Elemental-Descriptor 1.0

(Metal, Nonmetal, Semimetal)

NANOBRIDGES
-A Collaborative Project

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Marie Curie Actions
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Background: Nanotechnology-based products found a large application in material science, medical research, cosmetic and clothing industry. Currently, more than 1000 manufacturer-identified (MNPs) nanotechnology-based consumer products are available in the market and still the production of other nano-materials (NMs) are increasing at a staggering rate due the growing demand of nano-based product on a larger scale. Quantitative Nanostructure-Activity Relationships (QNAR) modeling plays an important role in allowing rapid prediction of potential toxicities caused by diverse type of MNPs prior to the experimental evaluation. In order to develop the robust and statistically significant models, it is quite essential to have prior information of all the elements (Metals, non-metals and semimetals) present in the nano-based compounds in addition to the descriptors calculated by using some other software.

About the program: This program calculates the total 31 descriptors comprising the information of metal, nonmetal and semimetals obtained from periodic table and other literature sources [1-3]. This program computes the descriptors for those elements which are having atomic number less than 103.

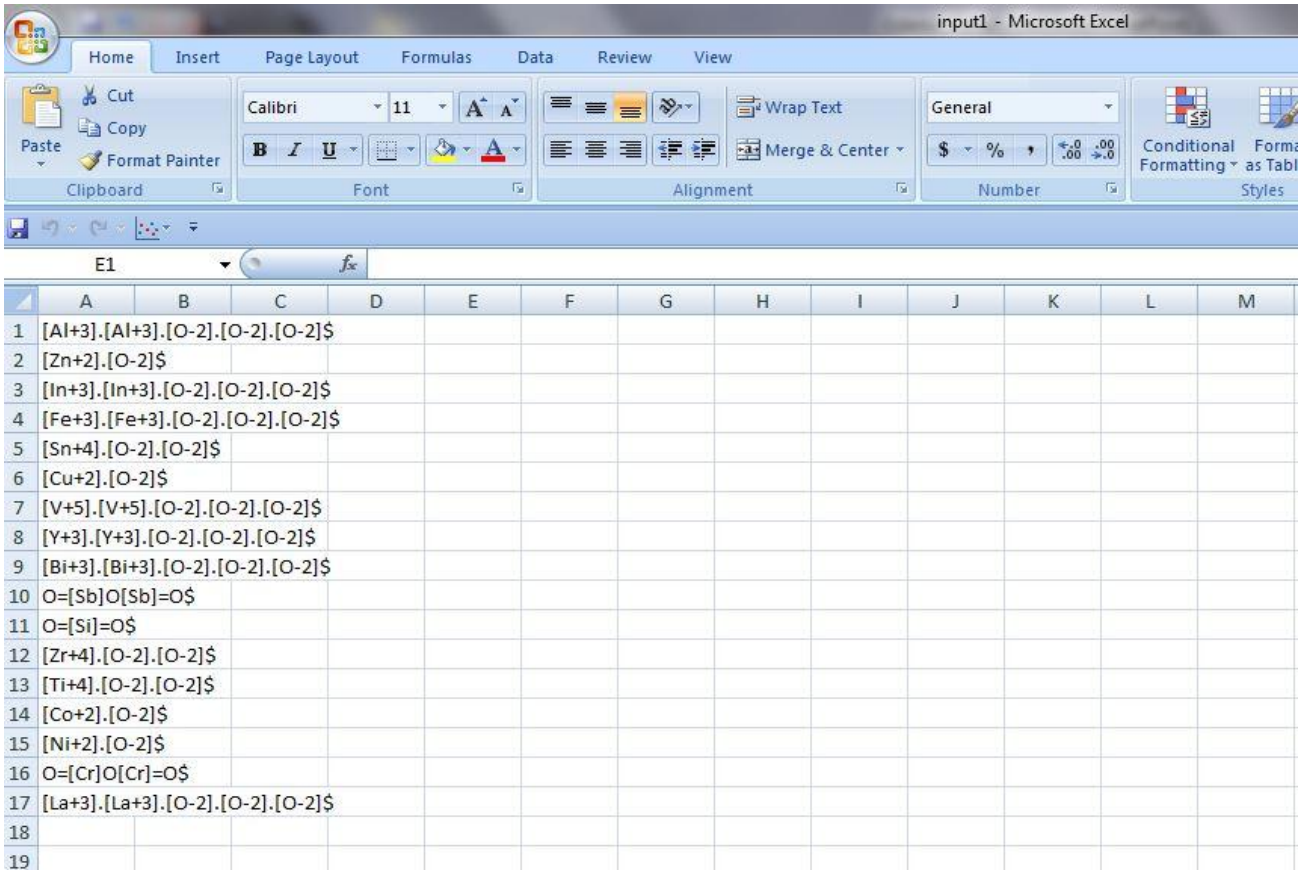
[Note: *Information of ionization potential, electronegativity, Vanderwaals radius, isotopes etc., for elements having atomic no. greater than 102 are not available in literature*]. Elements with least ionization potential energy of corresponding class (Metal/nonmetal/semimetal) are considered for the calculation of respective descriptors. These calculated descriptors could be used alone or combine with the other descriptors pool to develop the QSAR model. Following is the list of 31 descriptors:

Table 1. Names and description of the descriptors calculated using Elemental descriptor calculator.

Des No	*Descriptor Name*	*Description*
1	D1_Metals	Total no. of metals
2	D2_SemiMetals	Total no. of semi-metals
3	D3_HeteroNonMetals	Total no. of non-metallic heteroatoms (N, O, F, P, S, Cl, Se, Br, I, At) excluding hydrogen
4	Metals_SumIP	Sum of ionization potential energy (kJ/mol) of metals
5	SemiMetals_SumIP	Sum of ionization potential energy (kJ/mol) of semi-metals
6	Electrons_ActiveM	No. of electrons of active metal
7	AtWt_ActiveM	Atomic wt. of active metal
8	MassNo_ActiveM	Mass no. of active metal
9	Neutons_ActiveM	Number of neutrons of active metal
10	IP_ActivM	Ionisation potential energy (kJ/mol) of active metal
11	X_ActivM	Electronegativity of active metal
12	VWR_ActivM	van der Waal radius of active metal

13	Electrons_Activ_SM	No. of electrons of active metalloid/semi-metal
14	AtWt_Activ_SM	Atomic wt. of active metalloid/semi-metal
15	MassNo_Activ_SM	Mass no. of active metalloid/semi-metal
16	Neutons_Activ_SM	Number of neutrons of active metalloid/semi-metal
17	IP_Activ_SM	Ionisation potential energy of active metalloid/semi-metal
18	X_Activ_SM	Electronegativity of active metalloid/semi-metal
19	VWR_Activ_SM	van der Waals radius of active metalloid/semi-metal
20	Electrons_Activ_NM	No. of electrons of active non-metal
21	AtWt_Activ_NM	Atomic wt. of active non-metal
22	MassNo_Activ_NM	Mass no. of active non-metal
23	Neutons_Activ_NM	Number of neutrons of active non-metal
24	IP_Activ_NM	Ionisation potential energy of active non-metal
25	X_Activ_NM	Electronegativity of active non-metal
26	VWR_Activ_NM	van der Waals radius of active non-metal
27	SuM_Active_M_SM	Summation of number of metals and semi-metal
28	SuMElectrons_Active_M_SM	Summation of electrons of active metal and semi-metal
29	SuMAtWt_Active_M_SM	Summation of At. wt of active metal and semi-metal
30	SuMMassNo_Active_M_SM	Summation of mass no. of active metal and semi-metal
31	SuMNeutons_Active_M_SM	Summation of neutrons of active metal and semi-metal

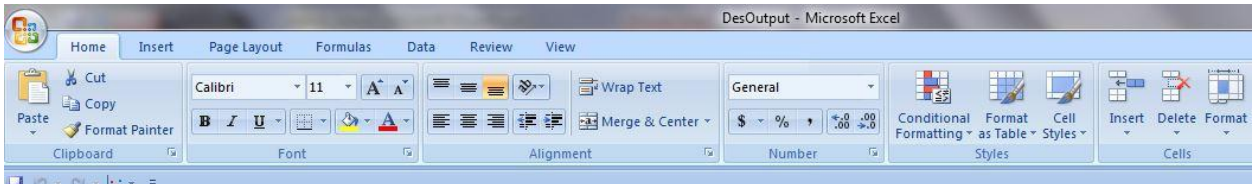
Input file format: This program takes a input from CSV file in SMILES format. So, it is important to enter the correct SMILES for all the compounds. At the end of each corresponding compound insert the symbol dollar ($) by using concatenate option provided in the excel file as shown in the input file snap.



	A
1	[Al+3].[Al+3].[O-2].[O-2].[O-2]$
2	[Zn+2].[O-2]$
3	[In+3].[In+3].[O-2].[O-2].[O-2]$
4	[Fe+3].[Fe+3].[O-2].[O-2].[O-2]$
5	[Sn+4].[O-2].[O-2]$
6	[Cu+2].[O-2]$
7	[V+5].[V+5].[O-2].[O-2].[O-2]$
8	[Y+3].[Y+3].[O-2].[O-2].[O-2]$
9	[Bi+3].[Bi+3].[O-2].[O-2].[O-2]$
10	O=[Sb]O[Sb]=O$
11	O=[Si]=O$
12	[Zr+4].[O-2].[O-2]$
13	[Ti+4].[O-2].[O-2]$
14	[Co+2].[O-2]$
15	[Ni+2].[O-2]$
16	O=[Cr]O[Cr]=O$
17	[La+3].[La+3].[O-2].[O-2].[O-2]$
18	
19	

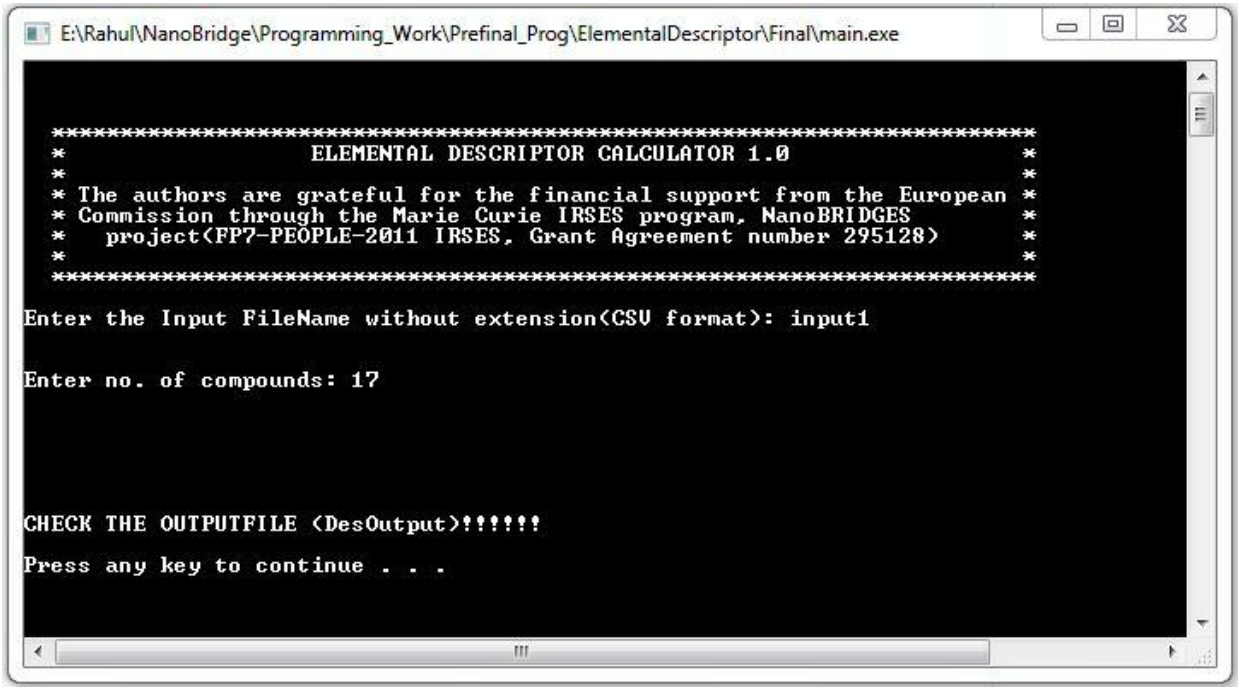
Output file format:

Descriptors having numerical value equal to NA, indicates that corresponding descriptor information is not available in the literature.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	CompNo	D1_Metal:	D2_SemiM	D3_Heter	Metals_Su	SemiMeta	Electrons_	AtWt_Acti	MassNo_A	Neutons_	IP_ActivM	X_ActivM	VWR_Acti	Electrons_	AtWt_Acti	MassNo_A
2	1	2	0	3	1154.8	0	13	26.982	27	14	577.4	1.5	0.143	0	0	0
3	2	1	0	1	904.5	0	30	65.38	65	35	904.5	1.6	0.138	0	0	0
4	3	2	0	3	1116.4	0	49	114.818	115	66	558.2	2	0.162	0	0	0
5	4	2	0	3	1522	0	26	55.845	56	30	761	1.8	0.126	0	0	0
6	5	1	0	2	708.4	0	50	118.71	119	69	708.4	1.8	0.162	0	0	0
7	6	1	0	1	743.5	0	29	63.546	64	35	743.5	1.9	0.128	0	0	0
8	7	2	0	3	1298.2	0	23	50.942	51	28	649.1	1.6	0.134	0	0	0
9	8	2	0	3	1252	0	39	88.9058	89	50	626	1.2	0.106	0	0	0
10	9	2	0	3	1406	0	83	208.98	209	126	703	1.9	0.152	0	0	0
11	10	0	2	3	0	1668	0	0	0	0	0	0	0	51	121.76	122
12	11	0	1	2	0	786.3	0	0	0	0	0	0	0	14	28.085	28
13	12	1	0	2	669	0	40	91.224	91	51	669	1.2	0.16	0	0	0
14	13	1	0	2	658	0	22	47.867	48	26	658	1.5	0.147	0	0	0
15	14	1	0	1	757	0	27	58.933	59	32	757	1.8	0.125	0	0	0
16	15	1	0	1	735	0	28	58.6934	59	31	735	1.8	0.124	0	0	0
17	16	2	0	3	1302.2	0	24	51.996	52	28	651.1	1.6	0.127	0	0	0
18	17	2	0	3	1078	0	57	138.91	139	82	539	1.1	0.104	0	0	0

How to run a program:



Case study: A Nano-QSAR model has been developed from a dataset [4] of metal oxide using the calculated nano-descriptors.

Total No. of compounds: 17; Training set: 10; Test set: 7

Stepwise MLR model

$$pEC_{50} = 2.652(+/-0.241) - 1.342(+/-0.217)\text{" D3\_HeteroNonMetals"} + 2.014(+/-0.339)\text{" Sum\_ActiveM\_SM"}$$

D3_HeteroNonMetals: Sum of no. of nonmetallic hetero atoms
Sum_Active_M_SM: Summation of no. of metals and metalloids

R^2 =0.848, R_a^2 =0.804, SEE =0.238, $SDEP$ =0.278, Q^2 =0.705, R_{pred}^2 =0.902, $\overline{r^2_{m(training)}}$ =0.616; $\Delta r^2_{m(training)}$ =0.078; $\overline{r^2_{m(test)}}$ =0.844, $\Delta r^2_{m(test)}$ =0.066, $\overline{r^2_{m(Overall)}}$ =0.709, $\Delta r^2_{m(Overall)}$ =0.052; Golbraikh-Tropsha criteria: passed

Disclaimer

For academic purpose only.

The program Elemental-Descriptor 1.0 has been developed in C++ language and is validated on the known data sets. This program is compatible with both 32- and 64-bit Windows operating system. Please report for discrepancy of result for any other dataset. Contact us at any of the following addresses:

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3. http://www.ptable.com/
4. Puzyn, Tomasz, Bakhtiyor Rasulev, Agnieszka Gajewicz, Xiaoke Hu, Thabitha P. Dasari, Andrea Michalkova, Huey-Min Hwang, Andrey Toropov, Danuta Leszczynska, and Jerzy Leszczynski. "Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles." *Nature nanotechnology* 6, no. 3 (2011): 175-178.