Chemical Space Networks: Application Cases and Future Perspective

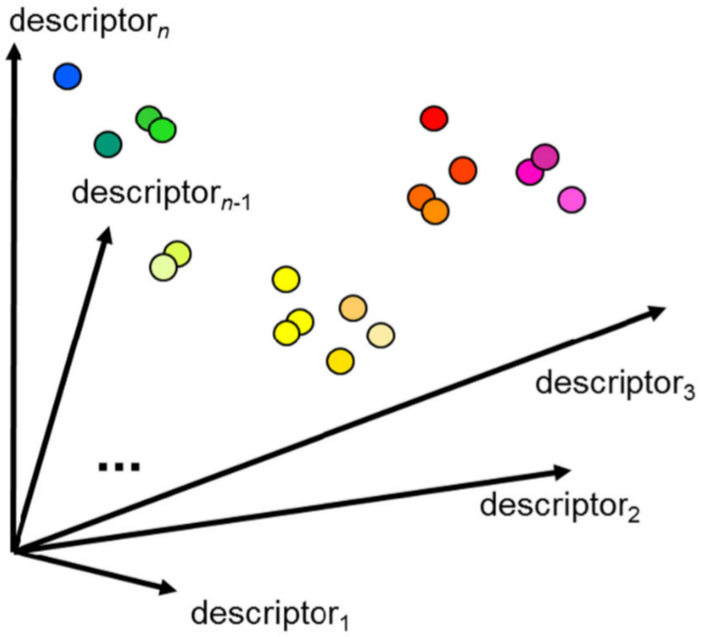
Presented by Aliaksandr Masny

Outline

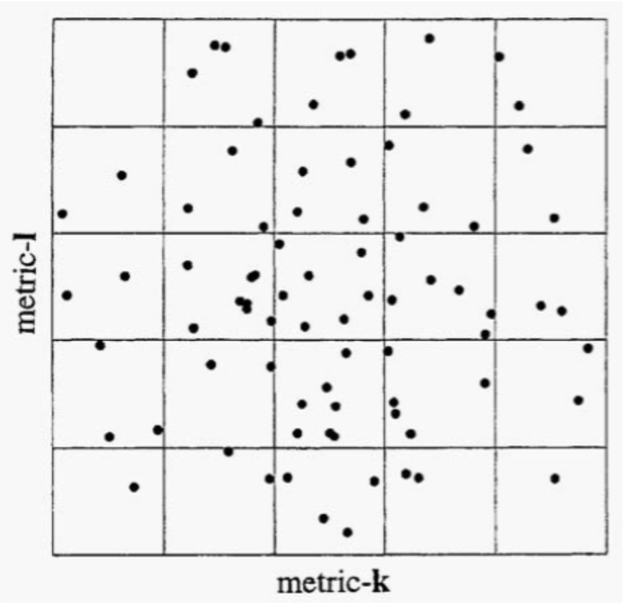
- Chemical Space Representations
- Measures of Similarity
- SAR Applications:
  - Networks
  - Hubs
- Bipartite Networks

Chemical Space Representations

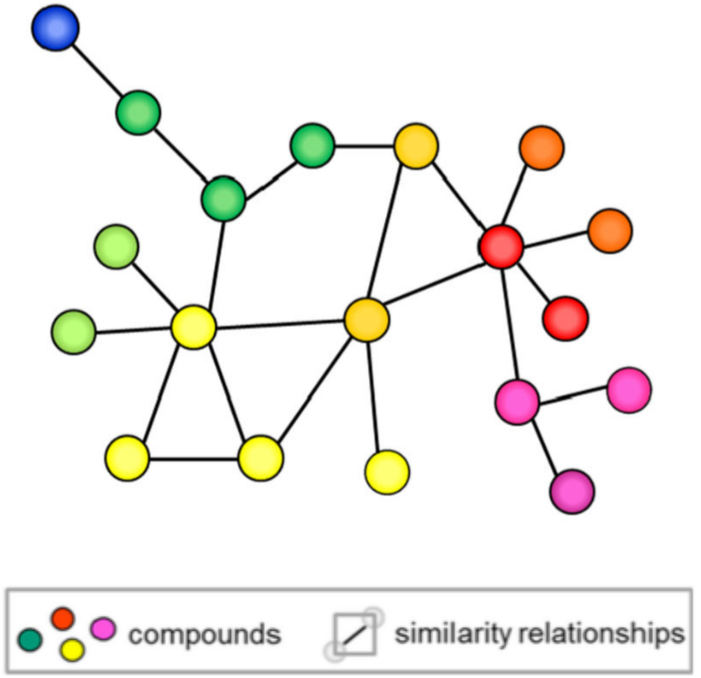
Coordinate-based model



Cell-based model

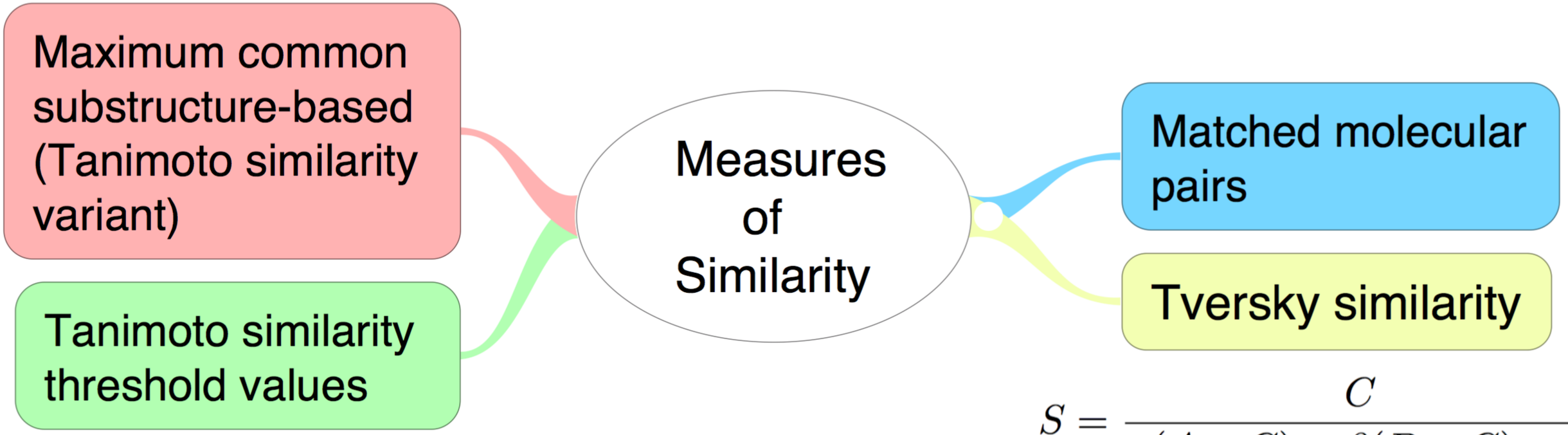


Network-based model



from Vogt, M. et. al., 2016 and Pearlman, R.S. et. al., 2002.

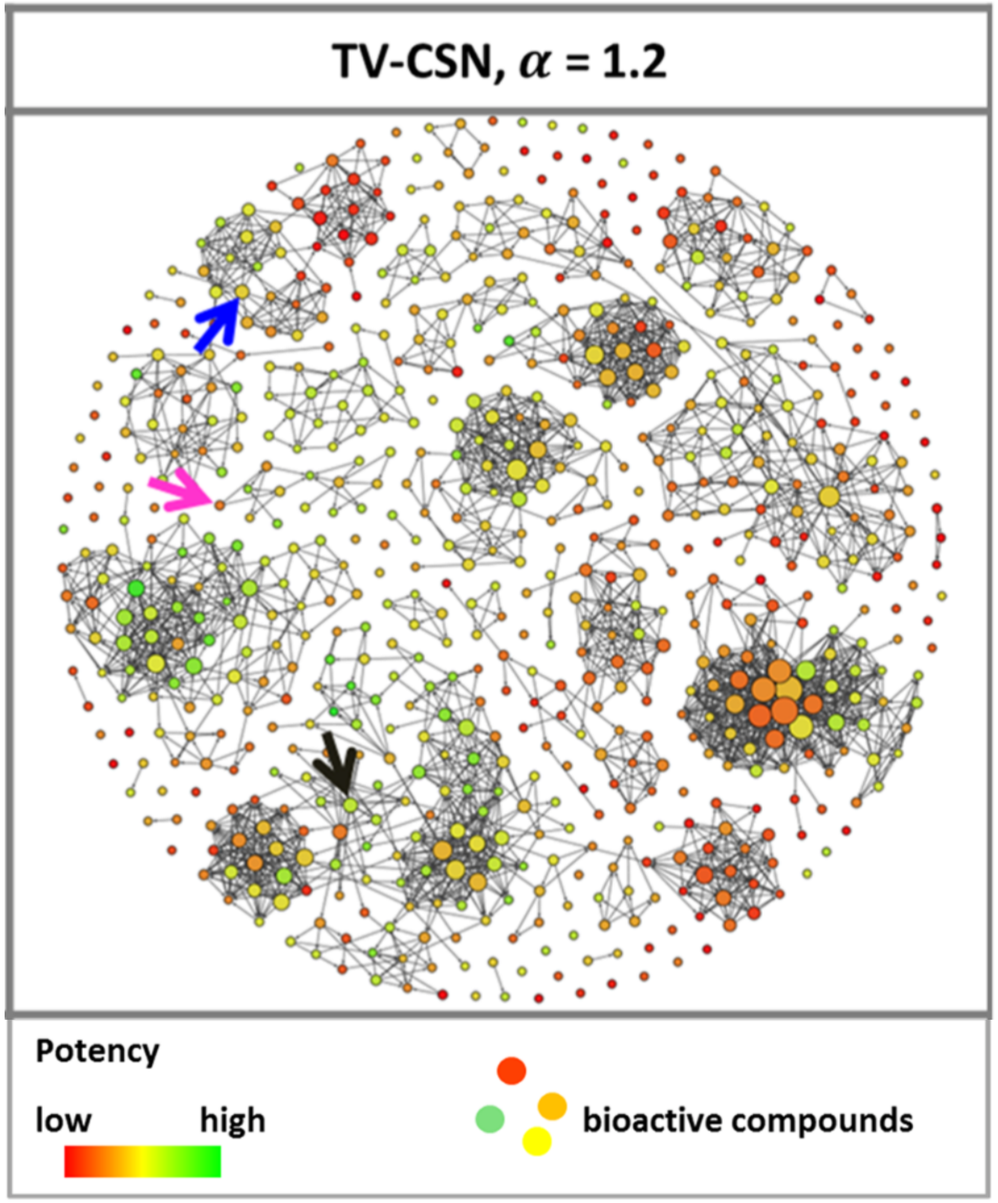
Measures of Similarity



$$S = \frac{C}{A + B - C}$$

$$S = \frac{C}{\alpha(A - C) + \beta(B - C) + C}$$

SAR Applications: Networks

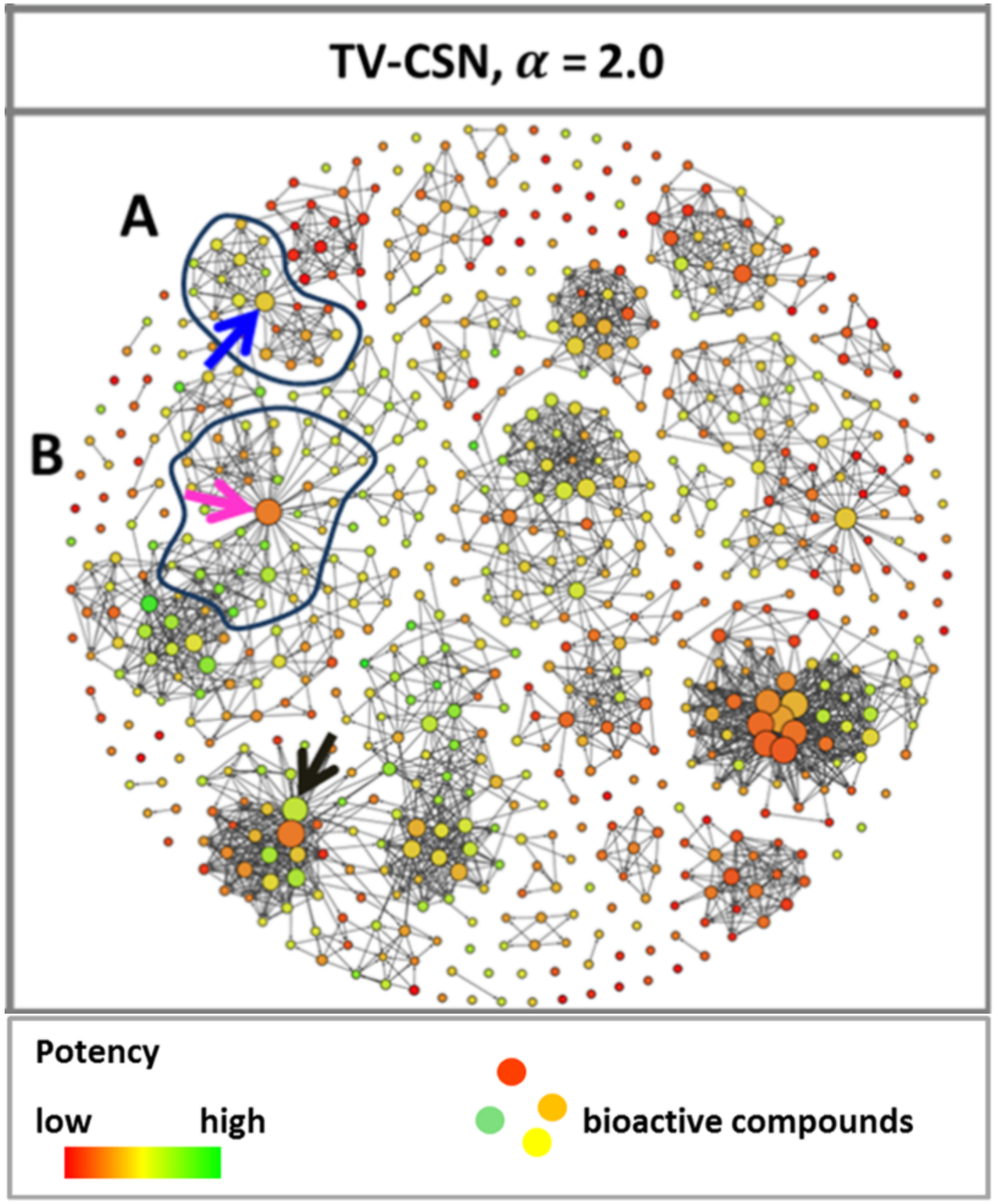


Chemical space networks based on Tversky coefficient (TV-CSN)

α (alpha) can be different

from Vogt, M. et. al., 2016

SAR Applications: Hubs

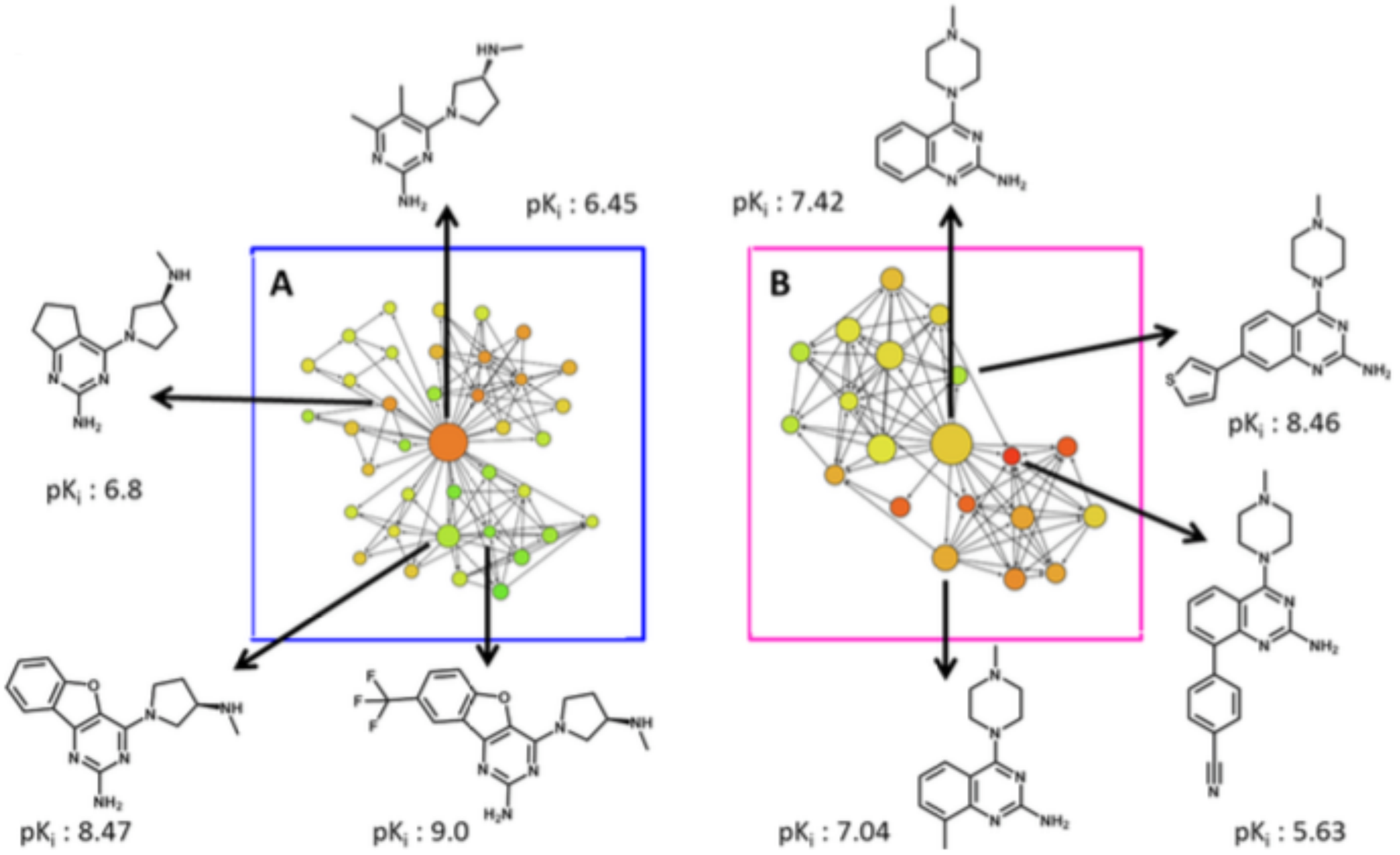


Hub – a node with a lot of connections from other nodes

Hubs become points of interests for SAR analysis

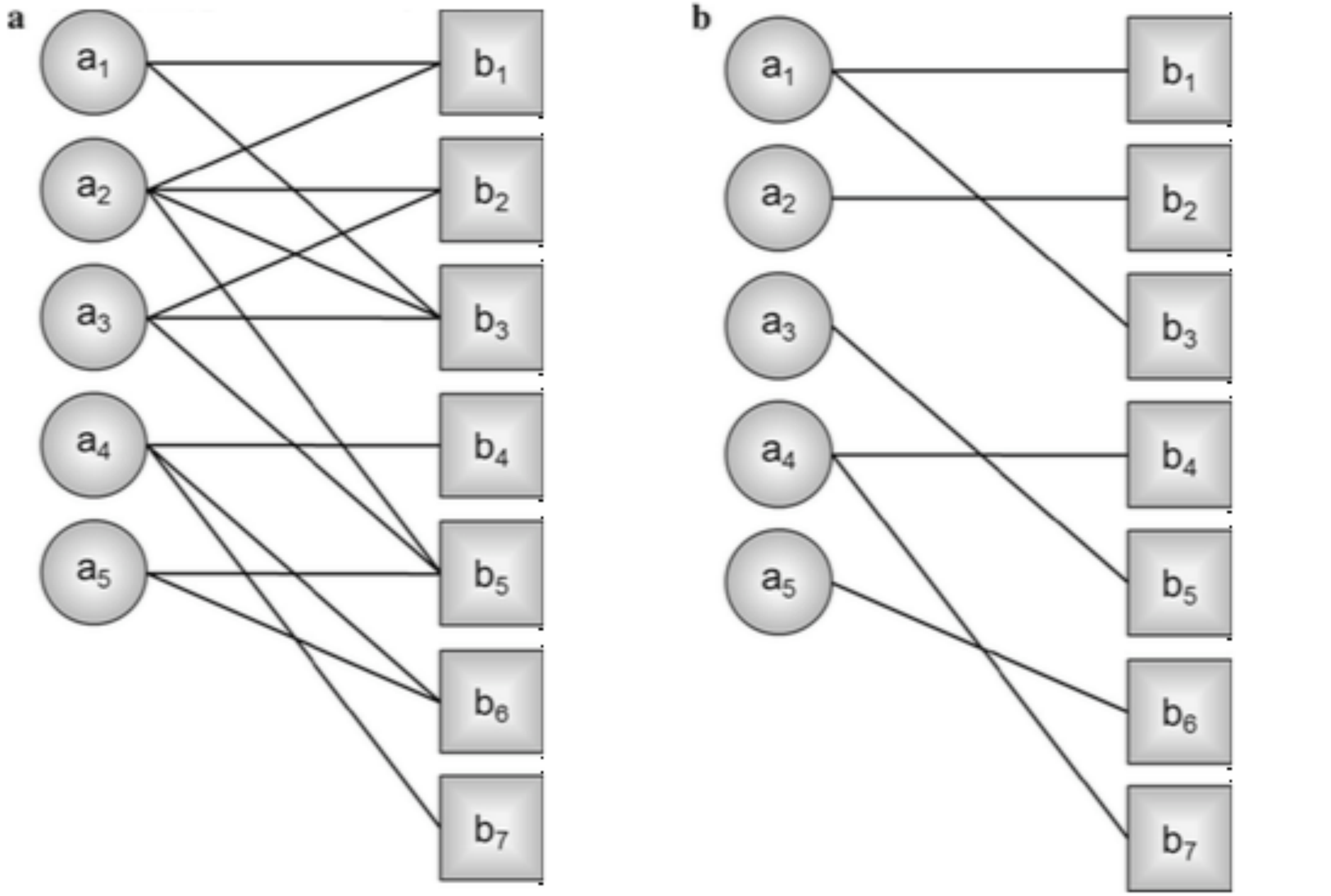
from Vogt, M. et. al., 2016

SAR Applications: Hubs



from Vogt, M. et. al., 2016

Bipartite Networks



Analysis based on mutual information between two sets of compounds

from Vogt, M. et. al., 2016

Conclusions

- Chemical space network as a representation without 'curse of dimensionality'
- Can be used for graphical or statistical analysis of structure-activity relationships (SARs)
- Bipartite network – one more way to analyse compounds sets

References

1. Vogt, M., Stumpfe, D., Maggiora, G. M., & Bajorath, J. (2016). Lessons learned from the design of chemical space networks and opportunities for new applications. Journal of computer-aided molecular design, 30(3), 191-208.

2. Pearlman, Robert S., and K. M. Smith. "Novel software tools for chemical diversity." In *3D QSAR in drug design*, pp. 339-353. Springer Netherlands, 2002.

Thank you
for your attention