

- *Design* low-dimensional reference spaces
- *Simplify* high-dimensional spaces
- *Reduce* their dimensionality

A. Modification and Simplification of chemical spaces

Fingerprints: family of descriptors

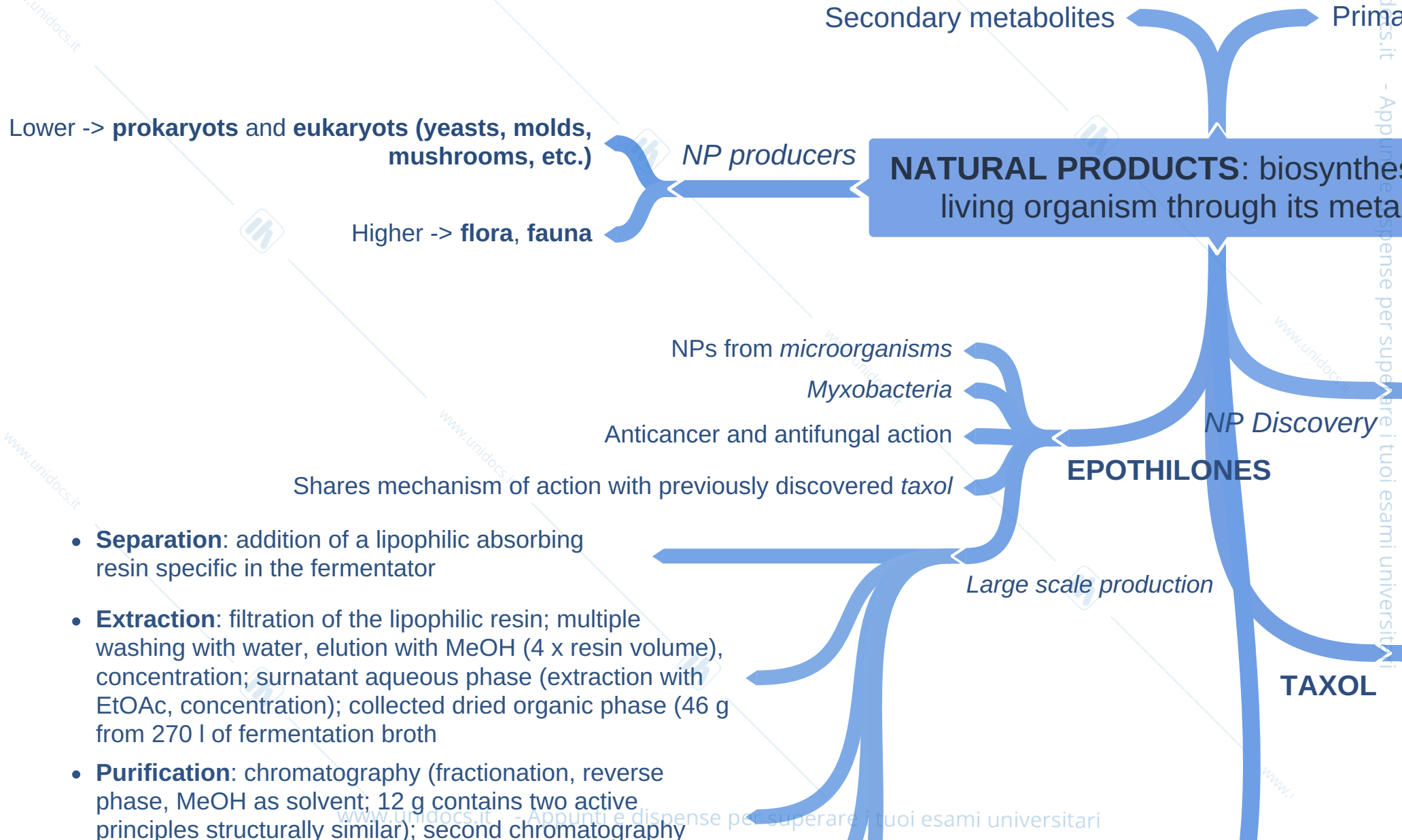
Hybrid
Substructure-based

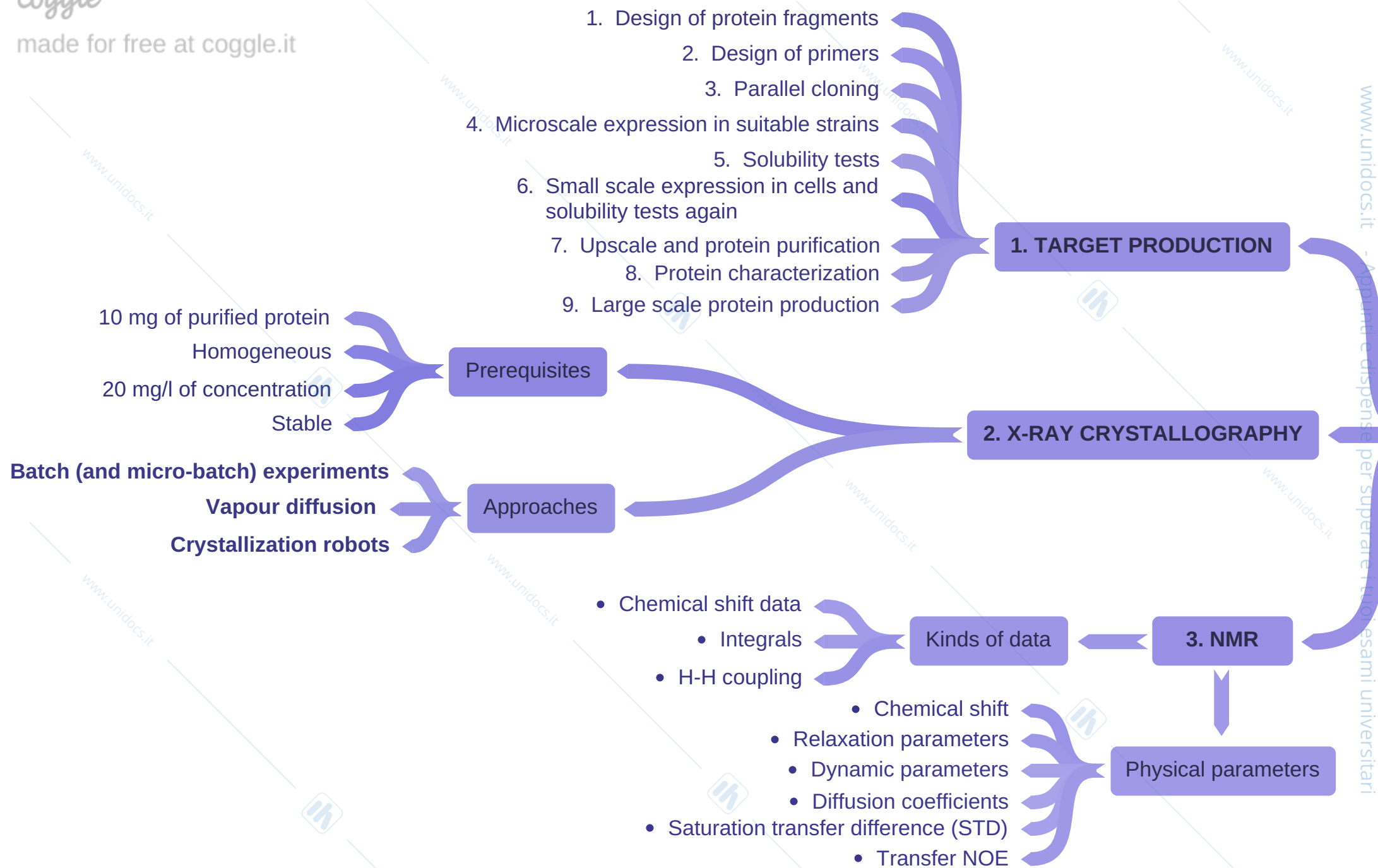
Circular pa
Topology b

**MOLECU
C**

**B. Con
S**

Activity-based sele





X-RAY: no size limit, structure can be very precise