

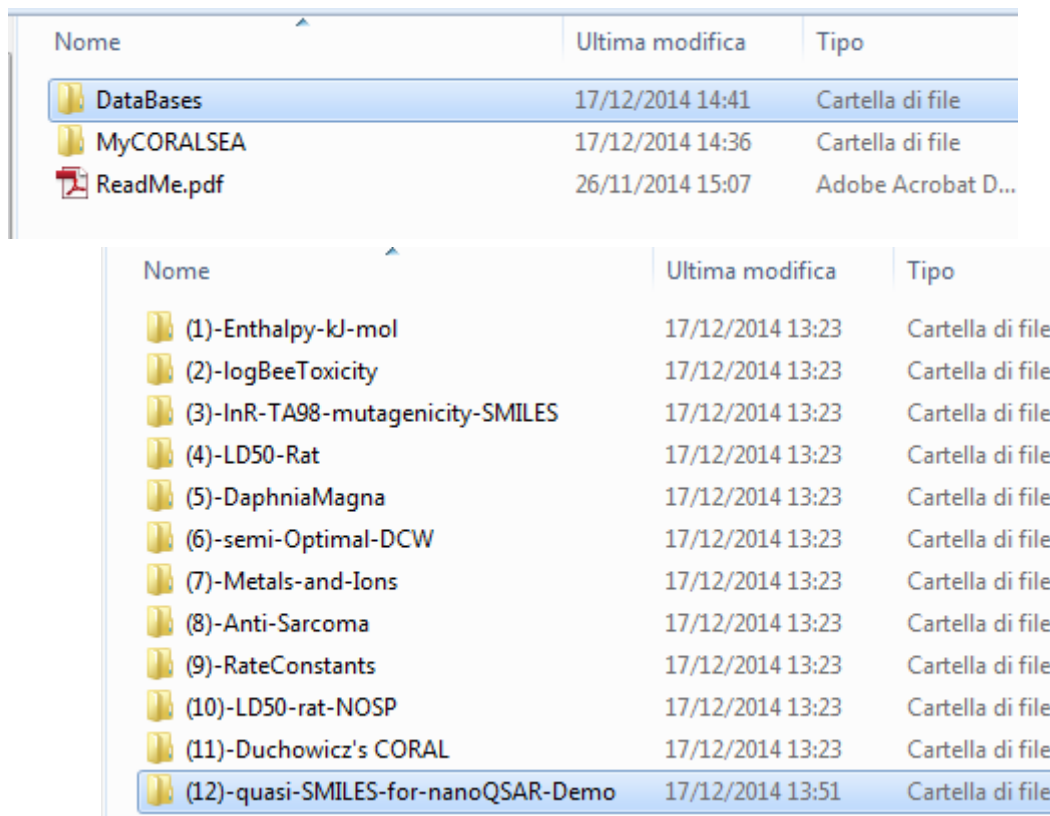
## An example of nano-QSAR based on the quasi-SMILES

Here the special version of the CORAL to build up a model of membrane damage caused by  $\text{TiO}_2$  nanoparticles under different conditions is represented.

Detailed description of this system quasi-QSAR (nano-QSAR) is available in PDF of article placed in this folder.

In order to check up the system please do the following:

1. Enter in folder “(12)-quasi-SMILES-for-nano-QSAR”;



Nome	Ultima modifica	Tipo
DataBases	17/12/2014 14:41	Cartella di file
MyCORALSEA	17/12/2014 14:36	Cartella di file
ReadMe.pdf	26/11/2014 15:07	Adobe Acrobat D...

Nome	Ultima modifica	Tipo
(1)-Enthalpy-kJ-mol	17/12/2014 13:23	Cartella di file
(2)-logBeeToxicity	17/12/2014 13:23	Cartella di file
(3)-lnR-TA98-mutagenicity-SMILES	17/12/2014 13:23	Cartella di file
(4)-LD50-Rat	17/12/2014 13:23	Cartella di file
(5)-DaphniaMagna	17/12/2014 13:23	Cartella di file
(6)-semi-Optimal-DCW	17/12/2014 13:23	Cartella di file
(7)-Metals-and-Ions	17/12/2014 13:23	Cartella di file
(8)-Anti-Sarcoma	17/12/2014 13:23	Cartella di file
(9)-RateConstants	17/12/2014 13:23	Cartella di file
(10)-LD50-rat-NOSP	17/12/2014 13:23	Cartella di file
(11)-Duchowicz's CORAL	17/12/2014 13:23	Cartella di file
(12)-quasi-SMILES-for-nanoQSAR-Demo	17/12/2014 13:51	Cartella di file

Nome	Ultima modifica
Model	17/12/2014 13:45
Search	17/12/2014 13:24
###TNadvice.txt	17/12/2014 13:45
#Input-1.txt	21/06/2013 16:34
#TRNCLBTST-1.txt	21/06/2013 16:34
AOs.txt	27/06/2011 08:23
Chemosphere 93 (2013) 2650-2655.pdf	13/11/2013 13:53
<b>CORALSEA.exe</b>	17/12/2014 13:11
METHOD.txt	17/12/2014 12:55
quasi-SMILES-comments.pdf	17/12/2014 13:49

2. Run CORALSEA.exe

3. Click “Load method”

**CORAL: Loading of method or system**

**Method:** Scheme: Additive or Multiplicative

**Sub-training set**  
 ...

**Calibration set**  
 ...

**Test set**   
 ...

**Place of compound (CAS) in graphical representations**

**Method options:**  
 Graph  G4O-type  HSG-type  SMILES  
 ec0  pt2  vs2  HFG-type  C7  s  
 ec1  pt3  vs3  nnc  C5  s s  
 ec2  C4  s s s  
 C3  BOND  
 NO SP  
 HALO  
 PAIR

**SMILES File (training-[calibration]-test sets)**  
 \*\*\*

**Target function for the Monte Carlo optimization:**  
 Classic Scheme  dR\_weight \*\*\*  
 Balance of correlations  Ideal C1, C1'  dC\_weight \*\*\*

**The field of search**  
 Classification  
 N\_epoch \*\*\*  
 Start threshold value..... \*\*\*  
 Maximal threshold value..... \*\*\*  
 Number of the Monte Carlo probes... \*\*\*

**System.txt**  
 W% N111 N110 N101 N100 Nall DEFECT  
 Split Info 

0	0	0	0	0	0	0
---	---	---	---	---	---	---

Outliers 5  
 DemoDCW  
 EvolutionCorr

#### 4. Click “Phase 2: Building up preferable model (T\*,N\*)”

**Method:** Additive scheme

**Phase 1: Search for preferable model (T\*,N\*)**

**Phase 2: Building up preferable model (T\*,N\*)**

**Method:** Additive scheme

**SMILES**

**Target function for the Monte Carlo optimization:**

Classic Scheme

Balance of correlations

Ideal C1, C1'

**The field of search**

Classification

**SMILES File (training-[calibration]-test sets)**

#TRNCLBTST-1.txt

**Split Info**

W%	N111	N110	N101	N100	Nall	DEFECT
0	0	0	0	0	0	0

#### 5. Insert Threshold =2

**Method:** Additive scheme

**Phase 2: Building up preferable model (T\*,N\*)**

Define preferable threshold and press Continue

**C0 =** 0 **C1 =** 1

**Method:** Additive scheme

**SMILES**

**Target function for the Monte Carlo optimization:**

Classic Scheme

Balance of correlations

Ideal C1, C1'

**The field of search**

Classification

**SMILES File (training-[calibration]-test sets)**

#TRNCLBTST-1.txt

**Split Info**

W%	N111	N110	N101	N100	Nall	DEFECT
0	0	0	0	0	0	0

6. Click (i) “Continue”; and (ii) “YES”

The screenshot shows the CORAL software interface with the title "CORAL: Building up preferable model". The main window displays several graphs (Sub-training set, Calibration set, Test set) and various configuration options. A "Confirm" dialog box is open in the foreground, asking: "There are files in 'model/\*.\*' which remain after previous calculations you can delete these files in order to avoid mixture of new files and files which remain after previous calculations. Delete these files?". The "Yes" button is highlighted with an arrow. In the background, the "Continue" button in the "Phase 2: Building up preferable model" section is also highlighted with an arrow.

7. Technical details for the obtained model you can find according to description from ReadMe.pdf

The screenshot shows the CORAL software interface with the title "CORAL: you must save system now". The main window displays the same graphs and configuration options as in the previous screenshot. The "Continue" button is now disabled, and the text "THE CALCULATION IS COMPLETED" is visible. A "Save system" button is highlighted with an arrow. The "Split Info" table at the bottom shows the following data:

W%	N111	N110	N101	N100	Na11	DEFECT
0	0	0	0	0	0	0
83	0	0	10	2	12	2,2557