



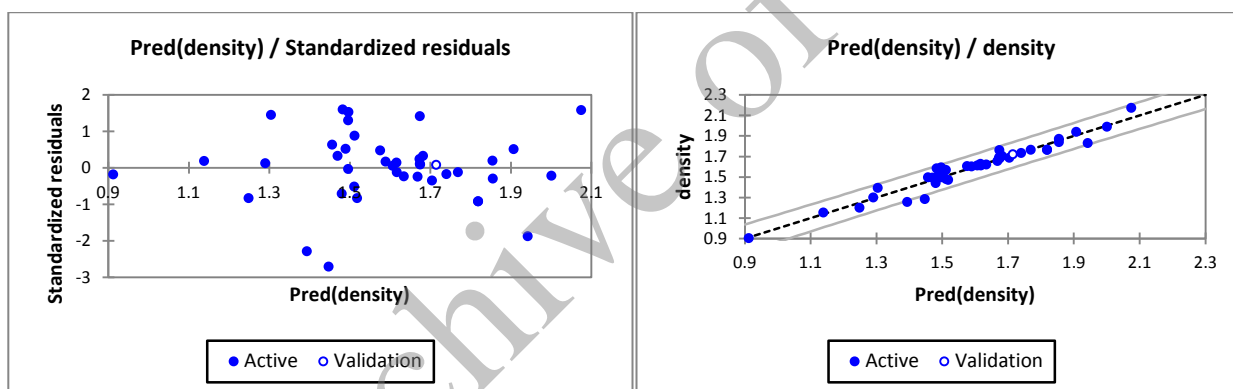
## New Method for Calculating Densities of Nitroaromatic Explosive Compounds and Prediction of their Biological Activity.

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Use nitroaromatic explosive compounds properties extensively in safety procedures, maintenance and improvement of the family better use of explosives, because of relevance to the structure and the ability to obtain explosives in the laboratory are very important [1, 2]. In order to get the best models causing the relationship between structure-property of explosives was an extensive study on the molecular descriptors to determine the important properties of explosives, such as density. In this study, a set of 42 nitroaromatic derived from QSAR models developed using multiple linear regression analysis (MLRA) was studied and density of "4-methyl-1,2-dinitrobenzene" as an external set was evaluated ( $d=1.444\text{g/cm}^3$ ). The biological activities of mentioned compounds were predicted. According to the method used, the values of  $R^2$ ,  $F$  and  $RMSE$  respectively; 0.941, 143.369 and 0.004 predicted and were obtained.



$$\text{Density} = 1.497 + 1.858 \text{ HATS1u} - 14.018 \text{ HATS1p} + 0.789 \text{ RTu} + 0.981 \text{ R3m}$$
$$N=42, R^2=0.941, \text{ Adjusted } R^2=0.934, \text{ RMSE}=0.004, F=143.369.$$

Biological Activity	$P_a$
<b>Pharmacologic al Effects</b>	
<b>Antiprotozoal</b>	<b>0.565</b>
Acaricide	0.541
Antiinfective	0.532
Antiparasitic	0.519
<b>Molecular Mechanisms</b>	
<b>Chloramphenicol O-acetyltransferase inhibitor</b>	<b>0.816</b>
Anthranilate-CoA ligase inhibitor	0.802
Pantoate 4-dehydrogenase inhibitor	0.760
3-Oxoadipate enol-lactonase inhibitor	0.714
<b>Side Effects and Toxicity</b>	
<b>Carcinogenic, group 3</b>	<b>0.777</b>
Mutagenic, Salmonella	0.770
Mutagenic	0.727
Carcinogenic, male mice	0.715

beta	B	HATS1u	HATS1p	RTu+
value	1.497	0.223	0.085	0.347
product	1.497	0.414	-1.192	0.274
density	<b>1.444 g/cm<sup>3</sup></b>			

### References:

- [1] M.H. Keshavarz, M.H. Moghadas, M.K. Terani, *Propel. Explos.Pyrotechn.* **2009**, 34, 136-141.
- [2] G. Fayet, L. Joubert, P. Rotureau, C. Adamo, *J. Phys. Chem. A*, **2009**, 113, 13621-13627.