# In silico evaluation using molecular descriptors

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### Organisation

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**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, 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

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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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