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In Silico Modeling, Prediction, and Designing of Some Anti-wear Lubricant Additives

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Abstract
For many decades, scientists in the field of boundary tribology have been working to find an excellent and environment friendly anti-wear additives to minimize wearing of the boundary equipment by improving the anti-wearing ability of the boundary lubricants. Four (4) anti-wear lubricant additives with better properties were carefully designed with the aids of QSPR and MD simulation methodologies. Out of the four newly designed additives, 2, 3, 5-trimethylheptyl acetate with the anti-wear property of 2.0802 mm was found to have better anti-wear lubricant property than its co-additives as well as the standard AW additive, Zinc dipropyl dithiophosphate (ZDDP). All the additives were found to have better boundary dynamic binding energy as well as high dynamic binding temperatures on steel-simulated coated surface than on DLC-coated surface. The boundary dynamic binding energy of all these anti-wear additives was found to be better than the ZDDP. And they could improve the anti-wear property of lubricant at elevated temperature without being decomposed since they have a high dynamic binding tribological temperature. Moreover, all these new anti-wear lubricant additives structures do not contain zinc (catalytic converters deactivator), sulfur (acidic oxide), and phosphorus (exhaust pipe ashes producer) and could be used to replace the widely used additive, ZDDP, which contains zinc and phosphorus and has less active (3.284 mm) additive property. Due to their better structures and properties correlation ability, these two methods could be used to provide a theoretical framework for engineers and other researchers to design a better anti-wear base oil additive before laboratory synthesis.

Keywords QSPR · Lubricant additive · DLC · MD · Dynamic binding energy · MD simulation

1 Introduction

Scientists in the field of boundary tribology have been working for many decades to find excellent and environment friendly anti-wear additives to minimize wearing of the boundary equipment, pollution, and consumption of energy by improving the anti-wearing ability of the boundary lubricants. It was reported by some scientists that 50 to 95% of the global energy is usually consumed by the machine's sliding components wearing of different types [1–3]. To improve the mechanical sliding components performance and curbing environmental pollution as well as to improve the global economy, wearing caused by the lubricating oil must be modified. Addition of anti-wear additives to the lubricating oil has been recommended by many researchers to modified working equipment lubricating oil wear since heavy duty sliding equipment has been reported to be damaged due to wearing of such equipment [4, 5]. Anti-wear lubricant additives are chemical compounds added to the base stock to improve the lubricating oil properties [1–8].

Since many decades ago, scientists in the field of boundary tribology have been working to find excellent and environment friendly anti-wear additive to minimize wearing of the lubricant boundary problems [9]. Since the last five decades, many different classes of anti-wear polar additive compounds like Organo-sulfur and organo-phosphorus, organo-molybdenum, and nanoparticles have been used in that order extensively. The usual disadvantage with these classes of boundary oil additives was due to their expensiveness and high level of corrosion properties [10–16]. Another most used anti-wear additive is the multipurpose base oil additive, Zinc dipropyl dithiophosphate (ZDDP). This additive is the most commonly used multifunctional additive in the oil industry since the Second World War. It protects the metal surfaces from wearing by forming sulfides and phosphates

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film. This multipurpose additive was reported elsewhere that its constituent phosphorus (P) restricts the function of catalytic converters, while zinc (Zn) often produces ashes in the exhaust emissions pipe [15, 16].

Therefore, in silico quantitative structure–property relationships (QSPR) is a computational method that could be used to provide a theoretical framework for engineers and other researchers to design a better anti-wear base oil additive that is devoid of phosphorus, zinc, and sulfur before laboratory synthesis. This QSPR method could be used to save resources by avoiding expensive laboratory trial and error. In silico QSPR could relate the additive's properties with their structures to produce a mathematical linear model that could be used to design novel base oil additives. In view of this, QSPR was used to design some excellent novel anti-wear additives, while molecular dynamic (MD) simulation method was also used to obtain the severe working boundary dynamic binding energies of some novel designed additives and boundary-coated equipment [17–19].

2 Experimental Section Details

2.1 Data Set Collections

The set of anti-wear lubricant additives data used for correlating the additive's anti-wear properties (mm) and the structures together was 25 compounds [20]. Unlike ZDDP, the experimental chemical structures of all the additives do not contain sulfur, phosphorus, and zinc which may produce harmful gases into the environment. These chemical structures of the additives were retrieved and drawn with the aids of Chemdrawn software (Fig. 1). All the two-dimensional drawn additive's chemical structures contained an excellent anti-wear property (Table 1).

2.2 Molecular Descriptors Generation and QSPR Model Building

The 2D additives chemical structures in Table 1 were saved in cdx file format in ChemDraw software and uploaded unto the Spartan 14 multipurpose software. Using B3LYP (level of theory) and 6–311 (basis set) of density functional theory, Spartan 14 software was used to perform geometrical optimization of all the 25 anti-wear lubricant additives. The optimized additives were saved in sdf and uploaded unto the dragon and padel toolkit software where 4832 molecular descriptors were generated [17, 21]. The 4832 generated molecular descriptors from 25 anti-wear additives were grouped into test (30) and training (70) sets. Using Molegro Data Modeler 3.0, 70% of the training data set was used to generate many mathematical linear QSPR models (Eq. 1), while the test data sets were used to identify the quality of the generated models.

$$Y = a_0 + \sum_{i=1}^{n} a_i x_i \tag{1}$$

Y predicted anti-wear lubricant additive property (pAW), a_0 equation's intercept, x_i developed molecular descriptors ,and a_i descriptors coefficients. To test the quality of the constructed/developed QSPR model, some QSPR parameters must be determined by subjecting them into statistical evaluation [22]. The Coefficients of internal additive set, R^2 (Eq. 2), adjusted R^2_{adj} (Eq. 3), *PRESS* (Eq. 4) cross-validated q^2/R^2_{cv} (Eq. 5), and external statistical validation R^2_{ext} (Eq. 6), must be less than one, but greater than 0.5 [22].

Moreover, the selected descriptors contribution to the constructed model was derived/identified in terms of mean effect (MF) value in Eq. 7 [23].

$$R^2 = 1 - \frac{\sum \left(Y_{obs} - Y_{calc}\right)^2}{\sum \left(Y_{obs} - \overline{Y}_{obs}\right)^2} \tag{2}$$

$$\text{Adjusted } r^2 = 1 - \left(1 - r^2\right)\frac{N-1}{N-P-1} \tag{3}$$

$$\text{PRESS} = \sum_{i=1}^{N} \left(x_{pred,i} - x_{obs,i}\right)^2 \tag{4}$$

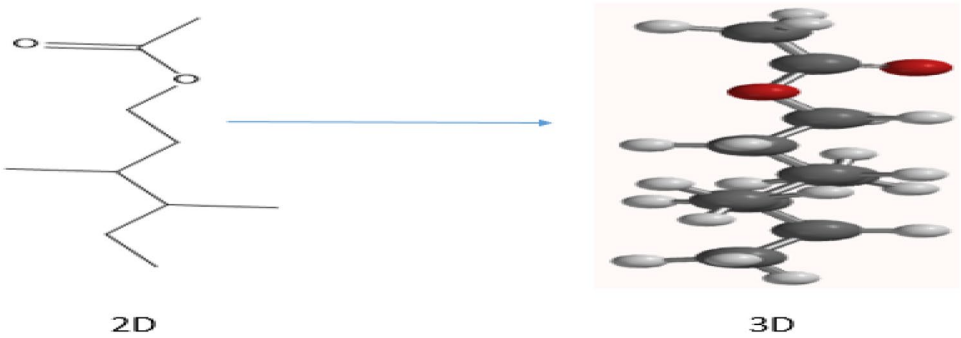


Fig. 1 2D and 3D of lubricant anti-wear additive

Table 1 Experimental properties, predicted properties, and anti-wear lubricant additives

S/N	Structures of anti-wear(AW) lubricant additives	Exp.AW properties (mm)	Pred. AW properties (mm)	Standard residual
1y	Butyl octanoate	2.4629	2.4187	0.487205
2y	Butyl decanoate	2.5733	2.52415	−0.41794
3y	Butyl dodecanoate	2.5225	2.51508	0.429716
4y	Butyl tetradecanoate	2.6152	2.64984	−0.89153
5x	Butyl dodecanoate	2.682	2.66954	−0.12079
6y	Butyl (E)-hexadec-9-enoate	2.6106	2.67809	−0.20694
7y	Methyl decanoate	2.4573	2.47989	−1.36449
8x	Methyl dodecanoate	2.5249	2.452	−0.12249
9x	Methyl palmitate	2.6327	2.65201	−0.81072
10y	Octyl acetate	2.2724	2.37463	0.132095
11y	Ethyl octanoate	2.4509	2.42896	−0.32698
12x	Ethyl dodecanoate	2.5952	2.5304	−0.37378
13y	Ethyl palmitatez	2.6759	2.66837	−0.7631
14y	2-ethylhexyl acrylate	2.3288	2.31195	3.076305
15x	8-methylnonyl methacrylate	2.4517	2.52683	−1.12679
16x	Heptadecyl methacrylate	2.7167	2.66143	0.763153
17y	Phenyl methacrylate	2.2965	2.28748	1.450739
18y	4-ethylhexyl methacrylate	2.4754	2.45584	−0.45276
19x	Isopropyl tetradecanoate	2.6327	2.47356	1.972354
20x	Isopropyl palmitate	2.6299	2.58933	1.461885
21y	Heptan-3-yl 3-(4-methoxyphenyl)propanoate	2.7554	2.69556	0.274287
22y	(6-oxabicyclo[3.1.0]hexan-3-yl)methyl6-oxabicyclo[3.1.0]hexane-3-carboxylate	2.4881	2.50211	-0.20996
23y	2-(oct-1-en-2-yloxy)ethyl heptanoate	2.5276	2.52664	0.252457
24y	(E)-4-oxohenicos-12-en-1-yl(E)-octadec-9-enoate	2.9109	3.85252	−0.54229
25x	Butane-1,4-diyl dioctanoate	2.6773	2.67283	0.20197

AW anti-wear, *x* test sets, *y* trainin sets

$$q^2 = 1 - \frac{\text{PRESS}}{\sum_{i=1}^{N} \left(x_{\text{obs,i}} - \overline{x_{\text{obs,i}}}\right)} \quad (5)$$

$$R^2_{\text{pred}} = 1 - \frac{\sum \left(Y_{\text{obs(test)}} - Y_{\text{pred(test)}}\right)^2}{\sum \left(Y_{\text{obs(test)}} - Y_{\text{training}}\right)^2} \quad (6)$$

$$MF_j = \frac{\beta_j \sum_{i=1}^{i=n} d_{ij}}{\sum_j^m d_{ij}\beta_j \sum_i^n d_{ij}} \quad (7)$$

where X_{pred} is the predicted additive variable, X_{obs} is the observed additive variable, Y_{obs} is the experimental training data set anti-friction additive properties, Y_{calc} is the calculated training data set on AW properties, $Y_{\text{obs(test)}}$ is the experimental AW additive properties for test set, $Y_{\text{pred(test)}}$ is the predicted data test set additive properties, N is the number of molecules in the data, R^2 is the determination coefficient, *and* p is descriptors number in the QSPR model, while $N-1-p$ is degree of freedom, j QSPR model's descriptor, β_j descriptor's coefficient, d_{ij} training set data matrix's descriptor value, m sum of model's descriptors, and n all training set's molecules.

2.3 Additive's Molecular Dynamics (MD) Simulation Methodology

The comprehension of the interactions of various greasing up oil added substances with this material isn't yet completely developed, but it was reported in the literature that high dynamic binding energy and sp3 hybridization between Diamond-like carbon (DLC) and lubricant additives does not accelerate base oil wearing [24–27]. DLC is an astounding covering material, and it has been accounted to be exceptionally compelling in dealing with the motors fuel energy utilization by forestalling mechanical seizure [28]. To understand, the structural and dynamic binding energy between the DLC/Steel-simulated boundary-coated surfaces and potentially designed lubricant anti-wear additives were accessed, and molecular dynamics (MD) simulation investigation was studied [17, 29, 30]. COMPASS II which is a

strong and well-created power field was determined depending on the fitting capacity against a wide scope of inorganic and synthetic organic compounds [31] selected from the studio of the materials 8.0 toolbar. MD simulation binding energy (B.E) calculations were done subsequently after presenting the minimized lubricating base oil additive compound unto the simulation vacuum slab of optimized DLC/Steel crystal (24.82 Å × 24.82 Å × 45.27 Å) surface at a high temperature of 350.15 K and over a range of inter-surface separations. The interaction dynamic binding energy was determined by using Eqs. 8 and 9 [31].

$$\text{B.E} = E_{\text{total}} - \left(E_{\text{Lubricant Additive}} + E_{\text{DLC Surface}}\right) \quad (8)$$

$$\text{B.E} = E_{\text{total}} - \left(E_{\text{Lubricant Additive}} + E_{\text{steel Surface}}\right) \quad (9)$$

3 Results and Discussion

A molecular modeling study was carried out to examine the property and structure relationship of 25 organic compounds as anti-wear base oil additives. Three QSPR linear models were developed with the aids of the material studio and molegro data modeler 3.0 software to help in designing some novel anti-wear lubricating base oil additives. After performing a diligent examination on all the three developed QSPR linear models, the second model was found to have better coefficients such as internal R^2_{internal} (0.90843), external/predicted R^2_{ext} (0.7209), adjusted R^2_{adj} (0.8507), and cross-validated R^2_{cv} (0.90843) [32]. Therefore, the second model was reliable and was used to design organic compounds with better anti-wear lubricant properties since there were no obvious variations between the experimental and predicted properties of the lubricating oil anti-wear p(AW) additives (Table 1).

3.1 1st QSPR Model

p(AW) = 0.95207 * **RNCS** − 0.85298 * "**Weta3.mass**" − 0.853297 * "**WV.mass**" + 0.85239* "**Weta2.eneg**" + 2.82097. R^2_{ext} (0.5692), R^2_{internal} (0.7432186), R^2_{adj} (0.5972), R^2_{cv} (0.64296).

3.2 2nd QSPR Model

p(AW) = 0.00993976 * **RNCS** + 0.162303 * "**Weta3.mass**" + 0.00431547 * "**WV.mass**" + 0.629144 * "**Weta2.eneg**" + 1.8537. R^2_{ext} (0.7209), R^2_{internal} (0.90843), R^2_{adj} (0.8507), R^2_{cv} (0.90843).

3.3 3rd QSPR Model

p(AW) = 0.09934965 * **RNCS** + 0.74298 * "**Weta3.mass**" + 0.00431547 * "**WV.mass**" + 0.629144 * "**Weta2.eneg**"—3.9753. R^2_{ext} (0.684), R^2_{internal} (0.6983), R^2_{adj} (0.7564), R^2_{cv} (0.8285).

The predicted internal ($R^2_{\text{internal}} = 0.90843$) value derived from molegro data modeler 3.0 software was consistentwith the predicted R^2 of 0.9084 obtained from the plotted graph (Fig. 2). Also, the external predicted ($R^2_{\text{external}} = 0.7209$) value obtained by using Eq. 6 was the same with R^2 of 0.7209 value obtained from Fig. 2 plot. Figure 3 also revealed the reliability of the developed QSPR model since the dispersion of coefficient of residual (Experimentally Predicted AW Lubricant Additives) anti-friction lubricant

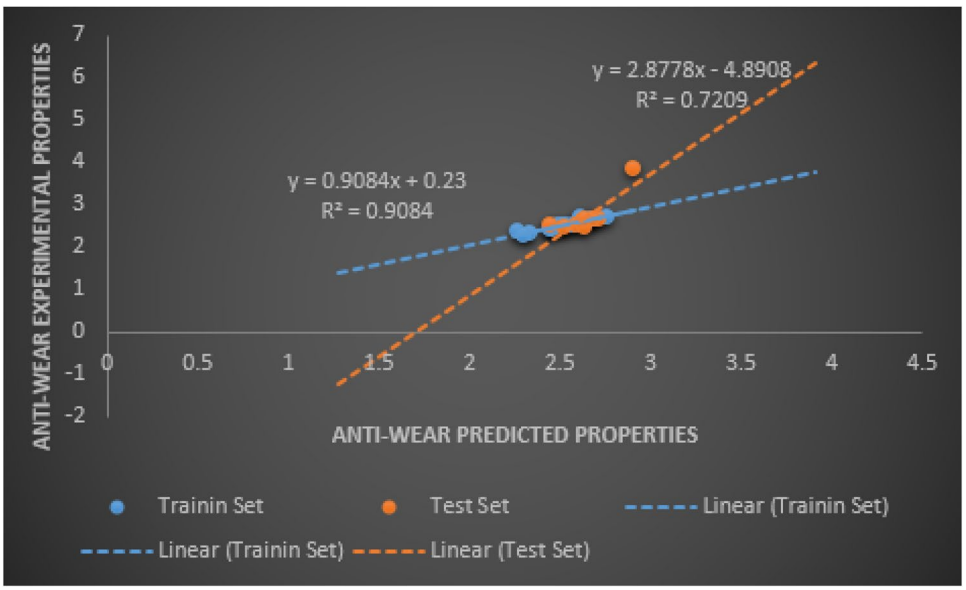


Fig. 2 Graph of experimental against the predicted properties of AW training and test sets

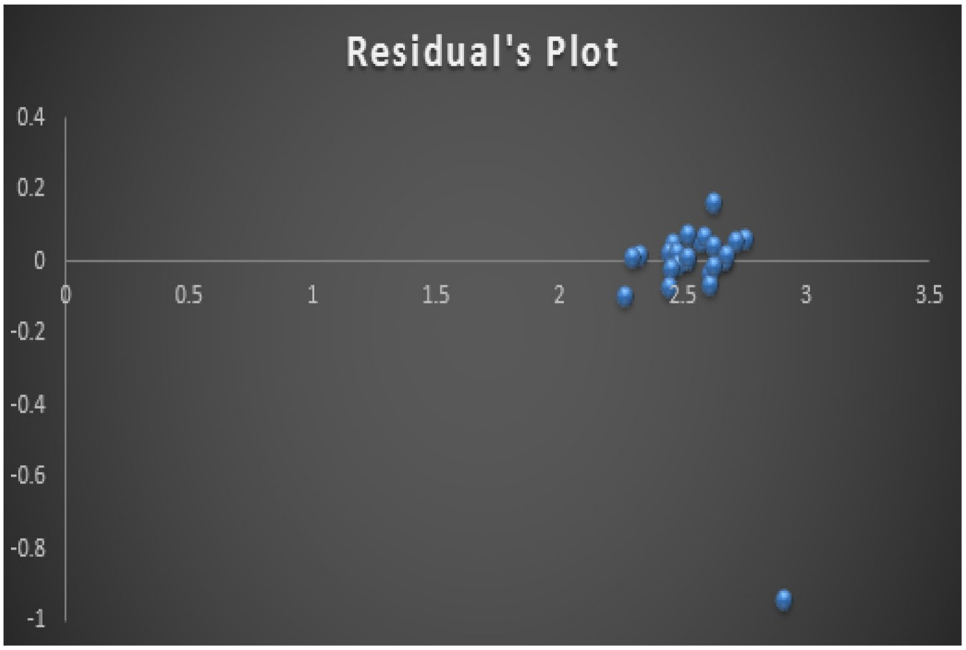


Fig. 3 Graph of Experimental against the residual properties of AW training and test sets

additives on the two sides of the plotted graph was observed [17]. Moreover, QSPR molecular descriptors' correlation analysis in Table 2 revealed that the coefficient correlation between the generated molecular descriptors was very low, and this was due to the non-significant inter-correlation among those molecular descriptors used in the development of AW QSPR model.

3.4 Evaluation of Designed Anti-wear Additives

The first two steps that were taken for the designing of some anti-wear lubricant additives were the identification of the most contributed molecular descriptor toward the developed QSPR model and selection of additive template from the pool of experimental lubricant additives in Table 1 [33].The excel worksheet of Molegro data modeler 6.3 was used to identify the most relevant descriptor out of the four molecular descriptors generated from the most reliable QSPR model (2nd QSPR model). Figure 4 represents a plot of relevancy values against molecular descriptors. From Table 2 and Fig. 4, it shows WV.Mass molecular descriptor contributed more to the development of the 2nd QSPR model due to high relevancy value than other co-descriptor [17].

Moreover, the second stage was the operation and statistical analysis of applicability domain to identify the set of molecular additives found within the domain and the outliers or influential additive compounds outside the domain, h^* (Eq. 10) [34] where m number of descriptors that appear in a QSPR linear model (4) and n is the number of training set molecule only (16).

$$h* = \frac{3(m + 1)}{n} \tag{10}$$

In Fig. 5, those AW lubricant additives that were found outside the leverage boundary, h^*, were called influential compounds because they were not similar to the majority of the lubricant anti-wear additives used for the QSPR model development.

From the applicability domain figure, anti-wear lubricant additives with a serial number 24 (standard residual of − 0.54229) were termed influential compounds [34]. The AW lubricant additive with serial number 10 was found to have a standard residual value of 0.132095 (Table 1 and Fig. 5) and was selected as design template (Fig. 5) to which other structural substituents were

Table 2 Used molecular descriptors correlation analysis

Descriptors	RNCS	Weta3.mass	WV.mass	Weta2.eneg	Descriptor's relevancy
RNCS	1				0.143366
Weta3.mass	0.094914	1			0.250078
WV.mass	− 0.43396	0.117192	1		0.868288
Weta2.eneg	0.244205	− 0.37503	0.116002	1	0.309499

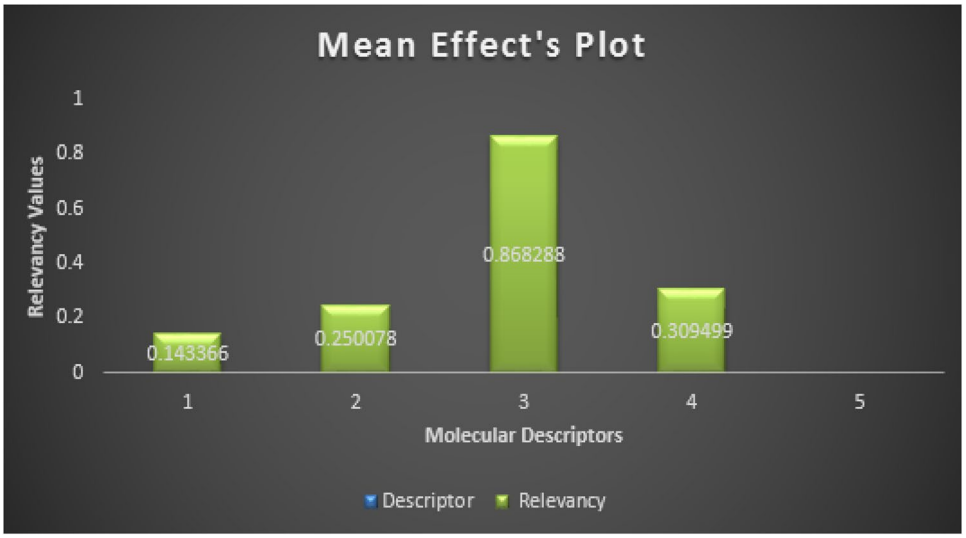


Fig. 4 Graph of molecular descriptor relevancy

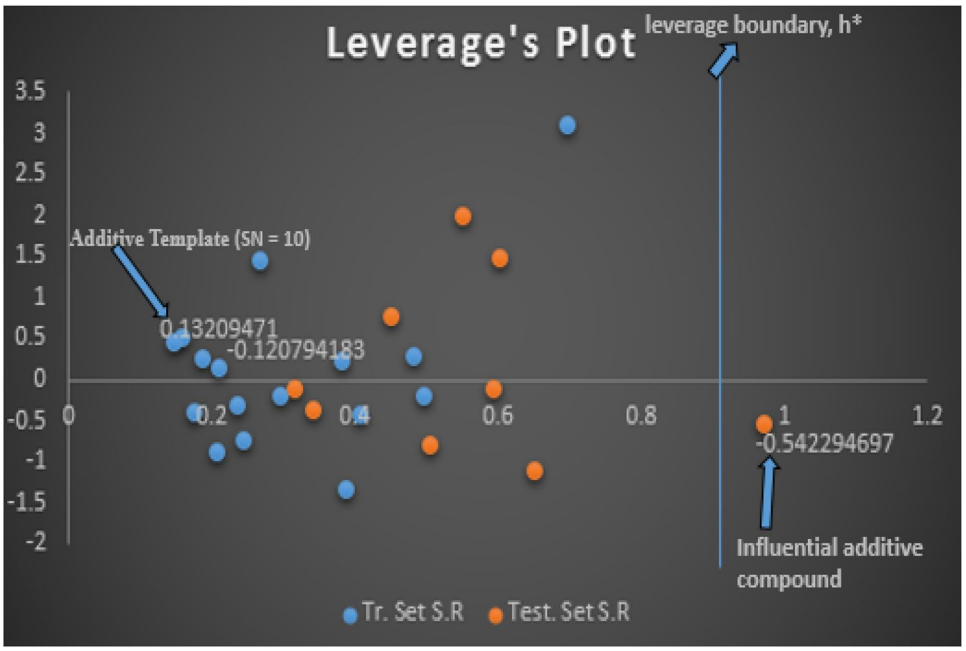


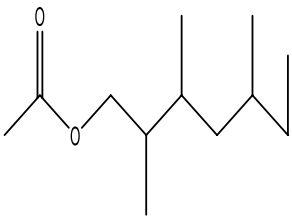
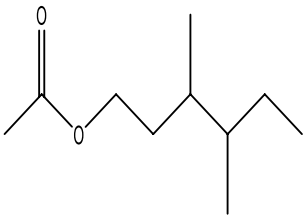
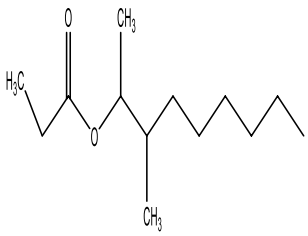
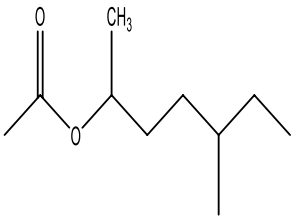
Fig. 5 The Williams plot of standardized residual versus leverage for the 2nd model

attached to this template on the information extracted from WV.mass (3D weighted by atomic masses) molecular descriptor (Table 2). WV.mass is a 3D hydrophobic or hydrogen bonding capacity descriptor [35]. The addition of substituents like $–CH_3$ or $–C_2H_5$ on the additive template was found to increase the AW lubricant properties of some four newly designed additives (Table 3). Out of these four, newly designed AW lubricant additives such as 2,3,5-trimethylheptyl acetate (2.0802 mm), 3,4-dimethylhexyl acetate (2.1135 mm), 3-methylnonan-2-yl propionate (2.1112 mm), and 5-methylheptan-2-yl ac`etate (2.1026 mm) were found to possess excellent anti-wear properties than the one reported by other researchers [35]. From Table 3, the lubricant additive with the highest anti-wear value was found to be 2,3,5-trimethylheptyl acetate (2.0802 mm).

3.5 Assessment of Molecular Dynamic Binding Energy

Material studio software was used to optimize all the four designed additives as well as simulated coated sliding surfaces of DLC and steel (Fig. 6) before dynamic energies were calculated one after the other. Equations 8 and 9 were used to calculate the dynamic binding energies between the designed anti-wear additives and DLC as well as steel-coated interfaces. The dynamic binding energies for the newly designed anti-wear lubricant additives on DLC

Table 3 AW lubricant additives properties and molecular dynamic simulation energies

S/N	Newly designed 2D AW lubricant additives	pAWLAP (mm)	DLC-AWLA		Steal-AWLA	
			Dynamic binding energy (kcal/mol)	Dynamic binding temperature (K)	Dynamic binding energy (kcal/mol)	Dynamic binding temperature (K)
1		2.0802	− 40.812	148.951	− 12562	148.691
2		2.1135	− 39.299	149.042	− 448.1	148.785
3		2.1112	− 29.299	149.011	− 1333	274.41
4		2.1026	− 47.066	149.08	− 9162.3	149.066

AWLAP Anti-wear Lubricant Additives Properties, *P* theoretical prediction, *DLC* Diamond-Like Carbon

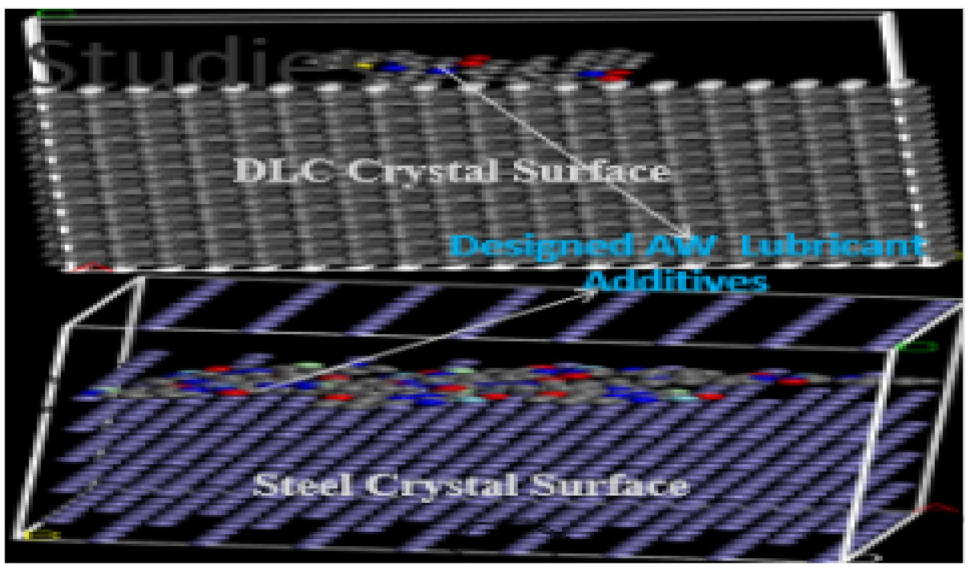


Fig. 6 Designed AW lubricant additives on DLC and steel crystal surfaces

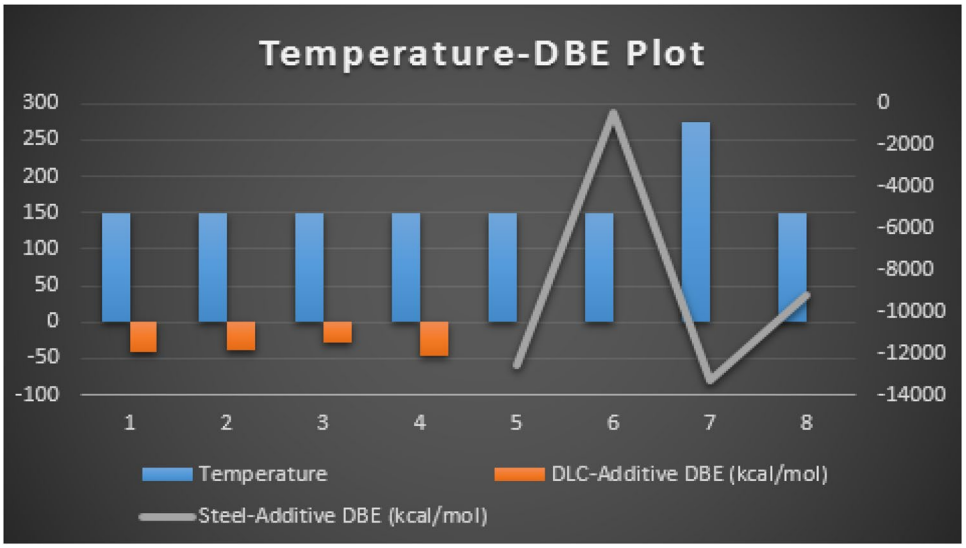


Fig. 7 The plot of dynamic binding energy and dynamic binding temperature of the newly designed additives

(−40.812, −39.299, −29.299, −47.066 kcal/mol) and steel (−12,562, −448.1, −1333, −9162.3 kcal/mol) simulated coated sliding surfaces (Table 3).

All the additives were found to have better boundary dynamic binding energy on steel-simulated coated surface than on DLC-coated surface. Moreover, Fig. 7 shows temperatures of various tribological dynamic binding energies . The boundary dynamic binding energy temperatures range from 148.691 to 274.41 K for all the four anti-wear lubricant additives **on both the DLC and steel surfaces. The 3-methylnonan-2-yl propionate with anti-wear lubricant property of 2.1112 mm and boundary dynamic binding energy of − 1333 kcal/mol were found to have better dynamic binding working temperature of 274.41 K than other co-additives (Fig. 7). The 3-methylnonan-2-yl propionate additive could improve the anti-wear property of lubricant at elevated temperature since it has a high dynamic binding temperature of 274.41 K.

4 Conclusion

Four (4) anti-wear lubricant additives with better properties were carefully designed with the aid of QSPR and MD simulation methods. Out of the four newly designed additives, 2,3,5-trimethylheptyl acetate with the anti-wear property of 2.0802 mm was found to have an excellent anti-wear lubricant property than its co-additives as well as standard additive, ZDDP (3.284 mm), and the one reported by other authors [20]. These four additives were found to have better boundary dynamic binding energy as well as high dynamic temperatures on steel-simulated coated surface than on DLC-coated surface. The boundary dynamic binding energy of all these anti-wear additives was found to be better than the standard anti-wear additive ZDDP and other researchers [36]. Also, the 3-methylnonan-2-yl propionate additive, in particular, could improve the AW property of lubricant at elevated temperature since it has a high dynamic binding temperature of 274.41 K. All the four new anti-wear lubricant additives' structures do not contain zinc (catalytic converters deactivator), sulfur (acidic oxide), and phosphorus (exhaust pipe ashes producer). Any of these newly designed additives could be used to replace the widely used additive ZDDP which contains zinc and phosphorus and has less active (3.284 mm) additive property. Due to their better structures and properties correlation ability, these two methods could be used to provide a theoretical framework for engineers and other researchers to design a better anti-wear base oil additive before laboratory synthesis.

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Compliance with Ethical Standards

Conflict of interest The authors declare that they have no conflict of interest.

Research Involving Human and Animal Participants This research does not contain any human or animal subjects.

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