

**Understanding & Probing [ Orvil Perl Library+AI::MXNet - Perl interface to MXNet Machine Learning Library ] in the Context of Bio-Chemical Information Systems Framework w.r.t R&D of Drug Design Aspects – An Interesting Insight into Perl Interfacing Concepts & Anticipatory Chemical Computing Paradigms.**

[ Understanding 'Scaffold Hopping' from Chemical Computing & ML View Point ]  
[ AI::MXNet - Perl interface to MXNet machine learning library ]

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**[I] Inspiration & Introduction :**

“Computational scaffold hopping: cornerstone for the future of drug design” ? -

Published Online:9 May 2017,<https://doi.org/10.4155/fmc-2017-0043> - Jürgen Bajorath.

“Rapid construction of virtual combinatorial library is a prerequisite for in silico library enumeration and design. Organic Virtual Library (ORVIL) is a perl programme to generate a combinatorial library using most frequently observed 200 organic substituents. It is designed to explore the organic chemical space in the given query structure without affecting the entire backbone of the molecule enabling minimum molecular complexities. Its particular features are its simplicity to use, portable SMILES format and high speed of library construction. Benchmarking of Tamoxifen (drug for breast cancer) was performed which revealed a compound having similar architecture of known drug analogue, Toremifene. “ [ **Source : Please see the link below** ] -

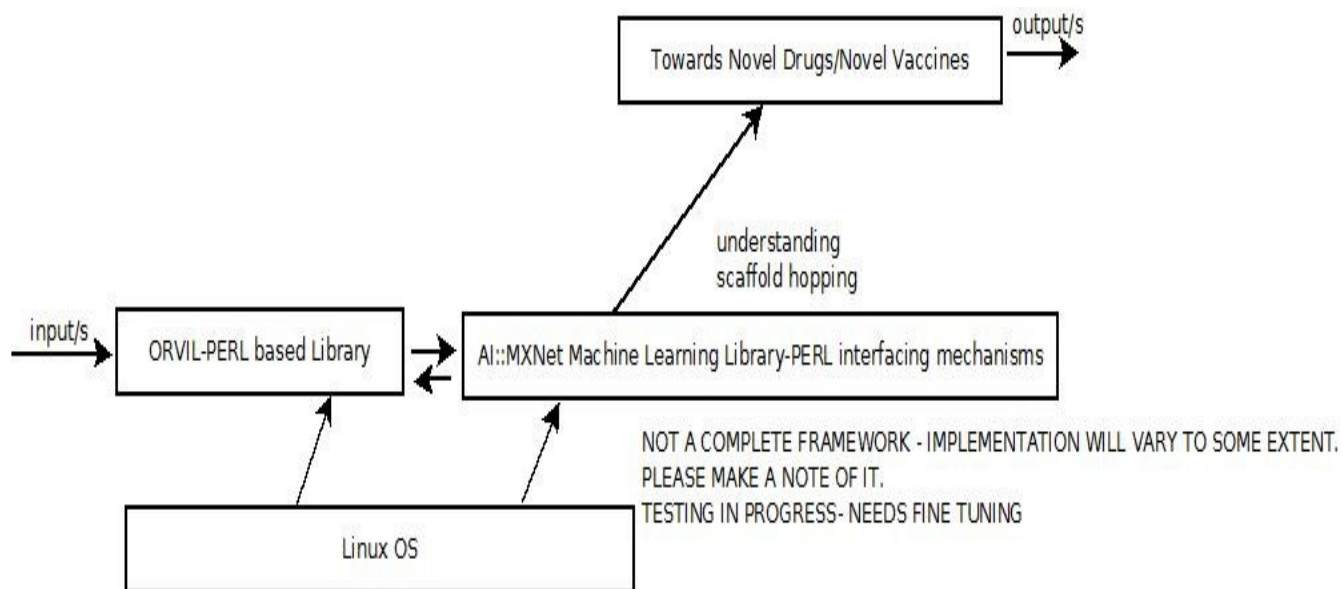
“Organic Virtual Library (ORVIL) – A Combinatorial Library Construction based on Organic Constituents and without Scaffold Hopping”. August 2011. DOI: 10.5958/j.0975-8070.2.2.012

“Toremifene, sold under the brand name Fareston among others, is a medication which is used in the treatment of [advanced breast cancer](#) in [postmenopausal](#) women.[\[5\]\[6\]\[3\]](#) It is taken [by mouth](#).[\[5\]](#)”

[ **Source : <https://en.wikipedia.org/wiki/Toremifene>** ]

**\*\*\* We need not write about the importance of Perl and Machine Learning Concepts in Chemical Computing/Bio-informatics R&D domains as there is lot of published scientific literature already available.**

### [II] Drug Design/Vaccine Design Informatics Framework Implementation :



A Simple Suggestion Explaining Our R&D Concept of Drug Design/Vaccine Applications  
Please Check & Satisfy Yourself  
Thanks - Dr.Nirmal

[ Chemical Computing Paradigms - Towards better Drug Designs Using PERL-MACHINE LEARNING CONCEPTS & TECHNIQUES ]

**[ Figure I – Our Total Idea – Only Partial Implementation of our Anticipatory Chemical Informatics Framework is Shown here. Actual implementation will vary – Please Check. ]**

<https://www.quora.com/I-am-good-at-Perl-and-machine-learning-To-become-a-data-scientist-is-it-compulsary-to-learn-Java-or-python>

<https://metacpan.org/pod/AI::MXNet#DESCRIPTION>

<https://metacpan.org/pod/Paws::MachineLearning>

<https://metacpan.org/pod/AI::MXNet>

<https://history.nih.gov/exhibits/genetics/sect3b.htm>

## For more info about the MNIST problem please refer to

L<<http://neuralnetworksanddeeplearning.com/chap1.html>>

[https://www.reddit.com/.../perl/.../machine\\_learning\\_book\\_for\\_perl\\_programmer/](https://www.reddit.com/.../perl/.../machine_learning_book_for_perl_programmer/)

<https://eswi.org/.../difference-between-vaccines-antivirals-and-antibiotics/>

<https://isoponline.org/wp.../Differences-on-drugs-and-vaccines.pdf>

<https://www.fda.gov/vaccines-blood-biologics/vaccines>

<https://www.futuremedicine.com/doi/abs/10.2217/fmb.10.168>  
<https://stm.sciencemag.org/content/2/50/50rv3.full>  
<https://www.pharmaceutical-journal.com/...vaccines-and-drug.../11050937>. article  
<https://www.eurekaselect.com/.../current-challenges-in-the-development-of- vaccines-and-drugs-against-emerging-vector-borne-diseases>  
[https://www.perlmonks.org/?node\\_id=1204349](https://www.perlmonks.org/?node_id=1204349) – *Machine Learning*

**\*\*\* [ *Future Extension/s With Ruby/Jruby -for IoT/HPC Heterogeneous Computing Environments is feasible/possible. Ruby - Perl interface to Ruby interpreter - RubyML Framework* ]**

Please see the references/links below for your own R&D :

<https://metacpan.org/pod/distribution/Ruby/lib/Ruby.pod>  
<https://metacpan.org/release/Ruby>

<http://vixra.org/abs/1906.0062> – *for information on Ruby based Machine Learning concepts.*  
<https://awesome-ruby.com/>  
[rubyml.org/](http://rubyml.org/)

<https://gist.github.com/gbuesing/865b814d312f46775cda>  
<https://www.mo-data.com/a-curated-list-of-awesome-machine-learning- frameworks-libraries-and- software/>  
<https://github.com/arbox/machine-learning-with-ruby>

### **[III] Acknowledgment/s :**

*The author has no relevant financial involvement with the subject matter or materials discussed in the manuscript. Non-Profit Academic R&D. Non Commercial Research.*

### **[IV] References + [ Information on Mathematics & Software Used/Useful ] :**

[a] <http://vixra.org/abs/1805.0120>

[b] <http://vixra.org/abs/1901.0027>

[c] <http://vixra.org/abs/1806.0075>

[d] <http://vixra.org/abs/1905.0186>

[e] <http://vixra.org/abs/1901.0157>

[f] <http://vixra.org/abs/1901.0177>

[g] [http://vixra.org/author/dnt\\_kumar](http://vixra.org/author/dnt_kumar)

[h] <http://vixra.org/abs/1903.0204>

**[ THE END ]**