

# CLASSIFICATION OF QUORUM-SENSING PEPTIDES

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1. Quorum-sensing

2. Quorumpeps®

3. Clustering

4. Conclusions

QUORUM-SENSING:

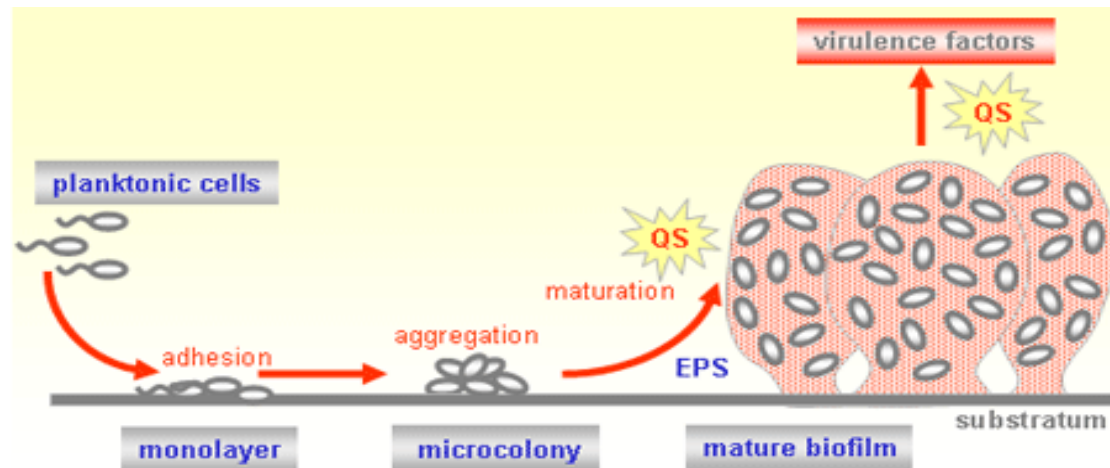
- Cell-cell communication between bacteria

- Regulate gene-expression:

Biofilm formation

Virulence factor secretion

...





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Interesting field:

- Recent evidence of interspecies communication
- Similarity to mammalian signalling pathways
- Peptides: promising group of drug candidates
- Pharmacologic manipulation
  - Receptor targeting

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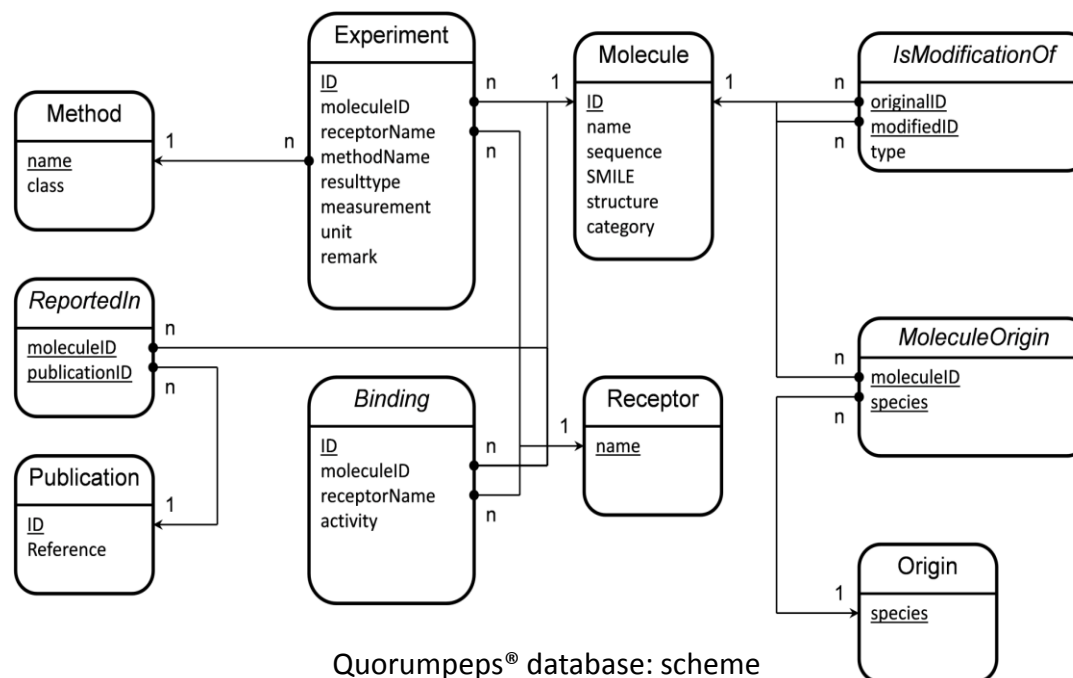
QUORUMPEPS<sup>®</sup> :

- Quorum-sensing peptide database
  - Keeping informed of expanding field
  - Tool to justify peptide choices
- Evaluating biological responses

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N-Acyl homoserine lacton derivatives	Quorum-sensing peptides	Boron-furanone derivatives
62 agonists	190 agonists	7 agonists
103 antagonists	57 antagonists	25 antagonists

(End April 2011)



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## CLUSTERING PEPTIDES:

(1) Primary structure

(2) Secondary structure:

Polak-Ribière conjugate gradient algorithm

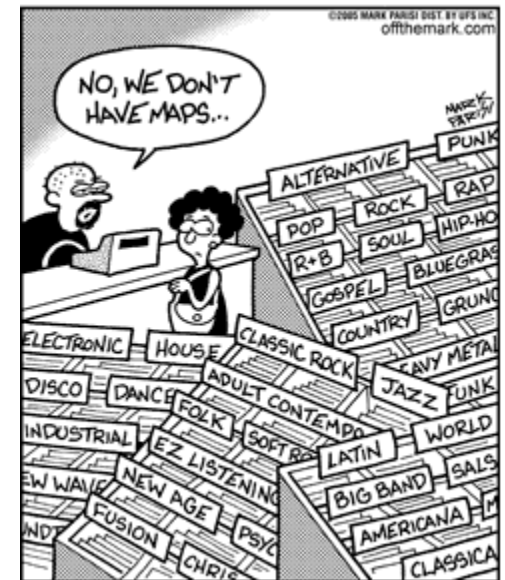
(3) Descriptor calculations:

3233  $\longrightarrow$  1517

(4) Data scaling: transformation

$$z_i = (x_i - \bar{x})/SD$$

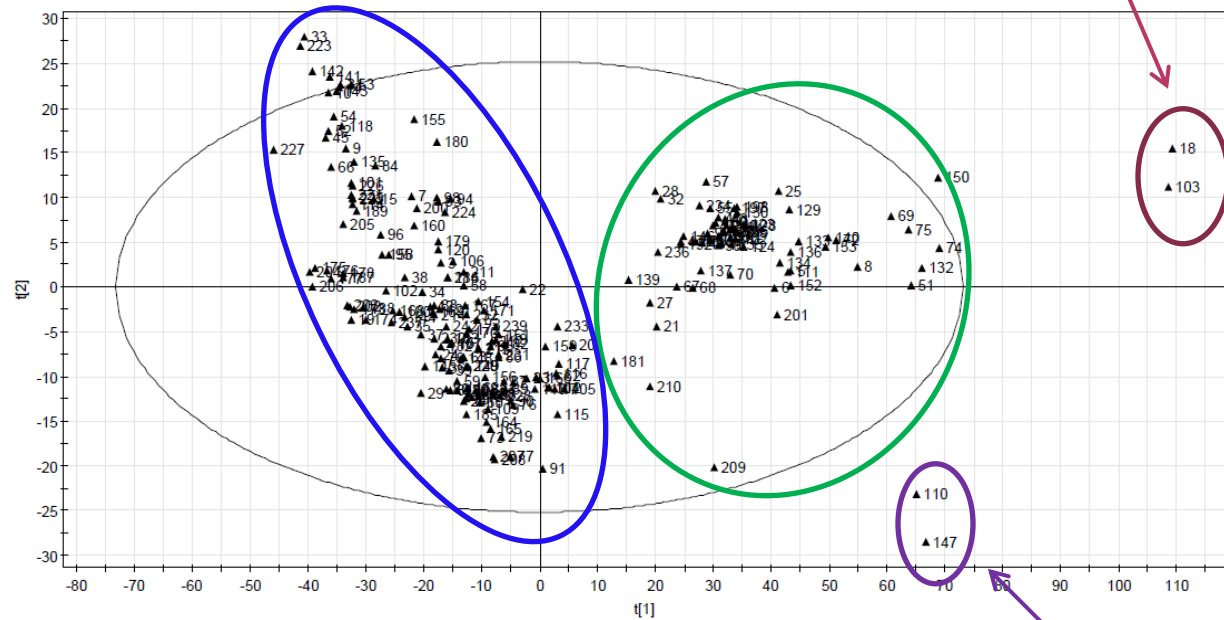
(5) Multivariate analysis: HCA + PCA



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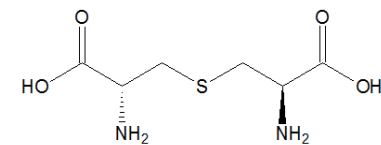
4 main clusters (PCA + HCA):



2 bacteriocins

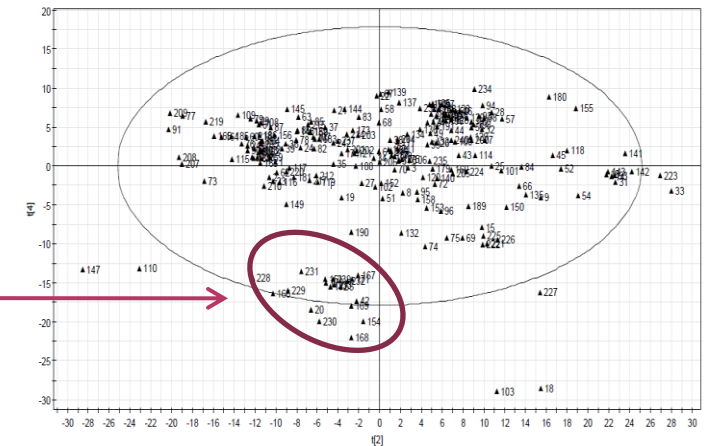
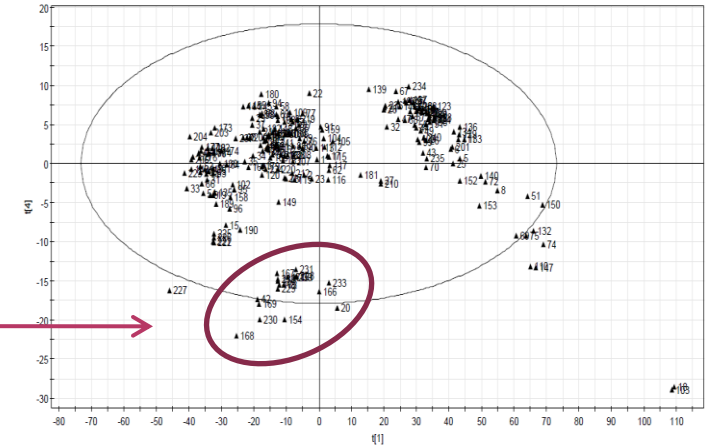
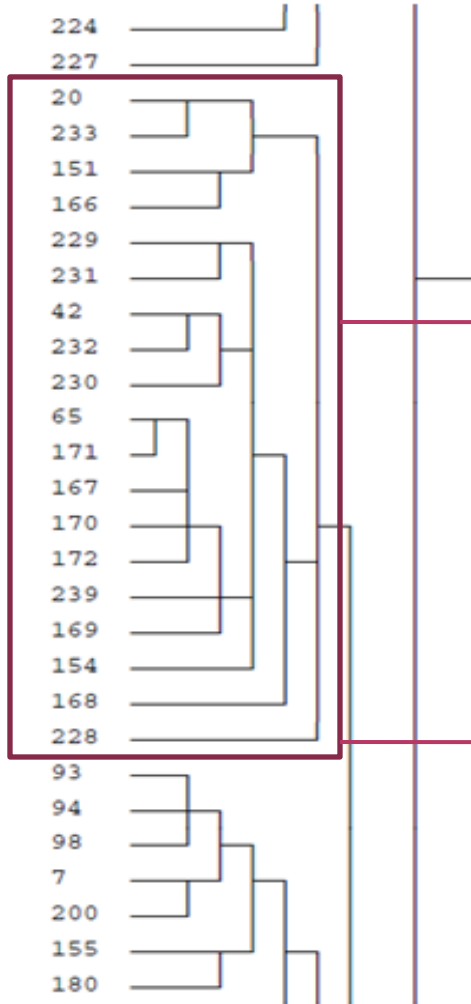
2 lantibiotics

+ subclusters



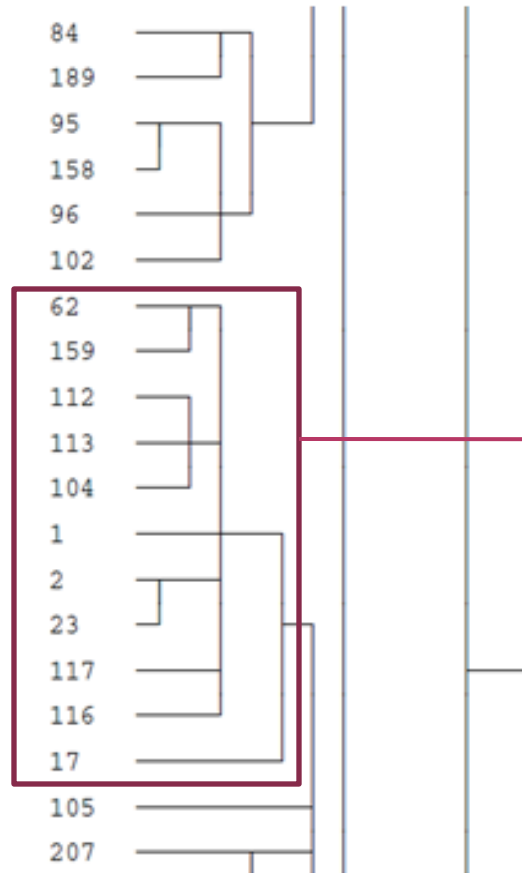


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ComX pheromones,  
produced by Bacillus

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Another cluster...

Gelatinase-biosynthesis-activating pheromone (GBAP # 62) + derivatives

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## CONCLUSIONS:

- Quorumpeps<sup>®</sup>: overview of quorum-sensing molecules

→ Available for researchers

- Clustering:

Chemical similarities

→ Biological coherence

Justification of peptide-choices (model peptides)

→ Biomedical functionality ?

**Thank you for your attention!**

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"PENICILLIN IS CALLED A 'WONDER DRUG' BECAUSE ANY TIME THE DOCTOR WONDERS WHAT YOU'VE GOT, THAT'S WHAT YOU GET."