

# In silico evaluation using molecular descriptors

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# **Organisation**

Name of the organisation Ghent University (UGent)

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**Country** Belgium

Geographical Area Flemish Region

### **SCOPE OF THE METHOD**

The Method relates to	Human health
The Method is situated in	Basic Research
Type of method	In silico

### **DESCRIPTION**

# **Method keywords**

in silico

molecular description
multi-variate analysis
clustering
Scientific area keywords
in silico
chemo-informatics
molecular space
clustering
Method description
Molecules are descripted by hundreds to thousands different descriptors (e.g. molecular weight, pl, log
P,) after which they can be clustered in different classes.
Lab equipment
Computer
Method status
Published in peer reviewed journal
PROS, CONS & FUTURE POTENTIAL
Advantages
No experiments needed, only <i>in silico</i> methods.

REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

References

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Wynendaele E., et al. (2015). Exploring the chemical space of quorum sensing peptides. Biopolymers. 104(5):544-51.

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