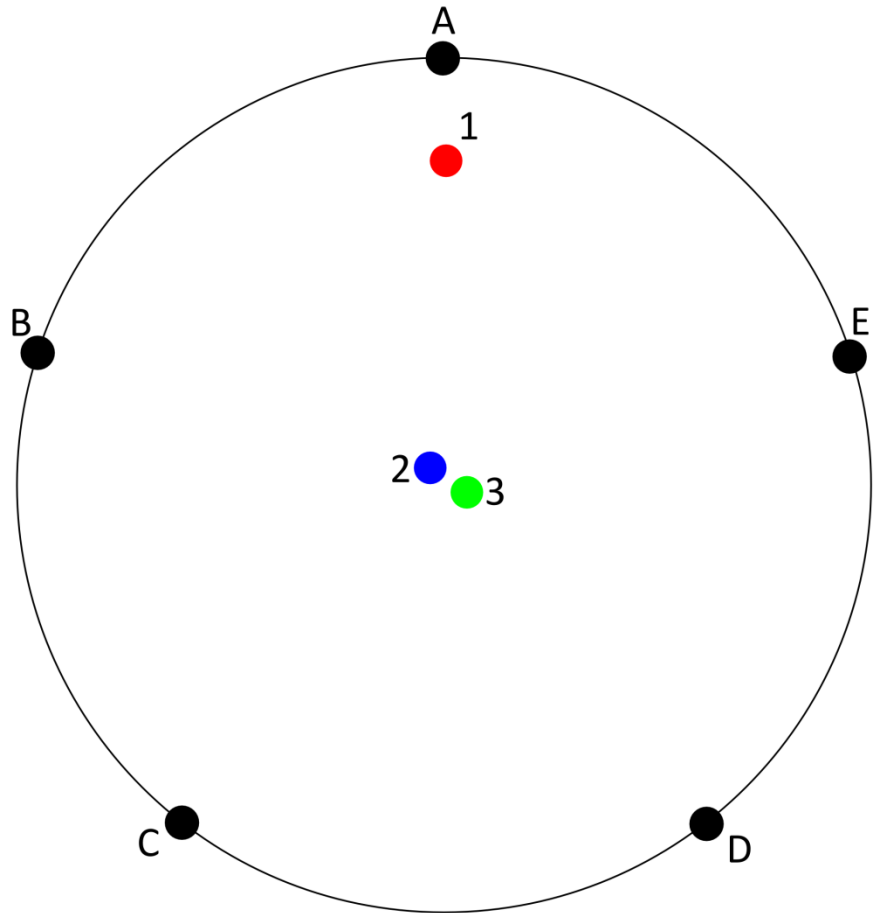www.sheffield.ac.uk/is
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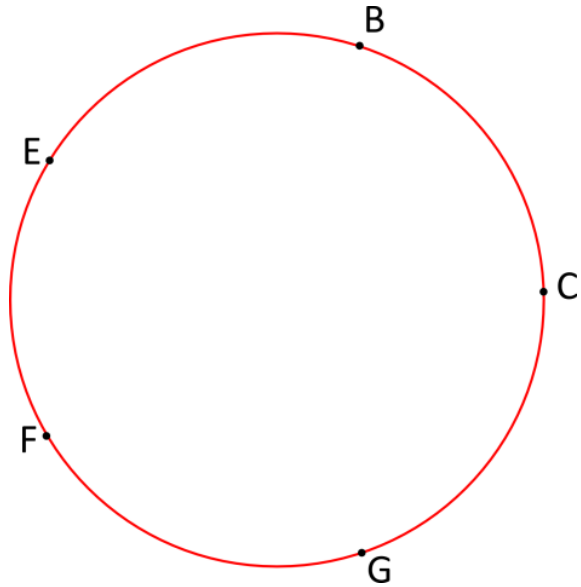University
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Radial coordinates

Features represented as dimensional anchors (A-E)

Position of a data point (1-3) depends on the position of the dimensional anchors and the value of the data point to each anchor
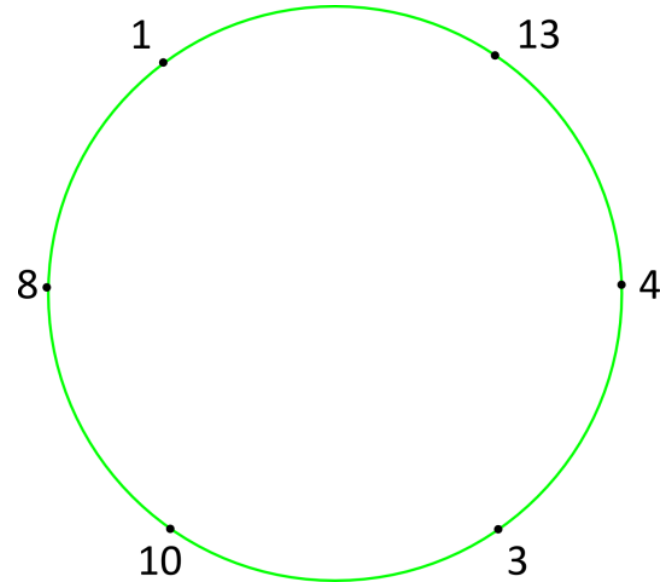
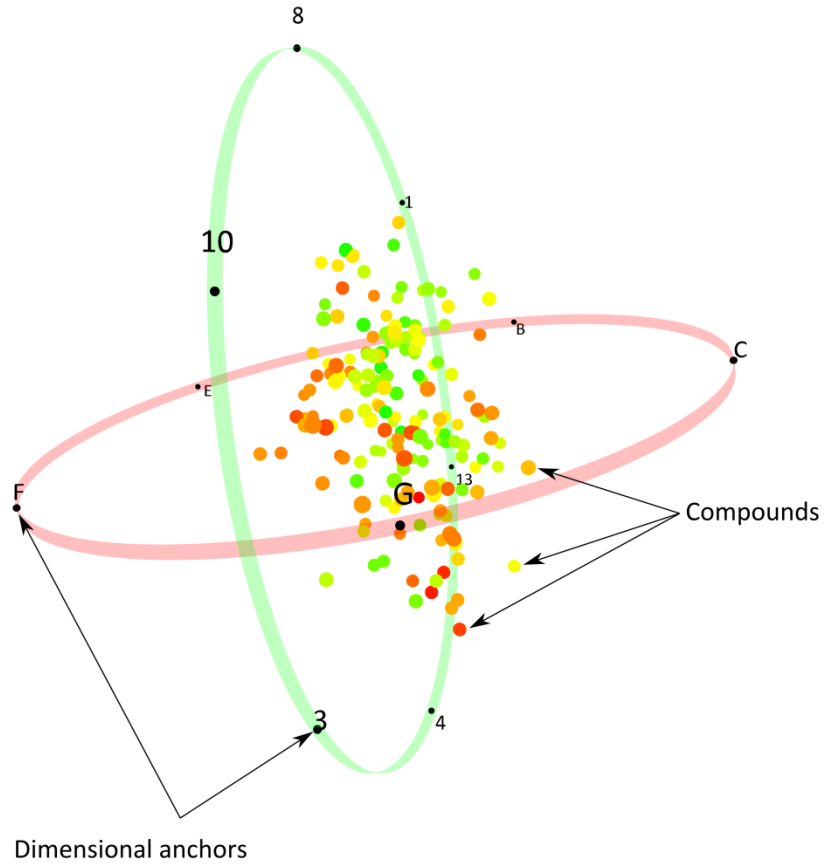Hoffman et al. IEEE Proceedings of Visualization '97, 437-441
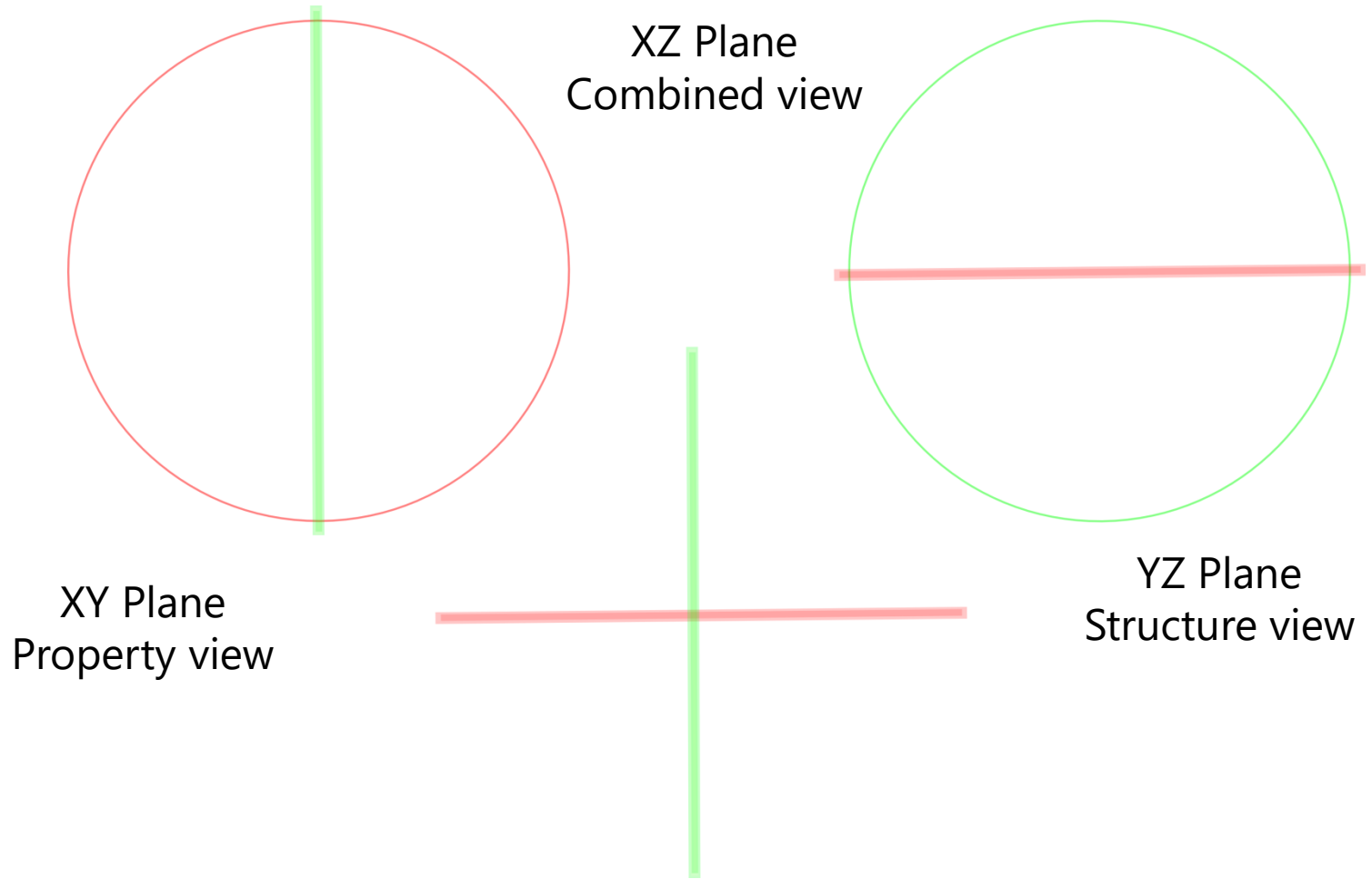
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Visualization generation

Property space

Structure space

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Visualization generation

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Views of the visualization

XZ Plane
Combined view

XY Plane
Property view

YZ Plane
Structure view

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Combined view

Different structure, similar properties

Similar structure,
different properties

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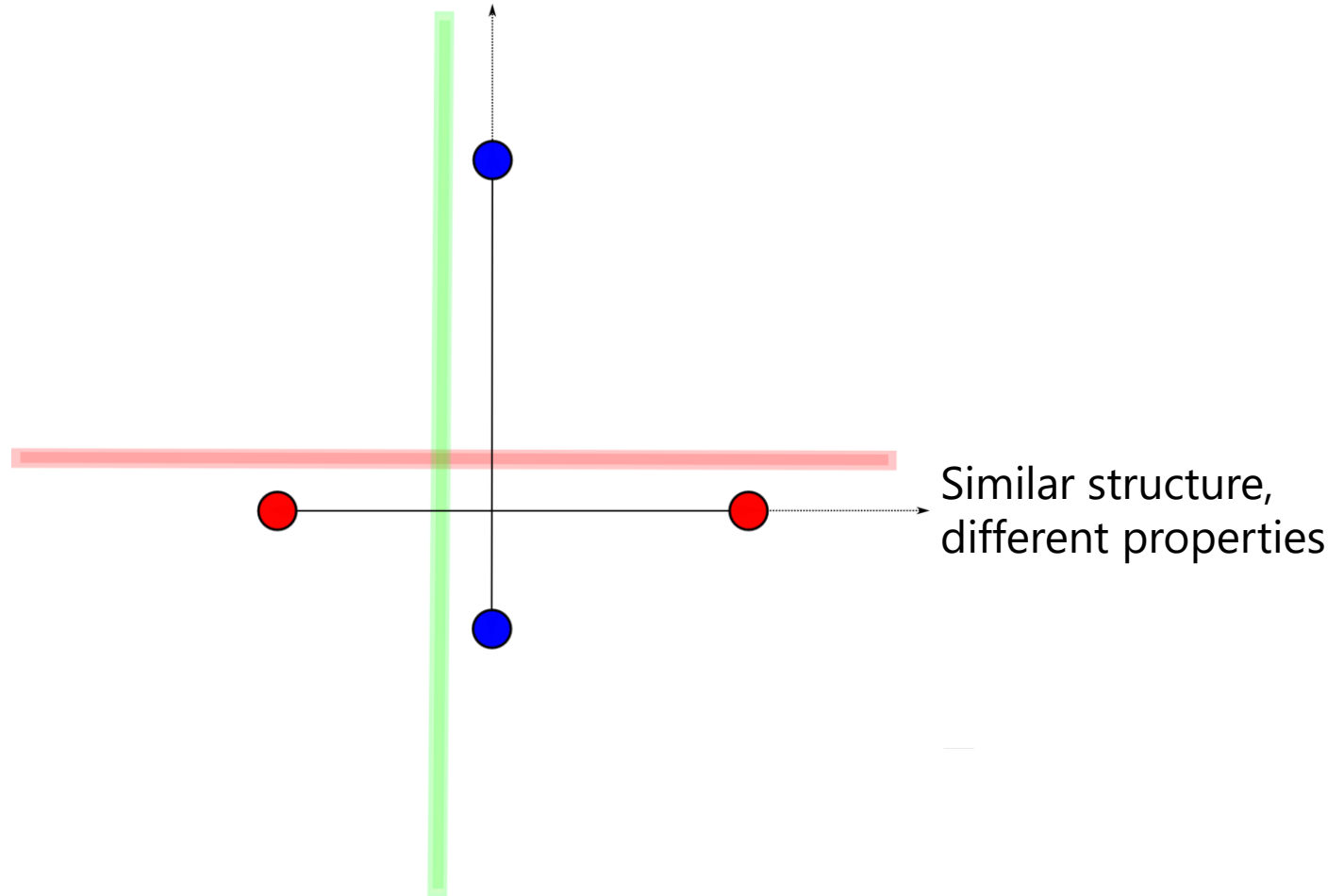
Screenshot of visualization
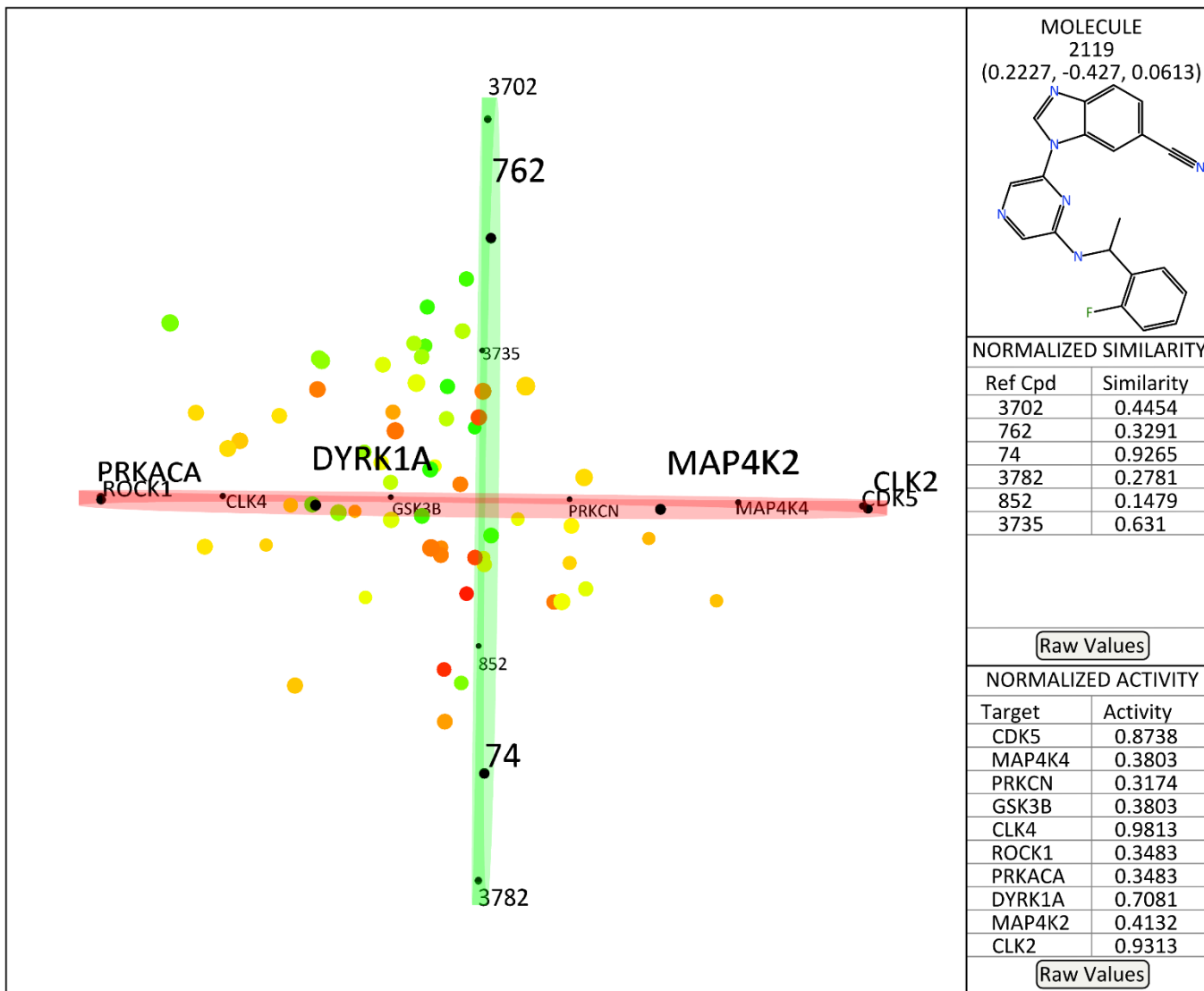
Thanks for your attention