

# In silico evaluation using molecular descriptors

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## SCOPE OF THE METHOD

<b>The Method relates to</b>	Human health
<b>The Method is situated in</b>	Basic Research
<b>Type of method</b>	In silico
<b>This method makes use of</b>	Animal derived cells / tissues / organs

## 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 described by hundreds to thousands different descriptors (e.g.

molecular weight, pI, 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 *in silico* methods.

## REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

### References

Taeavernier L., et al. (2017). Chemical Classification of Cyclic Depsipeptides. *Curr Protein Pept Sci.* 18(5):425-452.

Gevaert B., et al. (2016). Exploration of the Medicinal Peptide Space. *Protein Pept Lett.* 23(4):324-35.

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

### Associated documents

## PARTNERS AND COLLABORATIONS

### Organisation

**Name of the organisation** Ghent University

**Department** Pharmaceutical analysis

**Country** Belgium

**Geographical Area** Flemish Region

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