In silico evaluation using molecular descriptors

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Organisation

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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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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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