Evaluating the Effects of Volatile Organic Compounds from Vehicle Exhaust on the Endocrine System using Insilico Technique

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***Abstract*—Volatile organic compounds are emitted after combustion by petrol and diesel vehicles. Even after the use of various techniques to curb emission from vehicles, the presence of volatile organic compounds remains in the emissions. Air pollution from vehicles has been known to cause skin and eye irritation, respiratory disorders, inflamation, cardiovascular diseases and cancer. This article aims to evaluate the endocrine disrupting properties of these chemicals by using "Endocrine Disruptome" software. Common volatile organic compounds from petrol, diesel and also those running on biofuels have been chosen. This computational screening approach provides a rapid and cost-effective method to identify the toxic effects of volatile organic compounds on endocrine disruption. It has been found that a majority of the 66 volatile organic compounds emitted by vehicles have a harmful effect on the androgen receptor and aromatic compounds including polyaromatic and substituted aromatic compounds interacting strongly with several nuclear receptors in the endocrine system.**

***Keywords*—Endocrine-Disrupting Chemicals, Endocrine Disruptome, Volatile Organic Compounds.**

I. Introduction

The number of vehicles running on petrol, diesel or biofuels is 1.5 billion and rising every year. These vehicles run on petrol, diesel, biofuels and blended fuels. The exhaust from these vehicles contain a number of volatile organoc compounds. These have been known to cause skin and eye irritation, respiratory disorders, inflamation, cardiovascular diseases and cancer.

They disrupt many different hormones and are linked to adverse effects on human health like alterations in sperm quality and fertility, abnormalities in sex organs, endometriosis, early puberty, altered nervous system function, immune function, metabolic issues, diabetes, obesity, cardiovascular problems, growth, neurological and learning disabilities etc.

In this study, the effect of volatile organic compounds from the vehicle emissions on the endocrine system has been evaluated using a software, Endocrine Disruptome.

II. MATERIALS AND METHODS

Endocrine Disruptome [1] uses SMILES and docking is carried out with nuclear receptors. SMILES are obtained from the National Institute of Health website. The nuclear receptors are androgen receptor (AR), estrogen receptors α (ERα) and β (ERβ), glucocorticoid receptor (GR), liver X receptors α (LXRα) and β (LXRβ), mineralocorticoid receptor (MR), peroxisome proliferator activated recepor α (PPARα), β/δ (PPARβ/δ) and γ (PPARγ), progesterone receptor (PR), retinoid X receptor α (RXRα), thyroid receptor α (TRα) and β (TRβ). The software classifies the compounds based on the binding affinity as colour coded results, green corresponding to low probability of binding, followed by red, orange and red with the highest probability of binding.

Volatile organic compounds have been compiled using emission data from research papers chosen only from the past ten years.This has been done to take into account the compliance of vehicle emission to current environmental standards in the world. The studies employ advanced analytical techniques — primarily GC–MS, TD–GC×GC–MS and PTR–ToF–MS [3] to quantify both gas-phase and particle-phase VOCs.

III. Results And Discussions

The various volatile organic compounds in automobile exhaust have been segregated based on their functional groups. Their sources have been given as Petrol (P), Diesel (D), Biodiesel (BD) and Ethanol blended gasoline (EBG) in tables 1 - 13. Their and pathways of formation have been discussed very briefly.

TABLE 1 - ALKANES

Name of the Alkane	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Ethane	30.07	1.03	EBG	-
Propane	44.10	1.42	EBG	-
n-Butane	58.12	1.81	P	ARan
Iso-Butane	58.12	1.66	P, EBG	ARan
n-Pentane	70.13	1.97	P	ARan
Iso-Pentane	72.15	2.05	P	ARan
Hexane	86.18	2.59	P	ARan
Heptane	100.20	2.98	P	ARan
Octane	114.23	3.37	P	ARan
Iso Octane	114.23	3.08	P	ARan
Nonane	128.26	3.76	P, D, BD,BBD	ARan
Decane	142.28	4.15	D, BD,BBD	ARan
Undecane	156.31	4.54	D, BD,BBD	ARan
Dodecane	170.33	4.93	D	ARan
Tridecane	184.36	5.32	D	ARan
Tetradecane	198.39	5.71	D	ARan

Alkanes are the most abundant volatile organic compounds in

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petrol vehicle exhaust because of fuel evaporation and low reactivity. Unburned or partially oxidized hydrocarbons from diesel fuel and lubricating oils dominate intermediate-volatility fraction. The percentage of alkanes [2] in the exhaust of vehicles using biodiesel or blended biodiesel [6], [7] is reeduced relative to petro-diesel because biodiesel [6] burns more completely.

TABLE II- CYCLOALKANES

Name of the Cycloalkane	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Cyclohexane	84.16	2.34	D	ARan
Methylcyclohexane	98.19	2.59	D	ARan
Decalin	138.25	3.37	D	ARan

Cycloalkanes are formed from cracking of hydrocarbons in diesel [2]. They are responsible for total VOC load in diesel exhaust.

TABLE III - ALKENES

Name of the Alkene	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Ethylene	28.05	0.80	D	-
Propylene	42.08	1.19	D	-
1-Butene	56.11	1.58	P, D	ARan
Cis-2-butene	56.11	1.58	P	ARan
Trans-2-butene	56.11	1.15	P	ARan
Isobutene	56.11	1.58	P	ARan
Pentene	70.13	1.97	D, EBG	ARan
Hexene	84.16	2.36	EBG	ARan

Alkenes in petrol and diesel exhaust are by products of incomplete combustion [2]. They contribute to the formation of ozone in the exhaust. The concentration of alkanes and alkenes is reduced by 12–75% with E10 and higher blends [8], [9] due to oxygen-enhanced combustion.

TABLE IV - ALKYNES

Name of the Alkyne	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Acetylene	26.04	0.25	P	-

Alkynes are the markers of high temperature combustion inefficiency. The production of acetylene is monitored for this reason.

TABLE V - AROMATICS

Name of the Aromatics	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Benzene	78.11	1.69	P, D,BD,BBD, EBG	ARan
Toluene	92.14	1.99	P, D,BD,BBD, EBG	ARan
Styrene	104.15	2.33	D	ARan
Ethylbenzene	106.17	2.25	P, D,BD,BBD, EBG	ARan
o-xylene	106.17	2.30	P, D,BD,BBD, EBG	ARan
m-xylene	106.17	2.30	P, D,BD,BBD, EBG	ARan
p-xylene	106.17	2.30	P, D,BD,BBD, EBG	ARan
Trimethylbenzene	120.19	2.61	P	ARan

Monocyclic aromatic compounds in petrol and diesel exhaust [4], [5] come from incomplete fuel combustion and they are the major contributors of photochemical smog.These compounds contribute to secondary organic aerosol formation due to high reactivity and toxicity. The formation of aromatic compounds decreases by 40–70% due to lower aromatic content in biodiesel [6], [7] and by 40–60% in ethanol blended gasoline [8], [9] with ethanol replacing aromatic fractions.

TABLE VI - CARBONYL COMPOUNDS

Name of the Carbonyl compound	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Formaldehyde	30.03	0.45	P, D,BD,BBD, EBG	-
Acetaldehyde	44.05	0.21	P, D,BD,BBD, EBG	-
Acrolein	56.06	0.37	D,BD,BBD, EBG	-
Glyoxal	58.04	-0.62	BD,BBD	-
Propionaldehyde	58.08	0.60	P,BD,BBD	ARan
Acetone	58.08	0.60	P, D,BD,BBD, EBG	-
Butanone	72.11	0.99	P,BD,BBD	ARan

Oxygenated volatile organic compounds such as aldehydes, and ketones are produced from the oxidation of hydrocarbons in petrol and diesel exhaust [3] or the addition of additives such as ethanol and MTBE. Studies show that biodiesel combustion [6] produces fewer total hydrocarbons and aromatics but more oxygen-containing compounds. Their presence shows significant increase in biodiesel exhaust [7] from oxidation of residual unburned fatty acid methyl esters (FAMEs). The same is true for EBG with acetaldehyde being the dominant species.

TABLE VII - ALCOHOLS

Name of the Alcohol	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Methanol	32.04	-0.39	P, D, EBG	-
Ethanol	46.07	0.00	P, D, EBG	-
1-hexanol	102.17	1.56	BD,BBD	ARan
1-heptanol	116.20	1.95	BD,BBD	ARan
1-octanol	130.23	2.34	BD,BBD	ARan
Phenol	94.11	1.39	D	ARan
Cresol	108.14	1.70	D	ARan

Traces of alcohols in exhaust of diesel vehicles [3] are from oxidation of hydrocarbons and lubricant oil additives. They are also the direct products of incomplete oxidation of biodiesel [6], [7], hence unique markers for biofuel combustion.

TABLE VIII - ACIDS

Name of the Acids	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Formic acid	45.02	-1.00	D, EBG	-
Acetic acid	59.04	-1.24	D, EBG	-

Acids are found in the exhaust of diesel vehicles [3] from oxidation of hydrocarbons and lubricant oil additives. They are also present at trace levels, often from oxidation of ethanol in vehicles using ethanol or ethanol blended gasoline [8], [9].

TABLE IX - ETHERS AND ESTERS

Name of the Ether/Ester	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Ethyl formate	74.08	0.82	EBG	-
Ethyl acetate	88.11	0.57	EBG	ARan
Methyl tert-butyl ether	88.15	1.43	EBG	ARan

Ethers and Esters are formed [8], [9] by secondary oxidation of ethanol during combustion and aging.

TABLE X - FATTY ACID DERIVATIVES

Name of the Acids	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Methyl palmitate	270.45	5.64	BD,BBD	ARan
Methyl Oleate	296.49	6.20	BD,BBD	ARan, TRα
Methyl Stearate	298.50	6.42	BD,BBD	ARan

They are characteristic of high-biodiesel blends (B50–B100) formed by partially unburned or thermally decomposed molecules [6], [7].

TABLE XI- CHLOROCOMPOUNDS

Name of the Chlorocompound	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Chloromethane	50.49	0.86	P	-
Dichloromethane	84.93	1.42	P	-

Halogenated hydrocarbons in petrol engines are from traces from fuel additives or industrial contamination.

TABLE XIII - POLYAROMATIC HYDROCARBONS

Name of the PAH	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Naphthelene	128.17	2.84	D	ARan
Methylnaphthelene	142.20	3.15	D	ARan, MR, TRα
Anthracene	178.23	3.99	D	AR, ARan, ERβ, ERβan, GR, MR, TRα, TRβ
Phenanthrene	178.23	3.99	D	AR, ARan, ERβ, ERβan, GR, MR, TRα, TRβ
Pyrene	202.25	4.58	D	AR, ARan, ERα, ERβ, ERβan, GR, GRan, LXRβ, MR, TRα, TRβ

The main source of Polyaromatic hydrocarbons is exhaust from diesel vehicles [5]. They are products of incomplete combustion and associated with particulate matter in diesel exhaust.

TABLE XIII- NITRO AND OXY-AROMATICS

Name of the	Molecular weight	Log P value	Source	Nuclear Receptor/s that bind
Quinone	108.09	0.25	D	ARan
Nitrobenzene	123.11	2.12	D	ARan
Nitrophenol	139.11	1.82	D	ARan
Benzophenone	182.22	2.92	D	AR, ARan, GR, MR, PR, TRα, TRβ

Secondary oxidation and nitration products [3] are often found in aged or high-mileage emissions from diesel vehicles.

From the above data it is clear that most of the 66 volatile organic compounds show binding affinity to the androgen receptor ARan. Aromatic compounds, poly aromatic hydrocarbons in particular exhibit strong interaction [10], [11], [12], [13] with androgen receptors AR and ARan, estrogen receptor α- ERα and β- ERβ, ERβan, glucocorticoid receptors GR and GRan, liver X receptors β - LXRβ, mineralocorticoid receptor MR, thyroid receptor α and β - TRα, TRβ.

The same is true for oxy-aromatic compounds which interact [10], [11], [12], [13]with androgen receptors AR and ARan, glucocorticoid receptor GR, mineralocorticoid receptor MR, progesterone receptor PR, thyroid receptor α and β - TRα, TRβ

The value of log P is an additional information available in Endocrine disruptome software. We know that a negative value of log P indicates hydrophilicity. The higher the positive value, the higher indicates a higher probability for retention in the body for longer duration. From Tables 1 - 13, we can see that aromatic compounds, polyaromatic compounds, fatty acid derivatives and oxy-aromatic compounds would be interfering with the metabolic activities of the endocrine system and cause maximum harm [14].

IV. CONCLUSION

The endocrine system is responsible for functions like metabolism, regulation of blood pressure, blood sugar regulation, fluid and electrolyte balance and body temperature. It is also responsible for growth and development, sexual function, reproduction, sleep-wake cycle and mood. The interaction of the chosen 66 volatile organic compounds with the endocrine nuclear receptors were studied insilico using Endocrine Disruptome software.

Most of the 66 volatile organic compounds studied interact with the androgen receptor ARan. Aromatic compounds, polyaromatic compounds, fatty acid derivatives and oxy-aromatic compounds interfere with androgen receptors AR and ARan, estrogen receptor α- ERα and β- ERβ, ERβan, glucocorticoid receptors GR and GRan, liver X receptors β -

LXRβ, mineralocorticoid receptor MR, thyroid receptor α and β - TRα, TRβ and progesterone receptor PR.

Log P values indicate that these compounds would tend to remain in the body longer and cause maximum harm. Endocrine Disruptome offers a fast and cost effective method to screen the harmful effect of pollutants.

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