

**Application of  
*in silico* genomic modeling  
in bioremediation processes**

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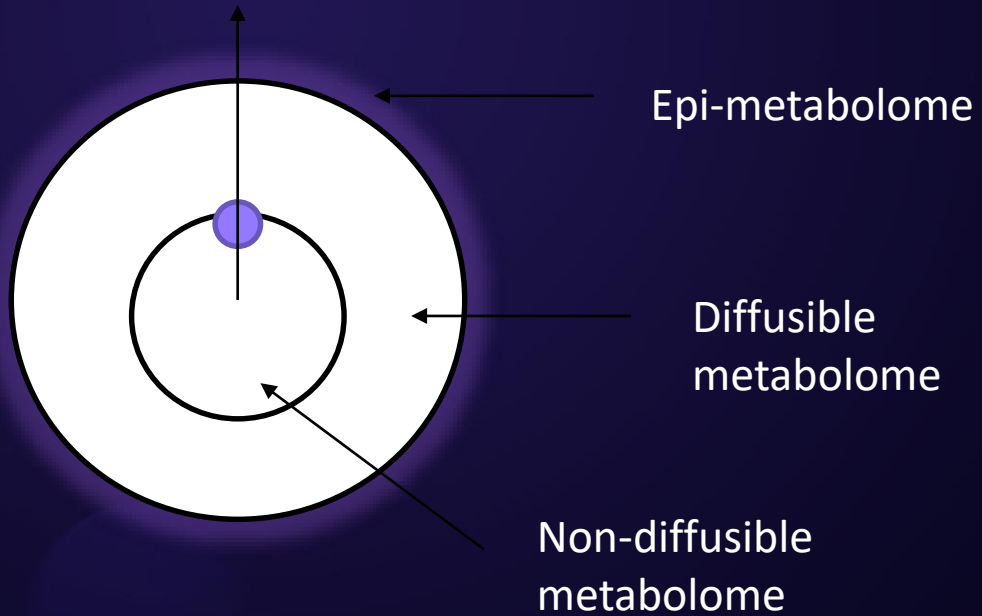
# Biomedication – the essence

- Types of bioremediation:
  - Natural bioremediation;
  - Biostimulation;
  - Bioamplification.
- Defies reductionist approaches

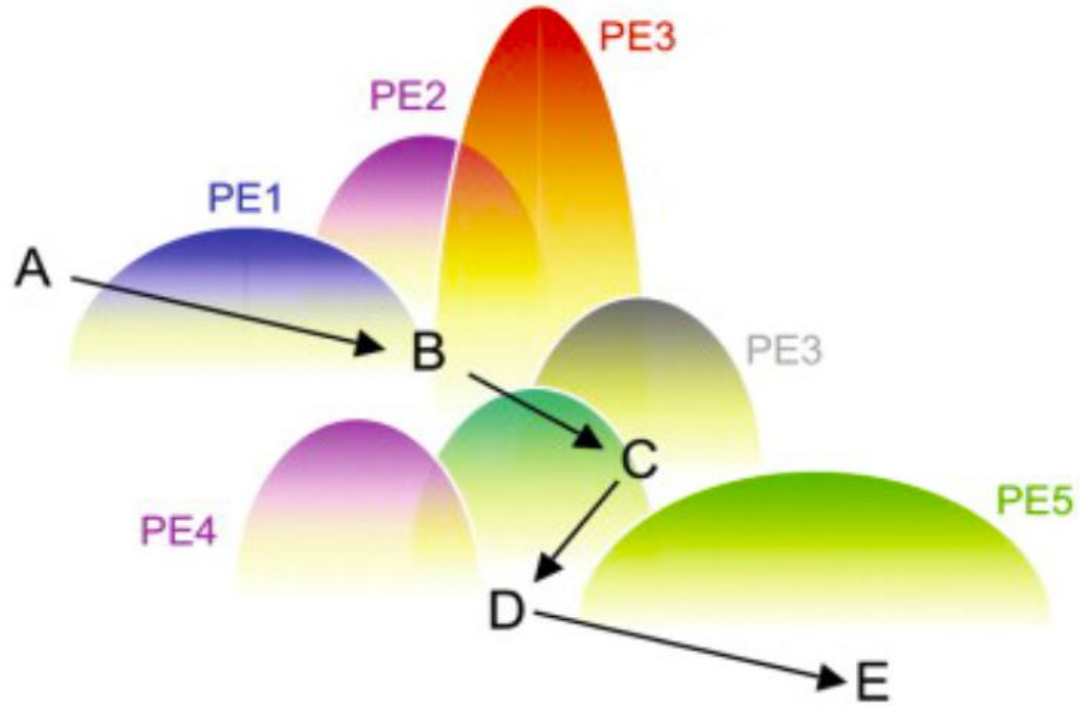
# The genome

- *Pseudomonas putida* – first steps towards cataloging all the components of the bioremediation process;
- Significant are the catabolic activities of the community, not the specific bacterial species ones.

# Epi-metabolome



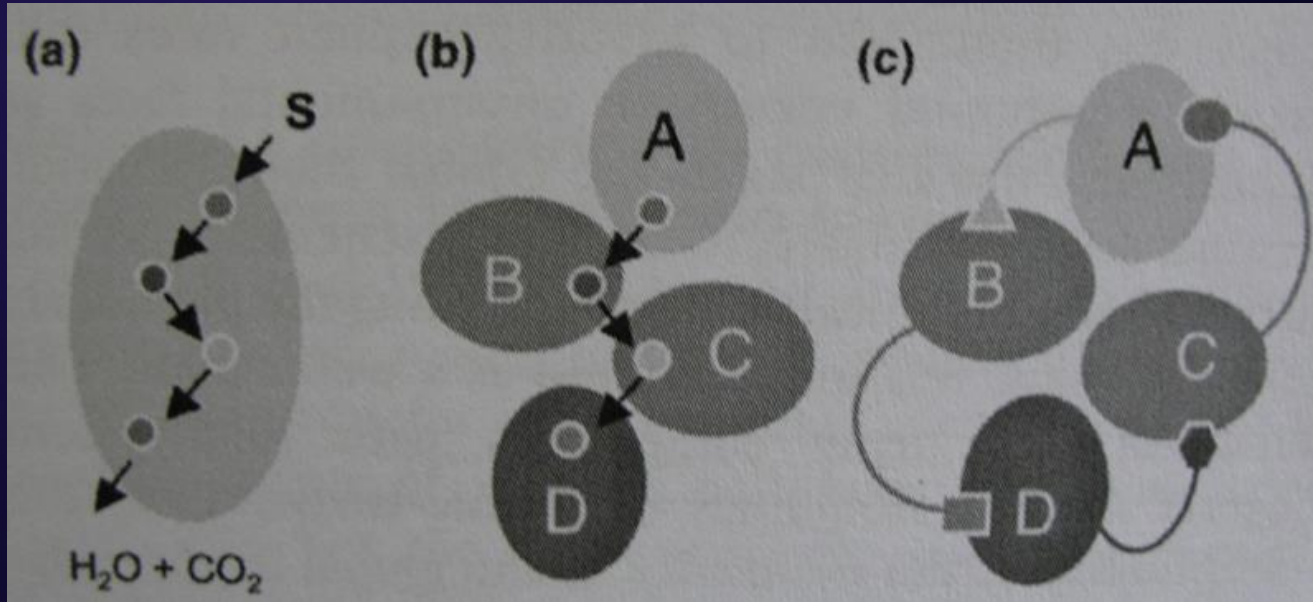
# Pan-enzymes



# *UMBBBD & The Global Biodegradation Network*

- *UMBBBD* - the University of Minnesota database for quantitative microbial transformation studies;
- *The Global Biodegradation Network* - encompasses and gives information on all known reactions that microorganisms can perform.

# *UMBBBD & The Global Biodegradation Network*



# *MetaRouter*

The MetaRouter system allows visualization of all possible paths where a large number of "foreign" chemicals can be transformed using known steps of all reactions taken from the UMBBD.



# Forecasting

- A huge number of new substances are synthesized by industry;
- The enzymatic activities of catabolic pathways affect *discrete molecular motifs* that may be *common* for many substances;
- Focusing on the reactivity of functional groups.

How to maintain a stable modified  
metabolic pathway in bacteria  
released into the environment?

# *Optknock*

- Suggests strategies to eliminate rival-responsive pathways as well as other mechanisms to compensate for the removed functions;
- Most modeling tools are aimed at generating products rather than biodegrading them.

# Applications

- Overexpression of the phytochelatine gene of *Arabidopsis thaliana* in *E. coli*;
- Co-expressions with the Cd-transporter gene;
- Insertion of the *mer* operon of *E. coli* in *Deinococcus geothermalis*;

# Applications

- Improvement of the catalytic capacity and substrate specificity of the enzyme organophosphate hydrolase;
- Translocation of the enzyme to the cell surface.