About the Natural-Product-Likeness Scorer

The **Natural-Product-Likeness Scorer** [1] was developed by Kalai Vanii Jayaseelan (Contact: kalai@ebi.ac.uk), Andreas Truszkowski, Pablo Moreno, Peter Ertl and Christoph Steinbeck to provide an open-source, open-data re-implementation of Peter Ertl's previous work [2].
Ertl originally developed this based on a close-data training set of natural products to screen large compound libraries for natural product likeness in drug designing studies. Our re-implemented NP-likeness scorer is using open source and open data to validate natural product likeness based on now publicly available sets of natural products described in [1]

The entire implementation is made as easy to use work-flows using CDK_Taverna2 an open source plug-in for Taverna-2.2 which is an open source work-flow management system.

- **Taverna**: http://www.taverna.org.uk/download/
- CDK-Taverna plugin for Taverna: http://www.ts-concepts.de/cdk-taverna2/plugin/
- The **NPLikenessScorer-1.4.1.jar** is a standalone Java ARchive offering the functionality similar to the taverna workflows found here http://www.myexperiment.org/packs/183.html.

Usage:
Input [Options] [Targets] for the application are specified below.
usage:

Natural Product-likeness calculator v-1.4.1 calculates natural product-likeness of small molecules based on open-data of natural products. Input [Options] [Targets] for the application are specified below.

-help	Usage information
-in	Input SDFile
-out	Output SDFile
-outFragments	Output .txt file for reconstructed fragments. Specify only if 'reconstructFragments' is true.
-reconstructFragments	Optional boolean argument {true/false} to reconstruct fragments. If true fragments;scores are written out in SMILES format.
-v	Application info

If output file options (out/outFragments) are unspecified, auto generated output files will be written to the directory of the input file.

References:

[1] KV Jayaseelan, C Steinbeck, P Moreno, A Truszkowski, P Ertl, Natural product-likeness score revisited: an open-source, open-data implementation, *BMC Bioinformatics* 2012, **13**:106
http://www.biomedcentral.com/1471-2105/13/106/abstract

[2] P Ertl, S Roggo, and A Schuffenhauer, Natural product-likeness score and its application for prioritization of compound libraries., *J. Chem. Inf. Model*, 2008 vol. 48 (1) pp. 68-74
http://www.ncbi.nlm.nih.gov/pubmed/18034468