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DESIGN OF SOME ENERGETIC COMPOUNDS

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ABSTRACT

Due to the increasing production of modern explosive-resistant vehicles, materials, and equipment, the calls for improved energetic materials (EMs) with a more destructive energetic capability and high thermal stability for engineering and warfare have received tremendous attention from researchers. Weka version 3.8.5 machine learning software has been used in this research to carry out the accurate energetic velocities predictions and to develop and generate five (5) novel models from the seventy-one (71) experimental EM compounds. Also, the quantitative structural property relationship (QSPR) method was used to design five (5) new EM along with their new energetic velocities (EV) of 10.835 Km/s, 10.22 Km/s, 10.531 Km/s, 10.436Km/s, and 10.33Km/s. The energetic velocities of all the five newly designed EMs were better than those reported in the literature and also better than the standard energetic compounds, TNT. Because of their unique energetic properties, The energetic compounds such as N, N'-(3,6 dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)bis(N-fluoronitramide) should be given special consideration while synthesizing those compounds. Furthermore, the results of this research have proven the scientific importance of using QSPR as a research tool in the field of energetic materials.

Keywords: QSPR, Energetic Material, EM, Explosive, Energetic Velocity

INTRODUCTION

Over the past decades, the calls for improved energetic materials (EMs) with a more destructive capability of energy for warfare have received tremendous attention (Fayet *et al*., 2011; Bae and Snurr, 2011; Kreno *et al.*, 2012; Baati *et al*., 2013; Seth and Matzger, 2017; Chandrasekaran *et al*., 2019; Zhang *et al*., 2020 Liu *et al*., 2021). Several researches have shown that some nitrogen-containing heterocyclic explosive compounds have been synthesized over many decades (Wong *et al*., 2021; Liu *et al.*, 2021). But, 2, 4, 6-trinitrotoluene (TNT) has remained one of the most referenced and used energetic compounds (Wong *et al*., 2021; Liu *et al*., 2021). This is because of its unique properties of energetic velocity and high stability, the most important properties to be considered before the energetic compound's production (Liu *et al*., 2021; Szala *et al*., 2017).

EMs are chemical compounds with high thermal stability and huge structurally stored explosive energies (Millar, 2012; Guo *et al.*, 2014). This category of chemical compounds can initiate several thousand chains of reactions upon initiation or triggered by any mechanical stimuli (Deng, 2011; Millar, 2012; Kreno *et al*., 2012; Guo *et al*., 2014; Shreeve *et al.*, 2019). The Nitrated-Pyrazoles-based EMs are a group of heterocyclic compounds that can release highly stored energetic energies. This group of EMs possessed higher stability and higher energetic properties than the TNT (Fayet *et al.*, 2011; Baati *et al*., 2013; Bae and Snurr, 2011; Kreno *et al*., 2012; Kreno *et al*., 2012; Seth and Matzger, 2017; Zhang *et al*., 2020; Liu *et al*., 2021). It's a fact that the determination of explosives experimentally is often costly, dangerous, and non-eco-friendly (Muratov *et al*., 2010; Zhang *et al.*, 2019[c]; Jinshan, 2018; Wong *et al*., 2021; Liu *et al.*, 2021). The aim is to use another unique technique to screen or design novel EMs candidate and as well as predicting their unknown properties. In this case, the computational Quantitative Structure-Property Relationship (QSPR) has been widely in the field of petroleum, corrosion, and medicine (Abdulfatai, *et al*., 2018; Umar *et al*., 2020; Abdulfatai *et al.*, 2020; Ibrahim *et al.*, 2020; Umar *et al.*, 2021; Abdullahi, *et al*., 2020).

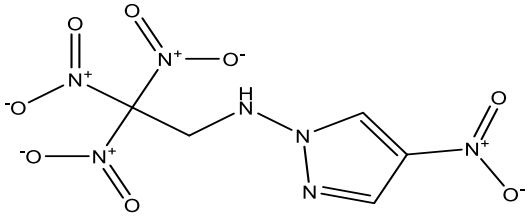
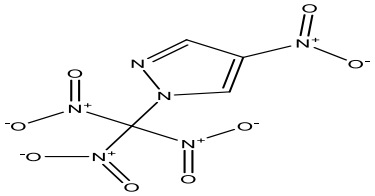
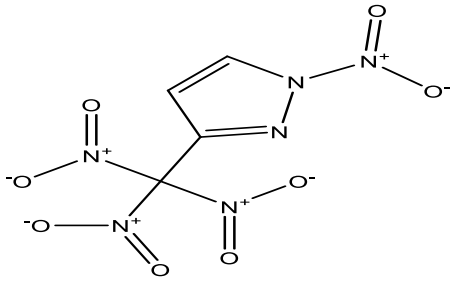
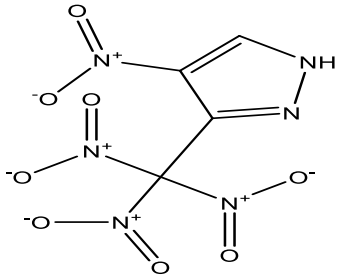
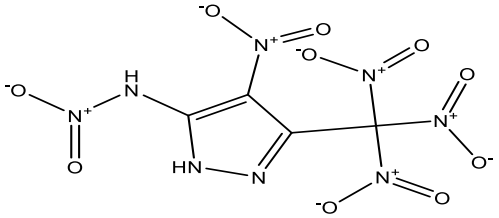
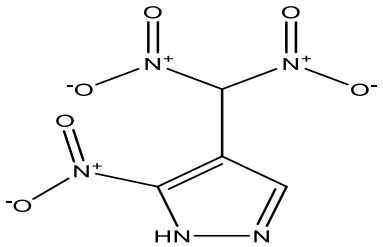
In recent years, accurate properties and chemical structure predictions have been easier via the QSPR method. (Muratov *et al.*, 2010; Fayet *et al*., 2011; Baati *et al.*, 2013). QSPR's main goal is to generate a functional model from the relationship between the compound's properties and structures of interest (Muratov *et al*., 2010; Fayet *et al.*, 2011; Baati *et al.*, 2013; Abdulfatai *et al.*, 20220; Ibrahim *et al.*, 2020).

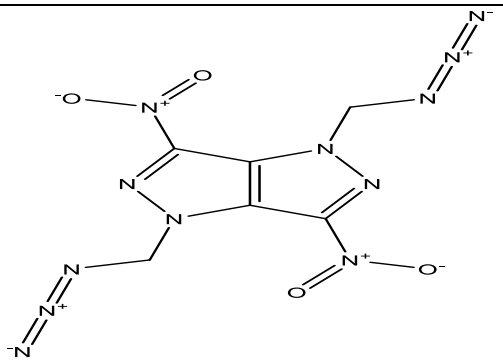
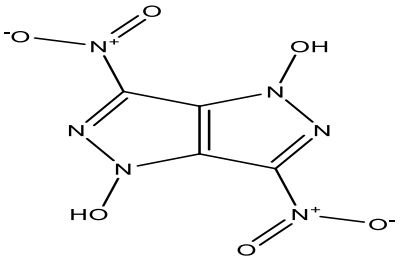
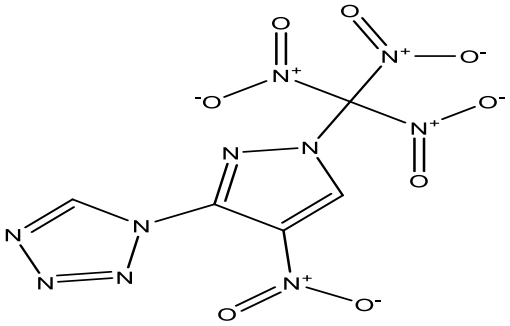
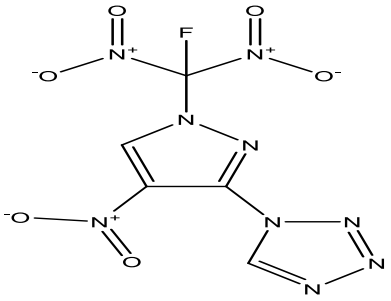
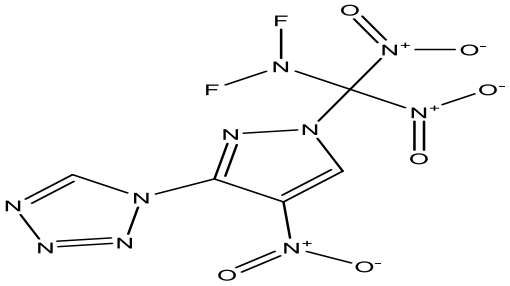
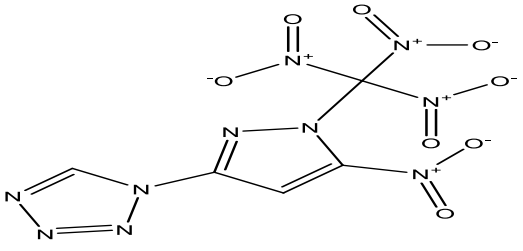
MATERIALS AND METHODS

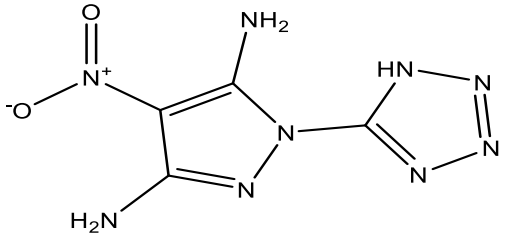
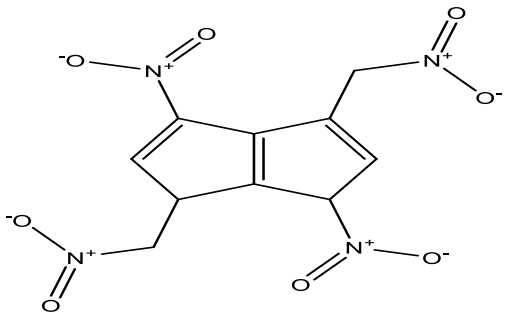
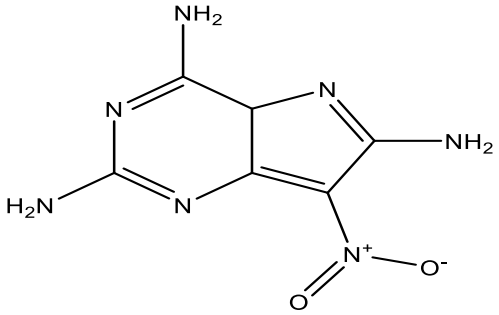
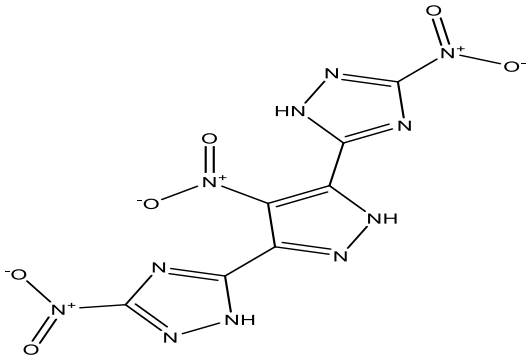
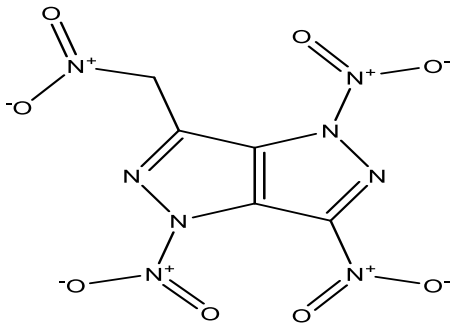
Compound's Stabilization, Properties Generation and EM data splitting

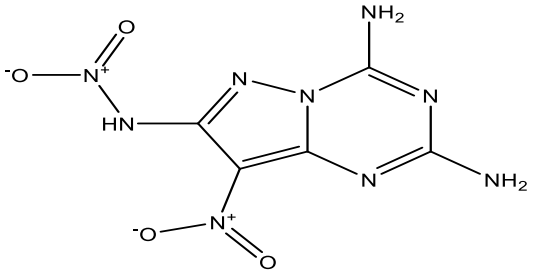
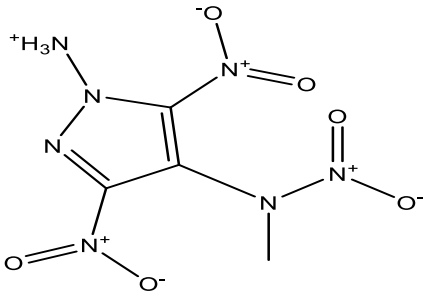
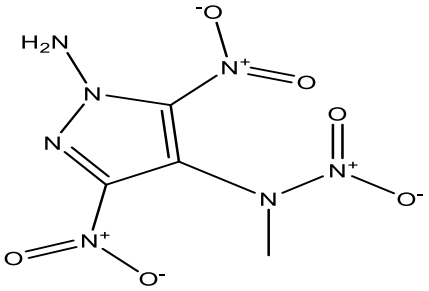
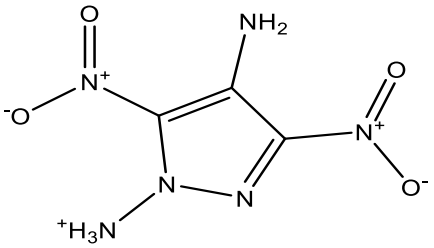
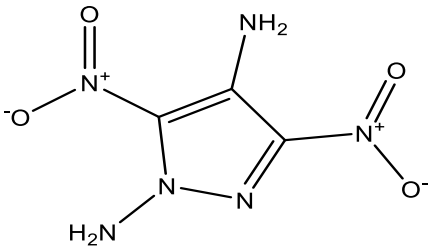
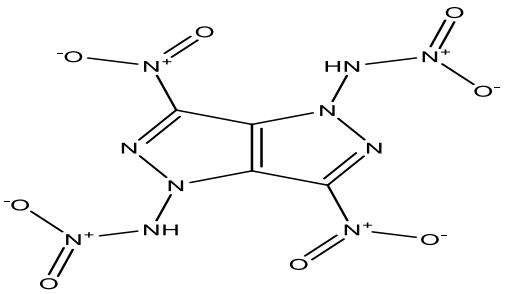
Seventy-one (71) EMs (Table 1) were sourced from the article (Zhang *et al*., 2020) along with their energetic velocity properties (Km/s). With the aid of B3LYP/6-311+ G basis set in Spartan 14 (Anonymous, 2013) software, EMs energy stabilizations were carried out successfully. About 3300 molecular descriptors were generated from the 71 EMs via Dragon and Padel (Yap, 2011) descriptor generators. This was followed by the normalization and grouping of the descriptors (20 tests and 51 training sets).

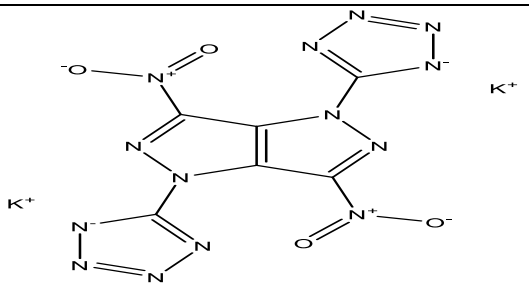
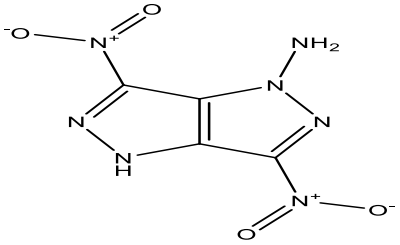
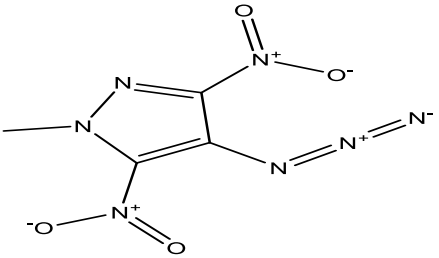
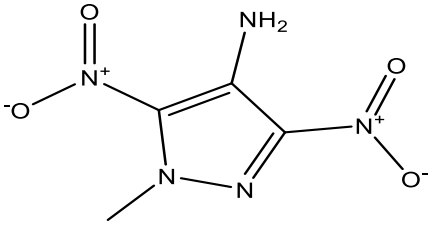
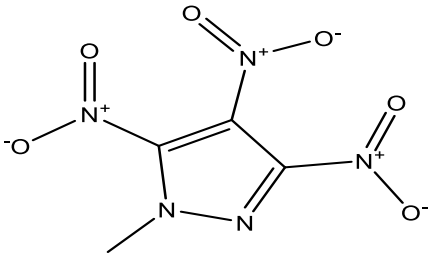
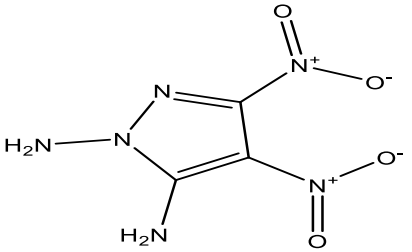
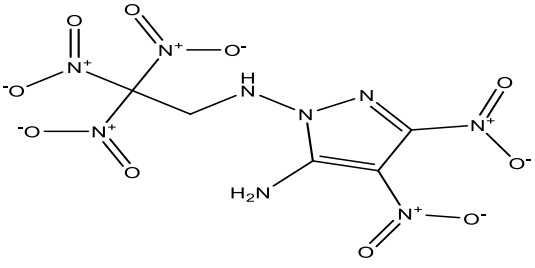
Table 1: The Experimental Energetic Compounds And Their Properties

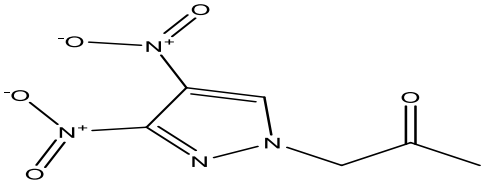
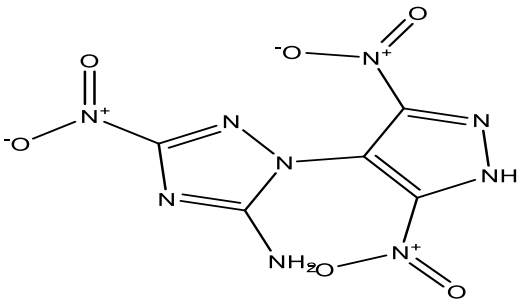
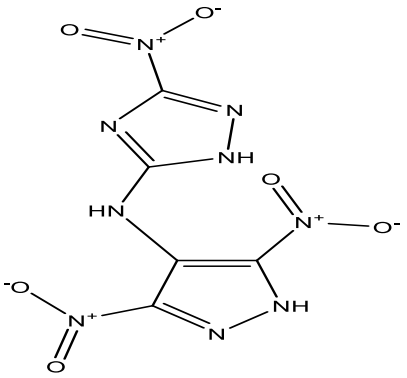
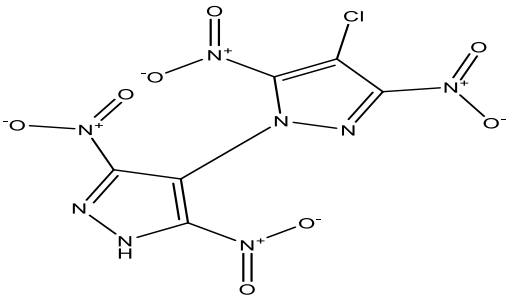
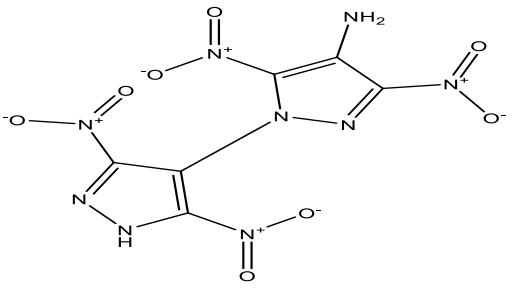
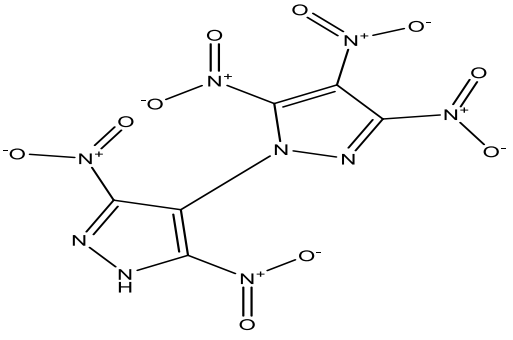
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
1		8.39	8.39
2		8.65	8.65
3		8.93	8.93
4		8.6	8.6
5		9.12	9.12
6		8.53	8.34

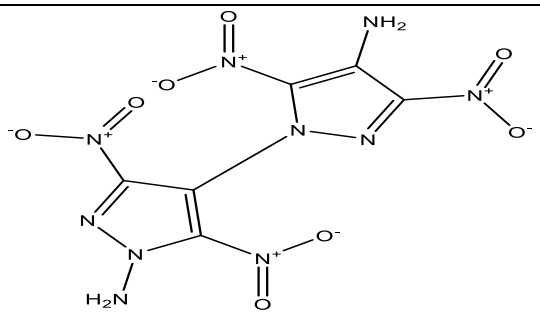
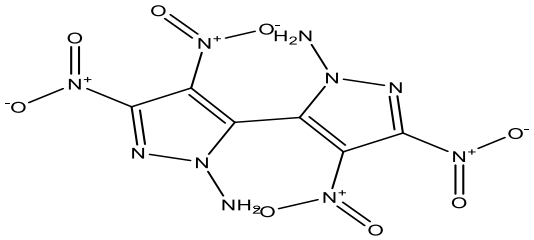
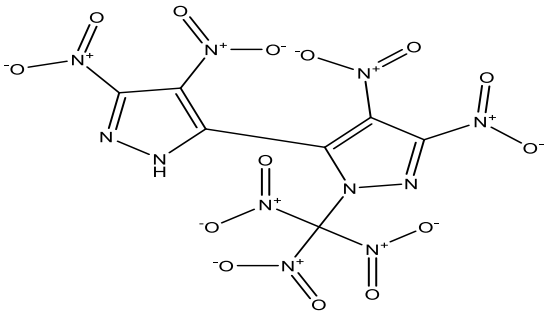
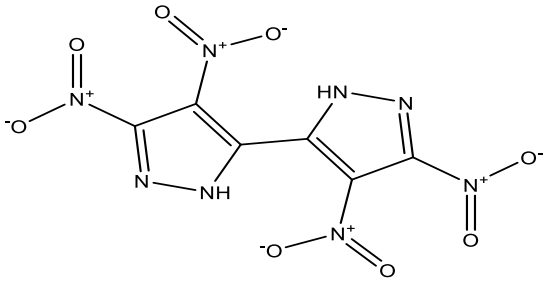
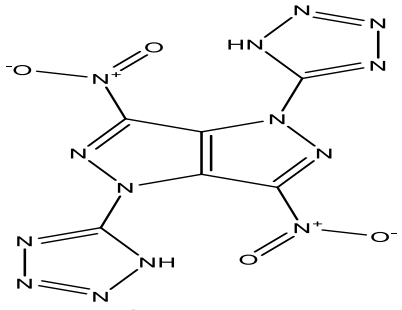
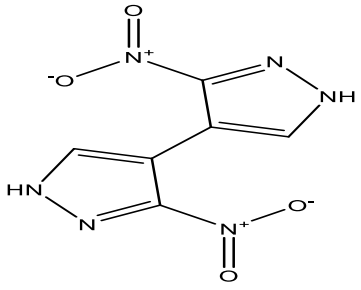
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
7		7.82	8.31
8		8.84	8.84
9		8.86	8.86
10		8.47	8.47
11		8.99	8.99
12		8.78	8.78

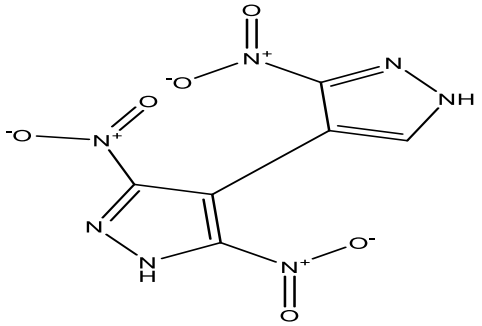
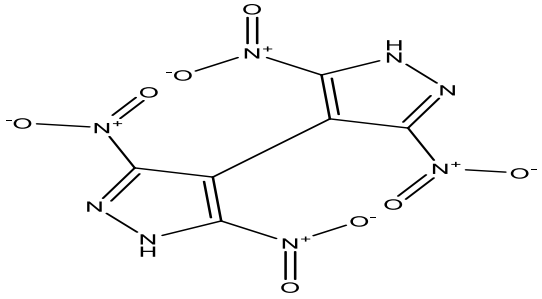
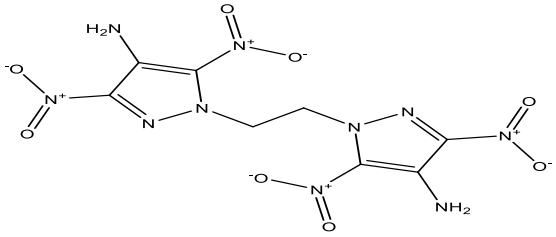
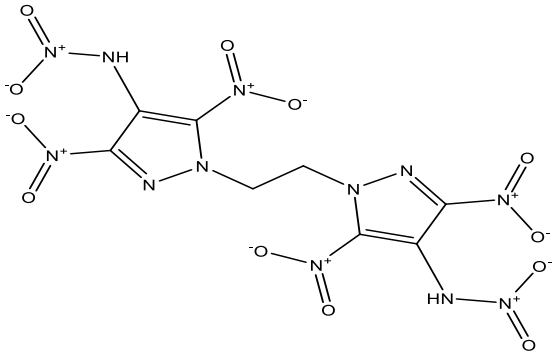
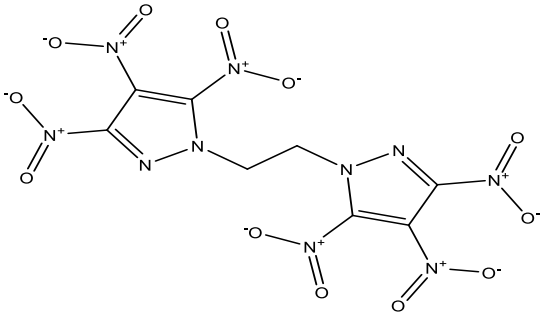
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
13		8.26	8.26
14		8.67	8.67
15		7.79	7.79
16		8.75	8.37
17		9.46	8.98

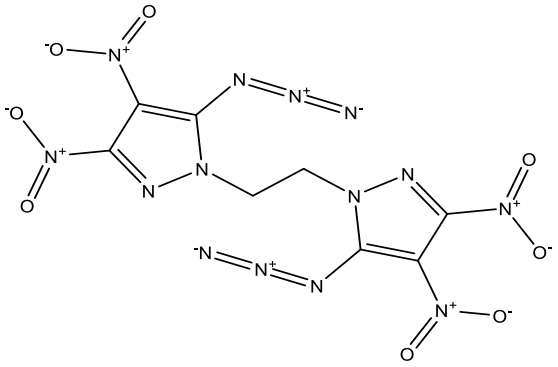
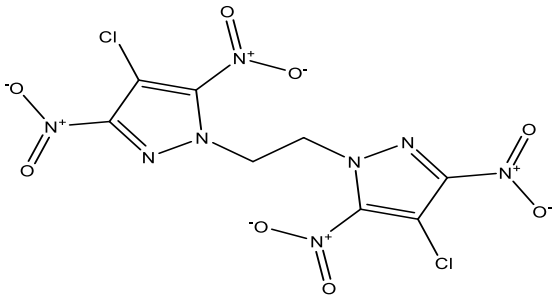
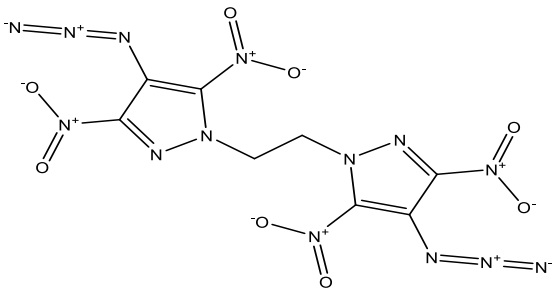
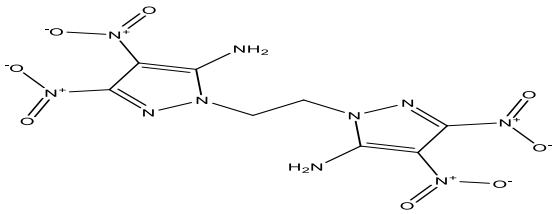
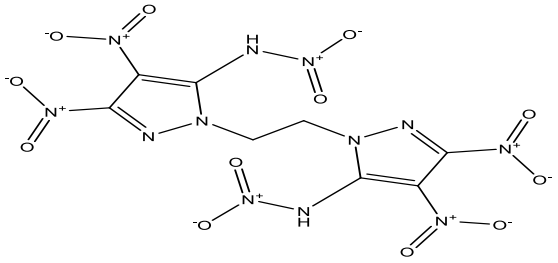
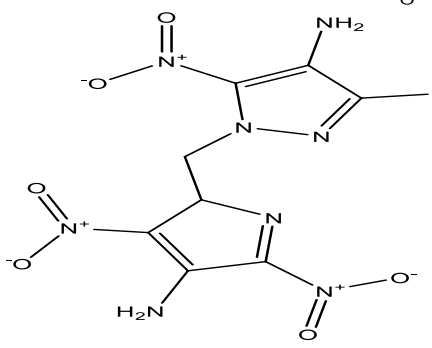
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
18		8.71	8.36
19		8.25	8.28
20		8.31	8.31
21		8.14	8.14
22		8.73	8.73
23		9.51	9.51

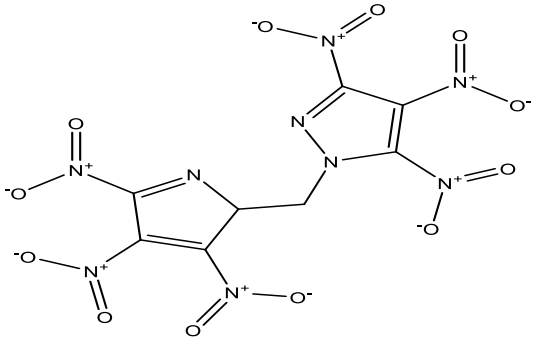
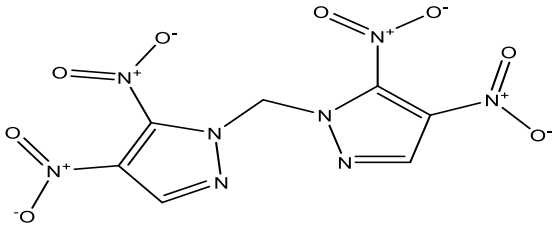
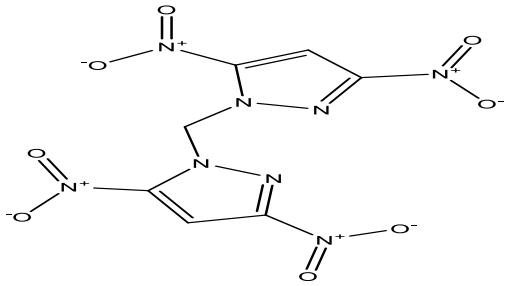
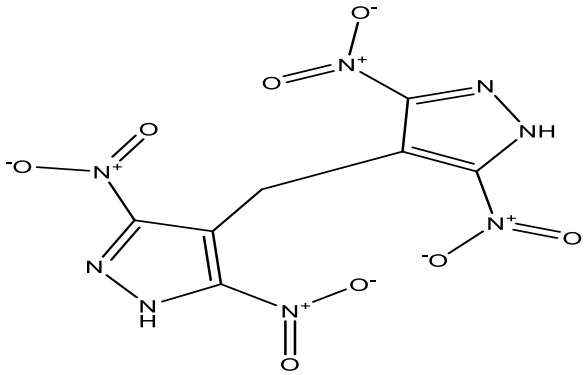
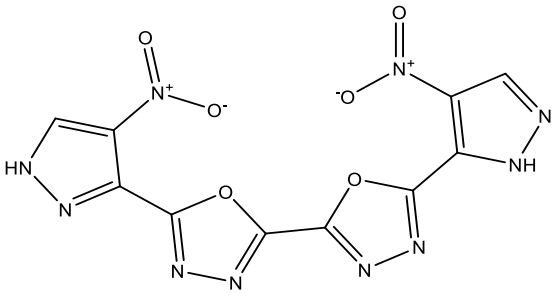
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
24		8.81	8.81
25		7.93	7.93
26		8.41	8.41
27		7.8	7.8
28		8.25	8.25
29		8.69	8.69
30		8.8	8.8

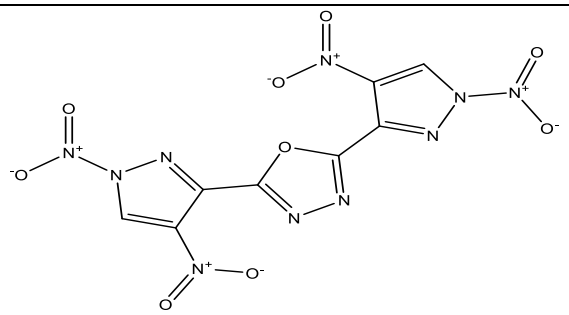
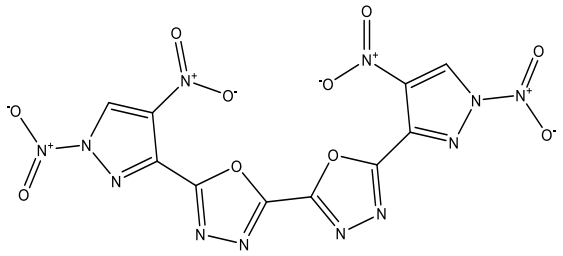
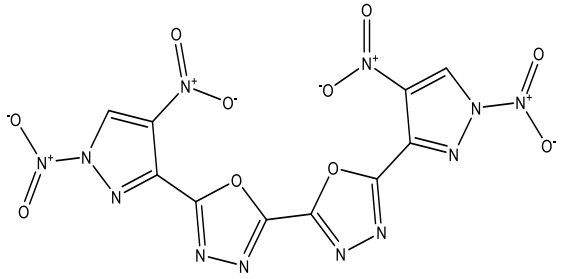
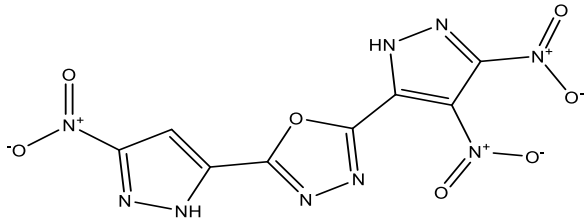
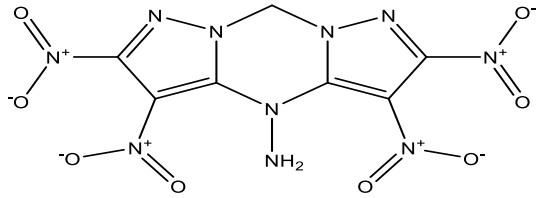
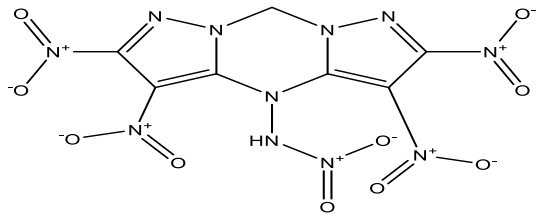
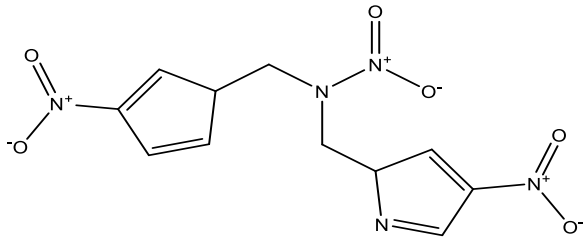
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
31		8.73	8.69
32		9.17	8.67
33		9.29	9.29
34		8.72	8.72
35		8.6	8.6
36		8.81	8.81

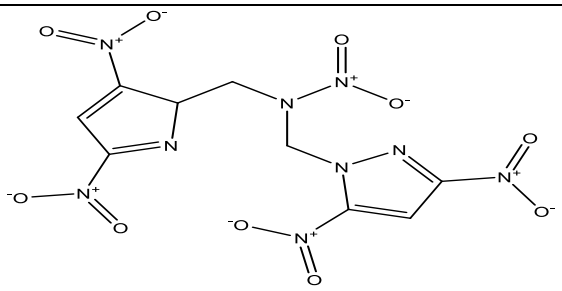
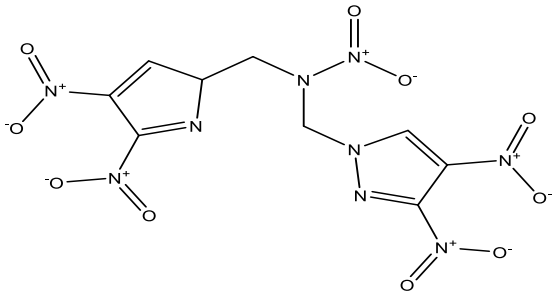
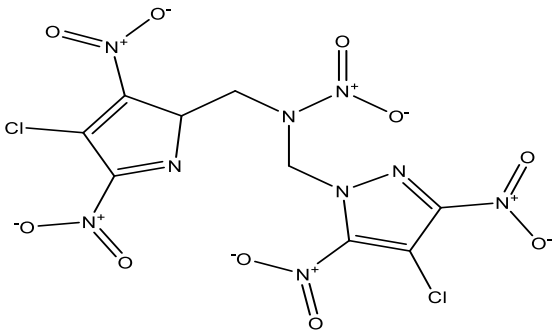
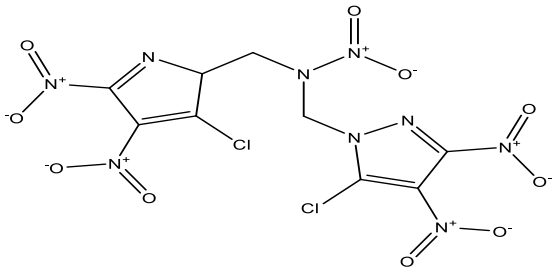
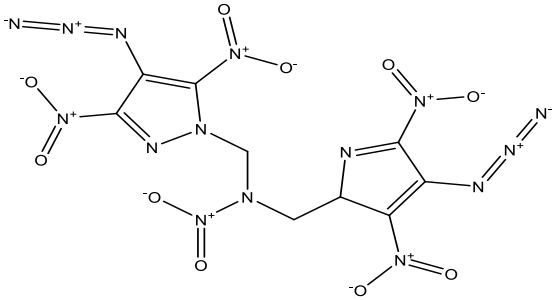
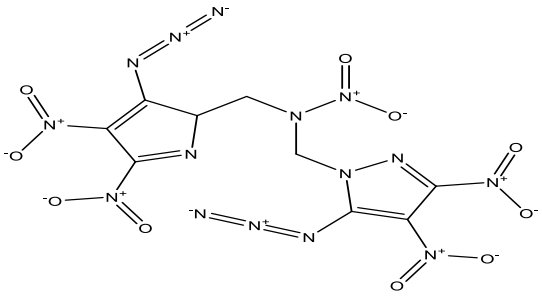
S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
37		8.65	8.65
38		8.5	8.5
39		8.99	8.99
40		8.04	8.04
41		8.72	8.72
42		7.53	7.53

S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
43		8.36	8.36
44		8.52	8.52
45		8.19	8.06
46		8.75	8.86
47		8.76	8.69

S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
48		8.8	8.54
49		7.88	7.98
50		8.56	8.56
51		8.13	8.13
52		8.71	8.71
53		8.33	8.33

S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
54		9.3	9.3
55		8.14	8.14
56		7.97	8.22
57		8.23	8.25
58		8.05	8.05

S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
59		8.86	8.86
60		8.77	8.77
61		8.71	8.71
62		8.54	8.54
63		8.36	8.36
64		9.23	9.23
65		7.87	7.87

S/N	2D Structures	Experimental Energetic Velocity,$_{P}EV$ (km/s)	Predicted Energetic Velocity, p*E*V (km/s)
66		8.26	8.26
67		8.27	8.27
68		8.06	8.30
69		8.04	8.36
70		8.72	8.84
71		8.72	8.72

QSPR Model Building and Validations

Software like Material Studio and Weka supporting Machine learning (ML) software were used to generate a robust QSPR model from the 51 compounds of training sets for its energetic velocity prediction. This ML software used an algorithm known as genetic function (GF) for the accurate prediction.

The ML-weka was used to calculate the predictive parameter (R^2_{int}), while the formally set aside 20 data were used to obtain external parameters ($R^2_{ext.}$) on the Excel (Ravichandran, 2011). Both parameter's values must be near 100% (1.0), but equal or above 50% (0.5). Also, the nearer the values of experimental and predicted properties to 100% (1.0), the nearer the R^2_{int} or R^2_{ext} values to 100% (1.0) (Ravichandran, 2011). The predictive parameters in equation 1 to 4 were used to ascertain the robustness of the generated models.

$$R^2_{int} = 1 - \frac{\sum(Yobs - Ypred)^2}{\sum(Yobs - Ytraining)^2} \quad (1)$$

$$R^2_{pred} = 1 - \frac{\sum[Y_{Pred\,(te)} - Y_{Pred\,(te)}]^2}{\sum[Y_{(te)} - Y_{m\,(tr)}]^2} \quad (2)$$

$$R^2_{adj} = 1 - (1 - R^2)\frac{N-1}{N-P-1} = \frac{(N-1)R^2 - P}{N-P+1} \quad (3)$$

$$Q^2_{CV} = 1 - \frac{\sum(Yp - Y)^2}{\sum(Y - Ym)^2} \quad (4)$$

From equation 1-4 (Ravichandran, 2011), observed/experimental property = Y_{obs} ,
Predicted/calculated property = Y_{pred},
Mean property observed = $Y_{training}$,
The predicted test set = Y_{pred}.(test),
Observed test set = Y(test),
Training set mean property value = $Y_{m(tr)}$,
Model descriptor's number = p,
Sample size = N,
Training set predicted property = Yp,
The training set observed property= Y, and
Training set of the mean property value = Y_m
The minimum systemic errors during model formation stages were determined with the aid of ML-weka software.

Novel EMs Designing Processes

After confirming the robustness of the generated model, mean effect (ME) analysis calculation was performed on an excel sheet and it was used to determine the descriptors' (independent variable) degree of contributors. After the actual independent variable had been ascertained, the applicability domain (Netzeva *et al.*, 2005) analysis was calculated to identify the specific compound's template from the 51 training compounds. The previously identified chemical descriptor with the highest magnitude/coefficient value was interpreted and the decoded information was used to perform structural modification on the EM template.

RESULTS AND DISCUSSION

QSPR Model Validations and Theoretical Properties Predictions

Four (4) regression QSPR models represented by equation 5 were built along with the EMs of 71 (Table 1). From models 1 to 4, the predictive parameters such as R^2ext, R^2int, R^2adj and Q^2_{CV} were compared and model 1 distinguished itself as the most robust and predictive (Ravichandran, 2011). Model 1's predictive parameters such as R^2int =0.9863 (98.63%) and R^2ext = 0.9400 (94.40%) correspond to the degree of agreement between EMs' calculated and observed properties (Table 1) (Ravichandran, 2011). The cross-validation parameter (Q^2_{CV}) value of 0.9764 and adjusted parameter (R^2adj) value of 0.9672 indicate the model's percentage stability of 97.64% and percentage reliability of 96.72% respectively. To further validate model one, the predictive R^2 of 0.9400 in Figure 1 was in agreement with the external parameter (R^2ext) of 0.9400. This implies that model 1 was predictive and robust and can be used to calculate both known and unknown chemical properties of interest (Abdulfatai *et al.,* 2018). Furthermore, the generated model 1's experimental error and the minimum expt. error for non-significant lack of fit, LOF (95%) were 0.0424 and 0.00 respectively. After this validation, model one was theoretically used to predict the energetic velocity ($_P$EV) properties of all the seventy-one compounds of EM (Table 1).

$$Y = a_0 + \sum_{i=1}^{n} a_i\chi_i \quad (5)$$

Where Y= $_P$D (Predictive energetic velocity property), ao = equation constant, xi = descriptor, ai = coefficient.

Figure 1: Test Set's Predicted Properties Vs Test Set's Experimental Properties

Designed Novel EM Compounds

To design a new compound, the selection of an actual descriptor that has the highest magnitude of contributions is the first step that needs to be taken into consideration after identifying the most stable and reliable model.

Model 1

pEV = - 0.143568583 ***SP-0** - 0.218421969 ***minaaN**+ 0.191336931 ***gmin** - 5.567341281 ***ETA_dEpsilon_C**+ 0.238327124 ***nHBAcc3**+6.889349. R^2ext = 0.9400, R^2int =0.9863, R^2adj =0.9672, Q^2_{CV} = 0.9764. Computed Experimental error = 0.0424. Min expt. error for non-significant LOF (95%) = 0.00000000

Model 2

pEV = - 0.155705492 * nAtom + 0.093498355 *nBondsS3 + 0.099624303 *gmin + 0.227599221 * nHBAcc3 + 0.312783501 *MLFER_S + 8.65103287. R^2ext = 0.5474, R^2int = 0.766349, R^2adj =0.738534, Q^2_{CV} = 0.676205. Computed Experimental error = 0.0424. Min expt. error for non-significant LOF (95%) = 0.00000000

Model 3

pEV = - 0.155327390 * nAtom + 0.061832477 *nBondsS3- 0.215264108 *minaaN + 0.132795219 * gmin + 0.318304922 *nHBAcc3+9.423419411. R^2ext = 0.5378, R^2int =0.763923, R^2adj =0.735818, Q^2_{CV} = 0.692243. Computed Experimental error = 0.0424. Min expt. error for non-significant LOF (95%) = 0.00000000

Model 4

pEV = - 0.627742977 * BCUTp-1l + 0.071135327 *ETA_Epsilon_4+ 5.220096825 * ETA_Epsilon_4 + 4.773889400 *ETA_BetaP_ns_d + 0.241238218 *MLFER_S+5.736935. R^2ext =0.51374, R^2int =0.76349, R^2adj =0.735334, Q^2_{CV} = 0.663824. Computed Experimental error = 0.0424. Min expt. error for non-significant LOF (95%) = 0.00000000.

To achieve this, mean effect statistical analysis was performed and the output of the analysis shows that the ETA_dEpsilon_C descriptor has the highest magnitude of contribution than the other co-descriptors present in model one (Table 2).

Table 2: Mean Effect Statistical Values

S/N	Regression Variables	Mean Effect Values
1	SP-0	0.393768
2	minaaN	0.237094
3	gmin	0.004097
4	ETA_dEpsilon_C	0.518564
5	nHBAcc3	0.145329

A literature search revealed that this descriptor (ETA_dEpsilon_C) was a topo-chemical descriptor that accounts for the need to have more electronegative atoms (Roy and Ghosh, 2004) substituents on the EM template structure. This descriptor was also found to be the first to be identified during the model building development by the material studio software 'generation counter (Figure 2).

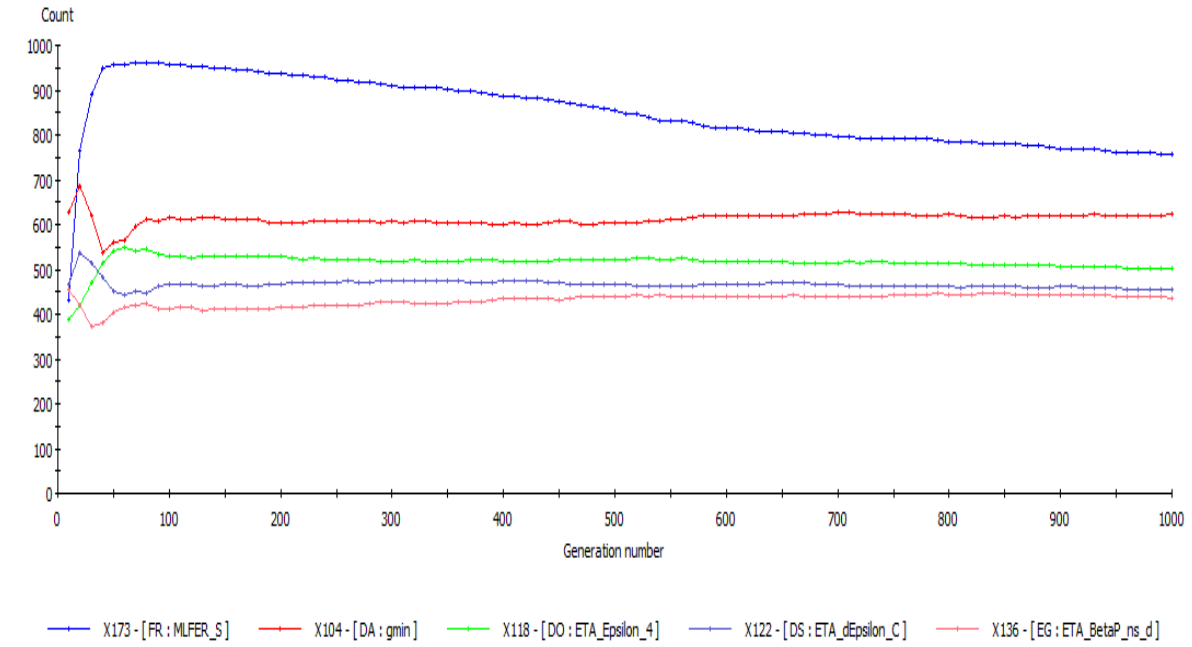


Figure 2: A Graph of Descriptors' Generation Number Vs Count Number

Also, to know the actual template compound for new compounds' structural modifications, the applicability domain leverage graph (Figure 3) was plotted and the template EM compound (Figure 3.4) was revealed to identify a compound with serial number 23 (Table 1) and the IUPAC name is N,N'-(3,6-dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)dinitramide.

The compound with a serial number 24 was found to have the standardized residual error and the leverage value nearness to zero (Figure 3). Moreover, the difference between the compound's experimental and predicted properties (Table 1) was also found to be zero (0).

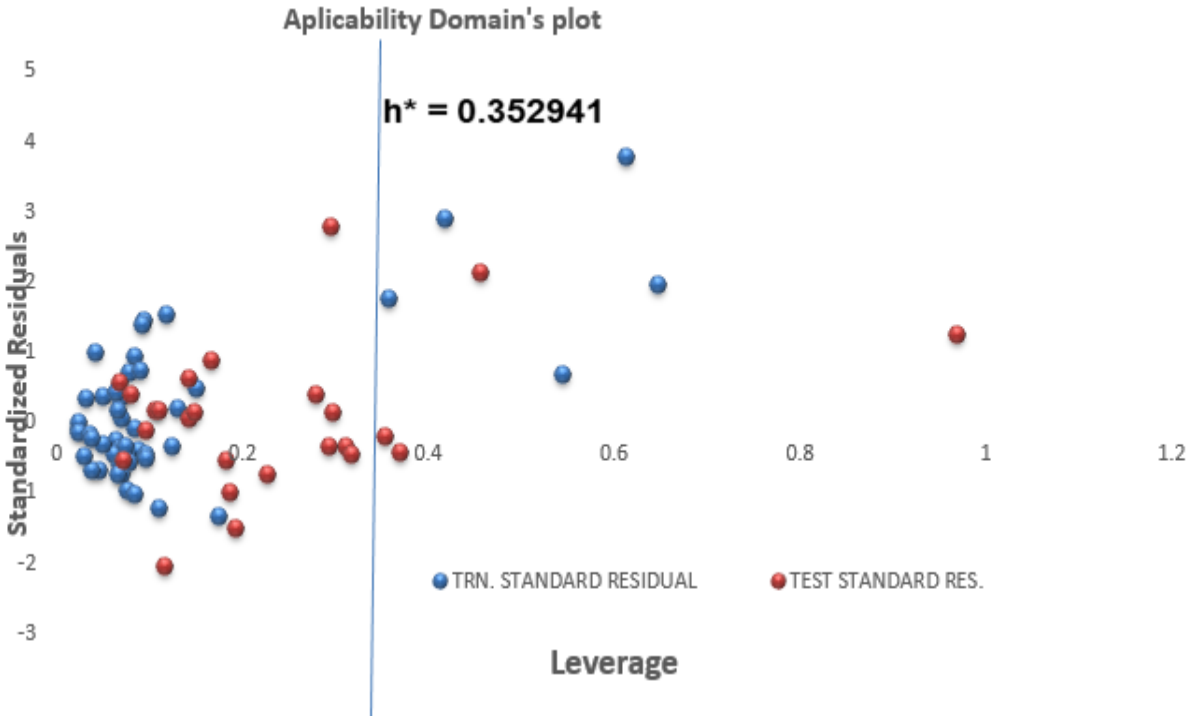


Figure 3: AD Leverage Graph

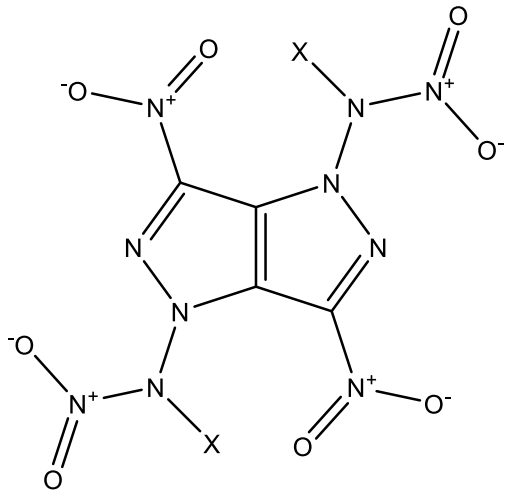
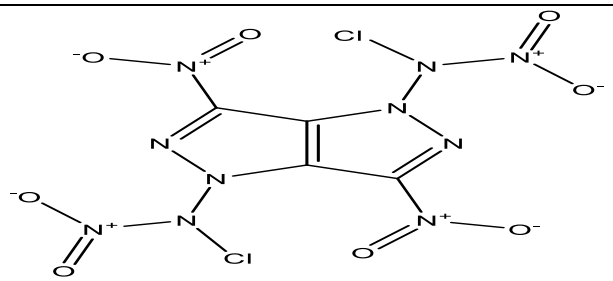
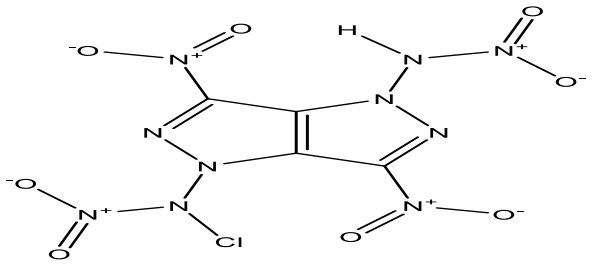
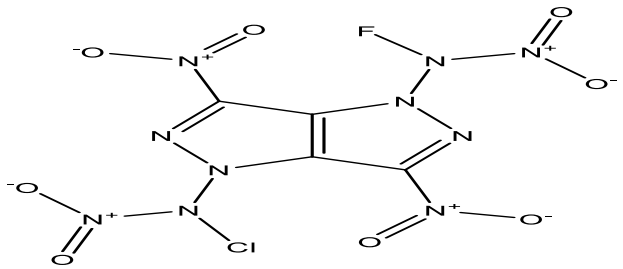


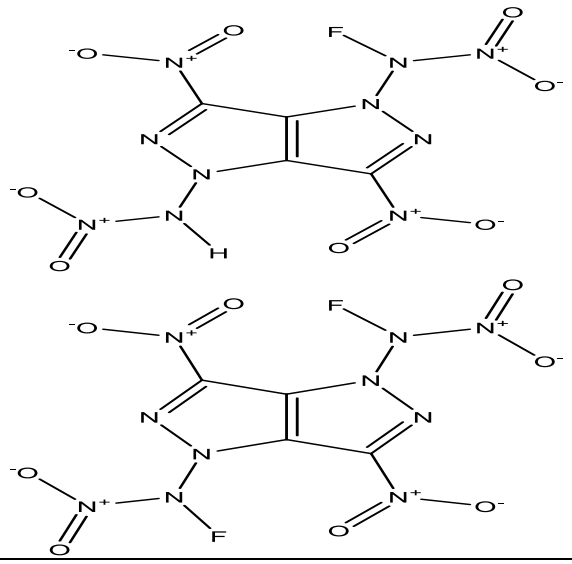
Figure 4: EM Template Compound

Newly Designed EM Compound's Energetic velocity Properties Calculations

After identify the need to add some electronegative compounds to the structural template, some electronegative atoms like F, Cl and O were systematically added to the attachment sites (X and Y) of the EM template compound in Figure 4. After that five new EVs were carefully designed (Table 3). All these five new EVs were subsequently subjected to geometric optimizations, and their molecular descriptors that decode the energetic information in the structures of those compounds were extracted and presented in the numerical values (Table 3). These molecular descriptors' numerical values were computed in equation 1 (Model 1). Subsequently, the energetic velocities (pEV) properties were calculated for all five newly designed structures.

Table 3: The Five Newly Designed Energetic Compounds with their Energetic Velocities

S/N	Novel 2D Structures	New Energetic Velocities, (pEV)
1		10.33
2		10.22
3		10.531
4		10.436

5		10.835

In Table 3., the newly designed EMs with serial number 1 were N, N'-(3, 6-dinitropyrazolo [4, 3-c] pyrazole-1, 4-diyl) bis (N-chloronitramide). This novel compound has a unique energetic velocity property of 10.33 Km/s. Other newly designed EMs were N-chloro-N-(3,6-dinitro-4-(nitroamino)pyrazolo[4,3-c]pyrazol-1(4H)-yl)nitramide with the energetic velocity of 10.22 Km/s, N-(4 (chloro(nitro)amino)-3,6-dinitropyrazolo[4,3-c]pyrazol-1(4H)-yl)-N-fluoronitramide with the energetic velocity of 10.531 Km/s, N-(3,6 dinitro-4-(nitroamino)pyrazolo[4,3-c]pyrazol-1(4H)-yl)-N-fluoronitramide with the energetic velocity of 10.436 Km/s and N, N'-(3,6 dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)bis(N-fluoronitramide) with the energetic velocity of 10.835 Km/s. When compared with the literature and with the standard energetic velocity(*EV* > 8.5 km/s), all the five designed EMs were found to have better energetic velocity properties of 10.22 to 10.835 km/s than the experimental EMs in Table 1 and those reported in the kinds of literature (Wong *et al*., 2021; Zhang *et al.*, 2020; Li *et al*., 2014; Yin *et al*., 2014). This means that the high magnitude of energetic velocity properties of all the newly designed explosive compounds implies that when the explosive compound explode they will have a devastating impact that can be felt in a distance of one kilometer apart radius than the TNT (Wong *et al*., 2021; Liu *et al*., 2021; Zhang *et al*., 2020).

CONCLUSION

An in-silico software such as Weka version 3.8.5 machine learning software has been used in this research to carry out the accurate energetic velocities predictions and to develop and generate four (4) novel models from the seventy-one (71) experimental EM compounds. Also, the quantitative structural property relationship (QSPR) research tool was used to design five (5) new EM along with their new energetic velocities (EV) of 10.835 Km/s, 10.22 Km/s, 10.531 Km/s, 10.436 Km/s, and 10.33 Km/s. The N, N'-(3, 6-dinitropyrazolo [4, 3-c] pyrazole-1, 4-diyl) bis (N-chloronitramide), N, N'-(3, 6-dinitropyrazolo [4, 3-c] pyrazole-1, 4-diyl) bis (N-chloronitramide), N-chloro-N-(3,6-dinitro-4-(nitroamino)pyrazolo[4,3-c]pyrazol-1(4H)-yl)nitramide, N-(4 (chloro(nitro)amino)-3,6-dinitropyrazolo[4,3-c]pyrazol-1(4H)-yl)-N-fluoronitramide, N-(3,6dinitro-4 (nitroamino)pyrazolo[4,3-c]pyrazol-1(4H)-yl)-N-fluoronitramide and N, N'-(3,6 dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)bis(N-fluoronitramide) were the five unique energetic compounds designed. The energetic velocities of all the EMs were better than those reported in the literature and also better than the standard energetic compounds i.e. TNT. Because of their unique energetic properties, energetic compounds such as N, N'-(3,6 dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)bis(N-fluoronitramide) should be given special consideration while synthesizing those compounds. Furthermore, the results of this research have proven the scientific importance of the usage of QSPR as a research tool in the field of energetic compounds.

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