

In silico evaluation using molecular descriptors

Created on: 10-10-2019 - Last modified on: 08-11-2019

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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 described 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 *in silico* methods.

REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

References

Taevernier 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.

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