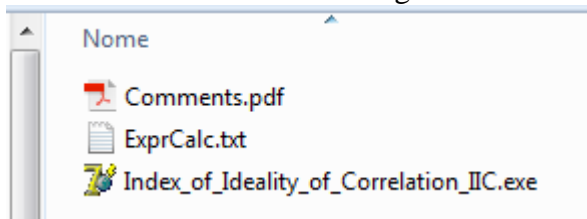


1. You should unzip, file “IIC.zip”.
2. Folder IIC has the following content:



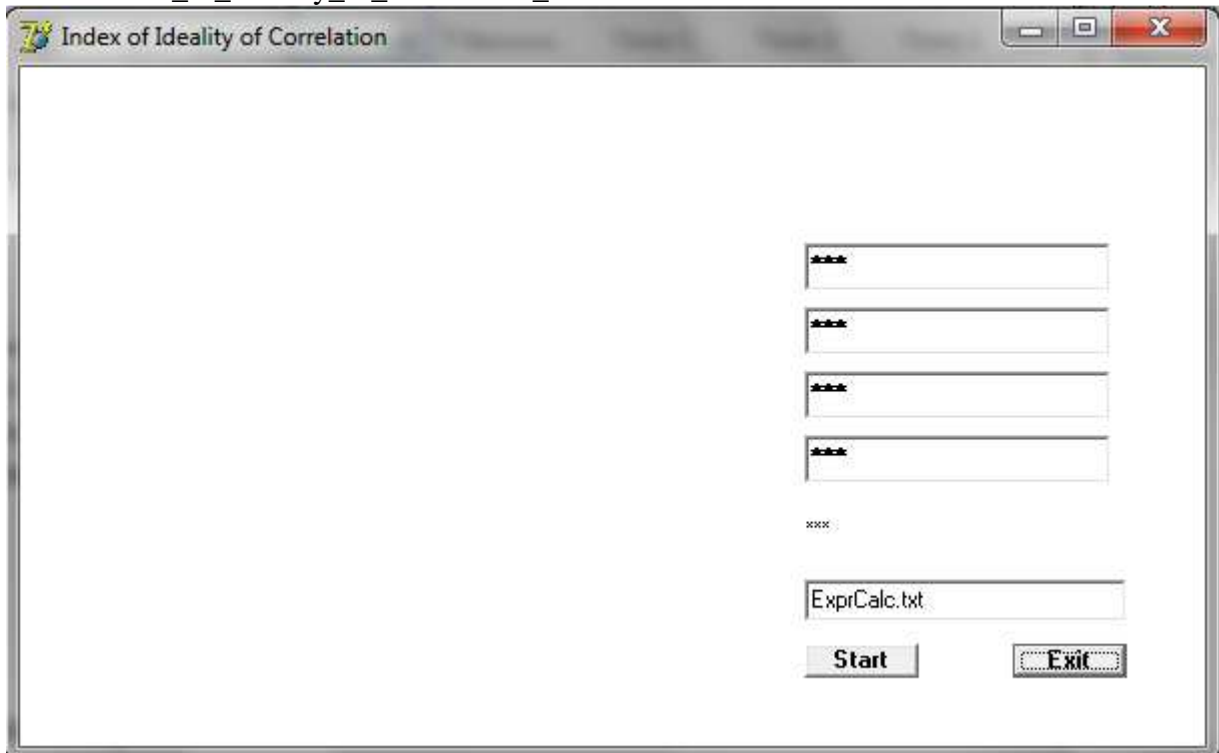
3. Insert in file “ExprCalc.txt” your data in the following format
N

```
expr1 calc1  
expr2 calc2  
...  
exprN calcN
```

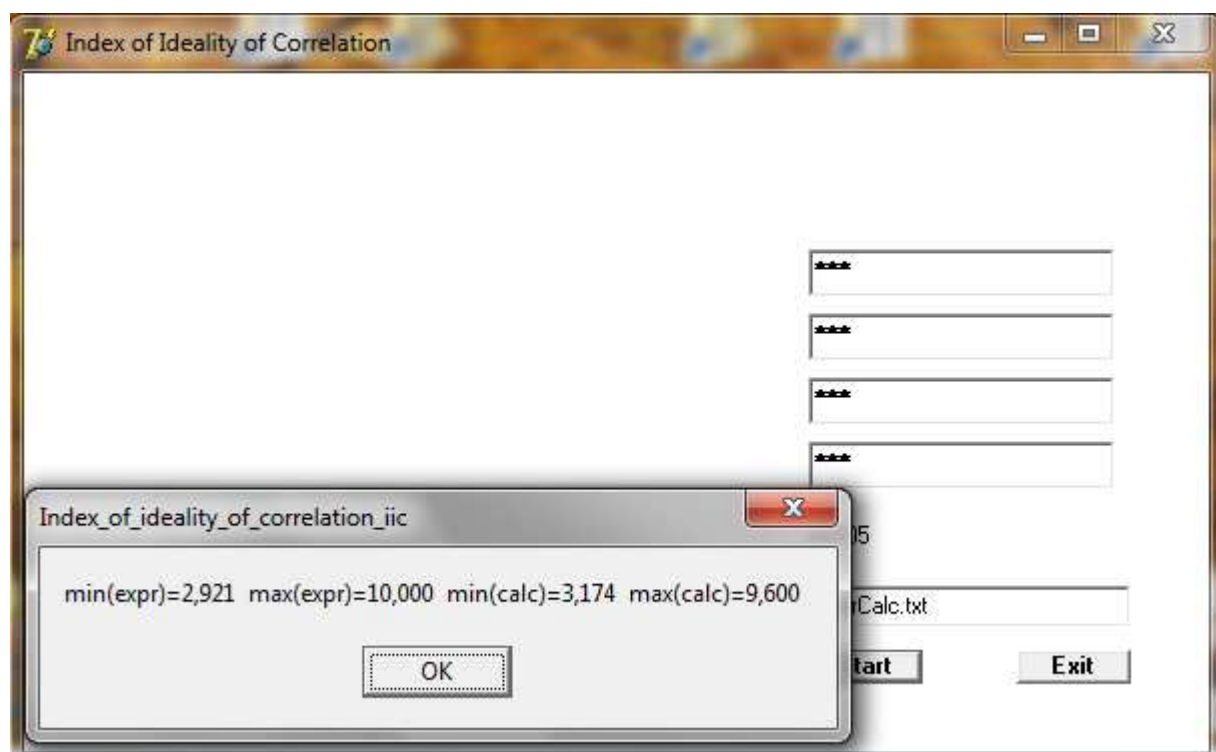
For instance, it can be the following:

```
10  
37.04 35.0  
51.70 50.00  
65.900 62.100  
77.200 80.900  
95.00 95.700  
110.70 111.20  
122.0 125.30  
141.060 140.500  
150.540 155.700  
173.2 187.88
```

4. Run Index_of_Ideality_of_Correlation_IIC.exe



5. Click button “Start”:



6. Click “OK”

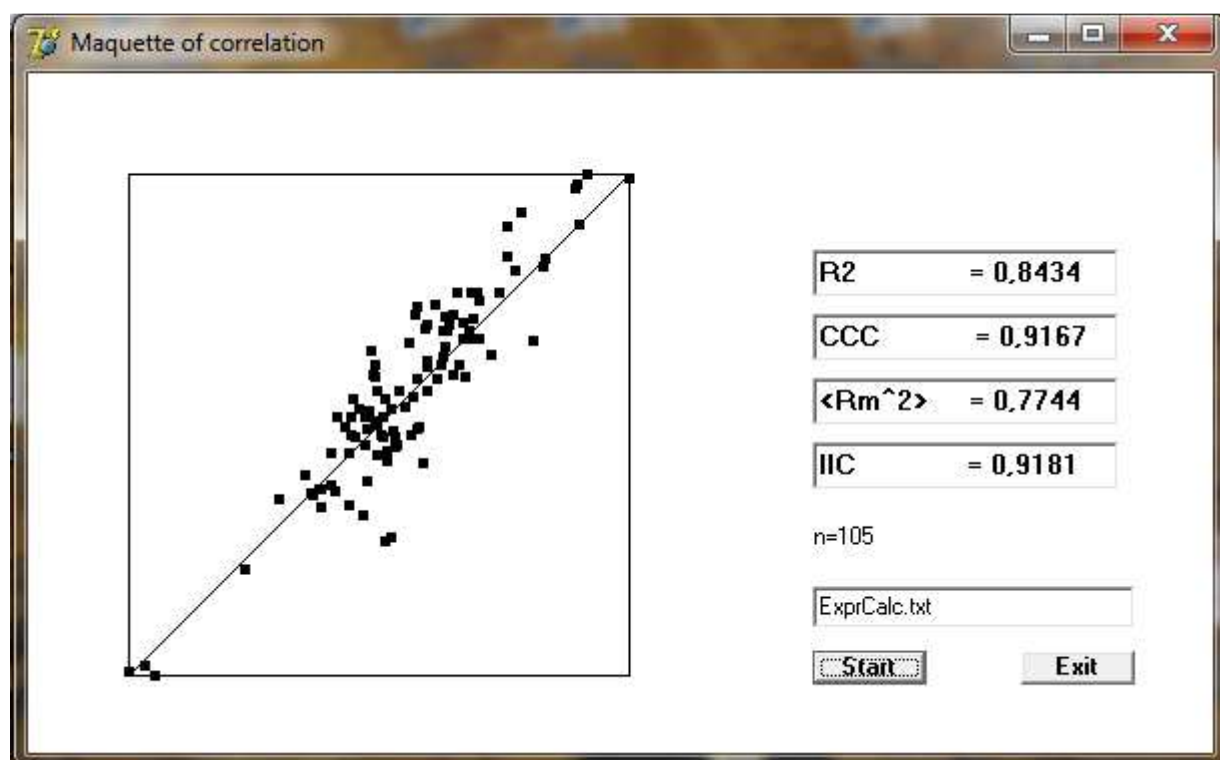


Table 1 contains clarification of calculated criteria for predictive potential for your model, which is inserted in file “ExprCalc.txt”.

Table 1

The x is vector of observed (experimental) values; the y is vector of calculated (predicted) values.

Formulae	Reference	Name
$r^2 = \left[\frac{n \sum xy - \sum x \sum y}{\sqrt{n \sum x^2 - (\sum x)^2} \times \sqrt{n \sum y^2 - (\sum y)^2}} \right]^2$	-	R2
$CCC = \frac{2 \sum (x - \bar{x})(y - \bar{y})}{\sum (x - \bar{x})^2 + \sum (y - \bar{y})^2 + n(\bar{x} - \bar{y})^2}$	[1]	CCC
$\langle r_m^2 \rangle = \frac{r_m^2(x, y) + r_m^2(y, x)}{2}$ $r_m^2(x, y) = r^2 \times (1 - \sqrt{ r^2 - r_0^2 })$	[2]	<Rm^2>
$IIC = r_{calibration} \times \frac{\min(-MAE_{calibration}, +MAE_{calibration})}{\max(-MAE_{calibration}, +MAE_{calibration})}$ $-MAE_{calibration} = \frac{1}{-N} \sum_{k=1}^{-N} \Delta_k \quad \Delta_k < 0, \quad -N \text{ is the number of } \Delta_k < 0$ $+MAE_{calibration} = \frac{1}{+N} \sum_{k=1}^{+N} \Delta_k \quad \Delta_k \geq 0, \quad +N \text{ is the number of } \Delta_k \geq 0$ $\Delta_k = observed_k - calculated_k$	[3,4]	IIC

References

- [1] I-Kuei Lin, L. A concordance correlation coefficient to evaluate reproducibility (1989) Biometrics, 45 (1), pp. 255-268.
- [2] Ojha, P.K., Mitra, I., Das, R.N., Roy, K. Further exploring r_m^2 metrics for validation of QSPR models (2011) Chemometrics and Intelligent Laboratory Systems, 107 (1), pp. 194-205.
- [3] Toropov, A.A., Toropova, A.P. The index of ideality of correlation: A criterion of predictive potential of QSPR/QSAR models? (2017) Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 819, pp. 31-37.
- [4] Toropova, A.P., Toropov, A.A. The index of ideality of correlation: A criterion of predictability of QSAR models for skin permeability? (2017) Science of the Total Environment, 586, pp. 466-472.