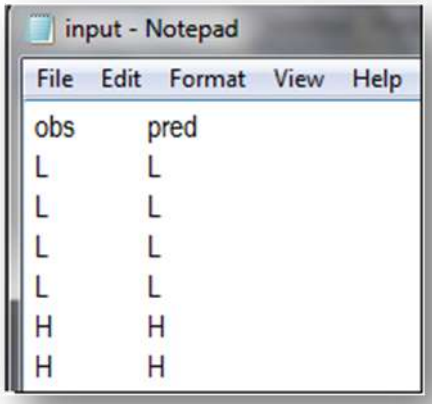
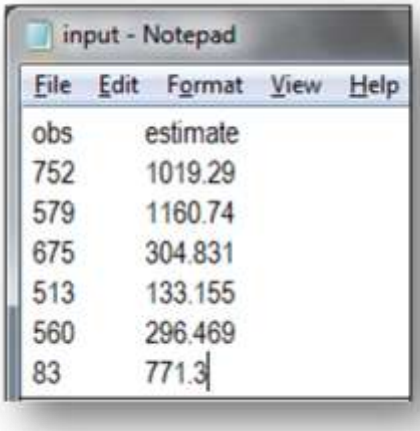
Single Program for determining qualitative validation parameters for both Linear discriminant analysis (LDA) and Pharmacophore model

1. This program calculates qualitative validation parameters for LDA and pharmacophore analysis such as *sensitivity, specificity, accuracy, precision, F measure, Matthews correlation coefficient (MCC), Geometric means (Gmeans), Cohen's kappa, Guner Henry score and Recall* for selected threshold based on the confusion matrix.
2. Copy and paste observed and predicted/estimate value in the *input.txt* file
   Input file format for LDA analysis (.txt format):
   Note: Header is must as shown below.



L: inactive/less active ; H: active/highly active

3. Input file format for pharmacophore analysis (.txt format):
   Note: Header is must as shown below. Data should not be in logarithmic unit.



4. **Disclaimer**
   For academic purpose only;.
   The program DTC_QualValid has been developed (C++ language) and validated on known data by Rahul Aher (rahulba26@gmail.com) of Drug Theoretics & Cheminformatics (DTC) Laboratory, Jadavpur University , Kolkata (2013).

5. References:

Kumar Ojha, P.; Roy, K. First report on exploring structural requirements of alpha and beta thymidine analogs for *PfTMPK* inhibitory activity using in silico studies. BioSystems, 2013, 113, 177-195.

Liu, Z.; Kelly, R.; Fang, H.; Ding, D.; Tong, W. Comparative Analysis of Predictive Models for Nongenotoxic Hepatocarcinogenicity Using Both Toxicogenomics and Quantitative Structure Activity Relationships. Chemical research in toxicology, 2011, 24, 1062-1070.