



Journal of Applicable Chemistry

2015, 4 (1): 1-98

(International Peer Reviewed Journal)



Focused information Reviews (Foc.Inf.Rev., FIR)

OmniMetrics

Part I: Applications of neural networks (Ma_NN) in Medicinometrics and pharmacometrics

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Accepted on 14th January 2015

(Dedicated with profound respects to Dr. S Brahmaji Rao, former professor of chemistry, SKD university, Ananthapur, AP, during on his *sahasra chandra darsanam* (thousand lunar months of life on the lap of mother earth))

ABSTRACT

The sub goals of medicine are diagnosis of a disease, treatment with pharmaceutical preparations/ surgery/intervention and probing into adverse drug effects on treated patients. The confidence in detection of cancer and discrimination from healthy individuals, onset of diabetes, diagnosis of HIV-AIDS, coronary diseases and hypertension are improved with NNs compared to model driven approaches. The prediction of colon cancer from metal ion concentration with NNs is better than even nonlinear-regression procedures. Survival analysis and clinical information of ICU patients improved with NNs. The pharmaceutical research is an iterative cyclic activity of discovering new drug like molecules, phase I to phase III clinical trials, approval, manufacture, quality control and modifying/ looking for new moieties. Both of these disciplines are inter- /intra- disciplinary with diverse paradigms. These sciences in loose/fused hybridization with metrics (information/mathematical/ statistical/ fuzzy/nature inspired protocols/ software/hardware/ robotics/ hyphenated instruments) are state-of-art- medicinoMetrics and pharamcometrics, qualimetrics, with a single ultimate goal of Pareto optimal human health from fetes stage to dot age. Neural networks (NNs), data driven computational second generation intelligent models entered pharmaceutical research and medical diagnosis in 1990s, and are now indispensable information tools. In different phases of product development like experimental design for operating conditions of a process, calibration of two or more compounds simultaneously, prediction of the drug in vivo, in vitro and prediction of dose in control drug design systems, NNs alone or in binary/ternary hybrid mode with other methods is laudable in routine laboratory/industry. Rational drug design (RDD) is more scientific in pruning biochemical/molecular descriptors to arrive at a drug compared to blind fold approaches of synthesis-test-modify cycles. In

different stages of drug development like probing into ADME(Tox), drug likeliness, drug activity, toxicity of a compound/metabolites, adverse effects of drugs, high throughput screening (HTS) and virtual libraries, the role of NNs is impressive. Selection of a compound for a drug, optimum safe limits of the dose, toxicity of a compound etc. are not only interwoven complicated procedures, but also inverse problems. It has been realized that modelling from first principles is not viable, in spite of noteworthy progress in the mechanistic/biochemical models for many of the micro-processes. Intestinal absorption, blood brain barrier (BBB), equilibria of drugs with DNA/active site are complex, but modelling and prediction using NNs do not collapse even with less/ distorted/ redundant/ sparse/ conflicting information. Structure activity/response relationship (SXR) with NN for physico-chemical properties, biological activity, and response to skin/eye irritants pave way to predict the behavior of a compound before synthesis and to develop hierarchical models.

Keywords: Medicinometrics, Pharmacometrics, Artificial Intelligence, Neural network models, Data driven models, Medical diagnosis, Treatment, Surgery, Intensive Care Unit, Non-invasive approach, Supportive tool, Machine-expert-assistant.
