



# DFT Calculations and Total Antioxidant Capacity Studies of some Substituted Monodentate Salicylaldimines

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## Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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## ABSTRACT

Three substituted monodentate salicylaldimines namely 5-chloro-N-[(2-methoxy) phenyl] salicylaldimine [I], 5-chloro-N-[(4-chloro)phenyl]salicylaldimine [II] and 5-chloro-N-[(2-methyl-5-chloro)phenyl] salicylaldimine [III] were synthesized and characterized by elemental analysis, IR, UV, <sup>1</sup>H and <sup>13</sup>C NMR. Theoretical calculations were also performed on the optimized structures of the compounds. The IR, NMR and UV spectra of the compounds were calculated and the results compared with the corresponding experimental spectra to augment the structural elucidation. The calculated IR, NMR and UV values were in agreement with the experimental results. The total antioxidant capacities of the compounds were determined by phosphomolybdenum assay.

**Keywords:** Salicylaldimines; antioxidant; theoretical calculations; substituents.

## 1. INTRODUCTION

Salicylaldimines are 2-hydroxyl Schiff bases formed by the reaction between a primary amine and 2-hydroxybenzaldehyde [1]. Schiff bases

were first reported by Hugo Schiff when reactions were carried out between carbonyl compounds and primary amines [2,3]. Schiff bases are similar to aldehydes or ketones except that the C=N is being substituted by C=O. They are

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compounds that have azomethine group (HC=N). They are also called imines or azomethines and have the general formula  $R_1H=NR_2$  where  $R_1$  and  $R_2$  are alkyl or aryl groups [1,4]. The imine group is important in explaining the mechanism of transamination and racemization reactions in living systems [2,4-6].

Schiff bases are among the most widely used organic compounds. They play essential roles in living systems as well as in coordination chemistry. They are of vital roles in living systems in combination with enzymes such as transaminases and tryptophan synthase [7-9]. Literatures revealed that Schiff bases derived from 2-hydroxybenzaldehyde and derivatives showed extensive range of biological properties. Some of the reported biological properties are antioxidant, anticonvulsant, antimalarial, antipyretic, antiviral, anti-inflammatory, antifungal, analgesic and antibacterial properties which make them attract attention [6,10-16].

Many Schiff bases have been synthesized for their pronounced biological activities. However, literatures search revealed that reports on the antioxidants activities are limited. Hence this study, which investigated the DFT and total antioxidant studies of some substituted monodentate salicylaldehydes. In addition to the experimental studies, quantum chemical computations were used to augment the experimental observations [17,18]. Thus, the molecular structures of the compounds were modelled and the theoretical calculations were carried out on the optimized structures. These were employed for the IR, UV-Visible and NMR spectra. A consideration of the similarities between the theoretical and experimental spectra of the compounds could further be utilized for structural elucidation.

## 2. MATERIALS AND METHODS

### 2.1 Reagents and Instruments

2-anisidine, 4-chloroaniline, 5-chloro-2-methylaniline, 5-chloro-2-hydroxybenzaldehyde were purchased from Merck and used as supplied. The solvent DMSO (dimethylsulfoxide) and absolute ethanol were of analytical grade and were used without further purification. Elemental analysis was carried out with Finnigan Flash EA 1112 series. The infrared spectra were recorded on a Perkin-Elmer 400 FT-IR/FT-FIR. The NMR spectra were obtained using a Bruker Avance 111 600 in solution with deuterated

chloroform ( $CDCl_3$ ) and DMSO using tetramethylsilane (TMS) as internal standard at 600 MHz. However, the electronic spectra were recorded on Shimadzu UV-2600 series in DMSO. Melting points were taken on Stuart Melting point apparatus SMP-3 but were not correct.

### 2.2 Synthesis of the Salicylaldehydes

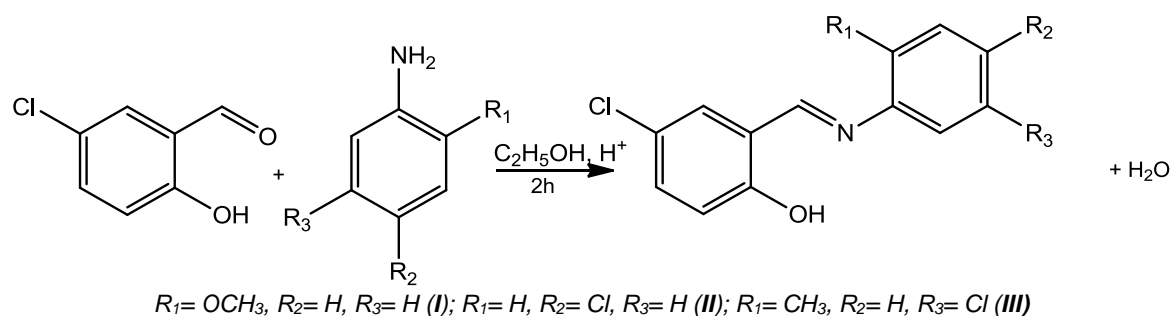
The salicylaldehydes were synthesized according to literature [15]. 0.015 mole of 5-chloro-2-hydroxybenzaldehyde in 10 mL absolute ethanol was added in drops to 0.015 mole of the corresponding amine in 15 mL of the same solvent. The resulting solution was stirred for 2 hours on addition of three drops of methanoic acid. The coloured solid precipitates were filtered and washed with cold ethanol, recrystallized from ethanol and dried in a desiccator over silica gel for two days.

### 2.3 Computational Method

The salicylaldehydes were modelled and optimized using Gaussian 09 and Spartan '14 computational software packages. Density Functional Theory (DFT) was employed for the geometry optimization, chemical shifts, electronic transitions and frequency calculations of the compounds based on preliminary conformational search of the molecules with molecular mechanics force field. The DFT calculations were performed on the most stable conformer in the ground state using Becke's three-parameter hybrid functional employing the Lee-Yang-Parr correlation functional (B3LYP) method with 6-31G\*\* basis set [9,19-21].

### 2.4 Phosphomolybdate Total Antioxidant Capacity Assay

The total antioxidant capacities (TAC) of the salicylaldehydes were determined by phosphomolybdenum assay and ascorbic acid was used as the standard. 1.0 mL of reagent (0.6 M sulphuric acid, 28  $\mu$ M sodium phosphate and 4  $\mu$ M ammonium molybdate) was reacted with a fractional part of the solution of the compounds (1.0 mL of 1000  $\mu$ g). The covered tubes were incubated at 95 °C in a water bath for 90 minutes after which the samples were cooled to room temperature and a UV spectrophotometer was used to measure the absorbance of the aqueous solution of each at 695 nm. The procedure was repeated for a blank solution containing 1.0 mL of reagent solution. The TAC studies were performed three times and the mean was expressed as equivalents of ascorbic acid [22].



Scheme 1. Synthetic route to compounds 1-III.

### 3. RESULTS AND DISCUSSION

#### 3.1 Characterization of the Salicylaldimines

**I** (5-chloro-N-[(2-methoxy)phenyl]salicylaldimine) =  $\text{C}_{14}\text{H}_{12}\text{ClNO}_2$ , Molecular weight: 261.70 g/mol, Yield 60.52%, IR ( $\text{cm}^{-1}$ ): 2939-2480 (O-H), 1616 (C=N), 1592-1466 (C=C), 1254 (C-O).  $^1\text{H}$  NMR (ppm): 13.90 (s, 1H, OH), 8.91 (s, 1H, C=N), 7.70-6.90 (m, 7H, C-H<sub>Ar</sub>), 3.81 (s, 3H, C-H<sub>methoxy</sub>).  $^{13}\text{C}$  NMR (ppm): 161.75, 160.12, 153.26, 136.36, 133.11, 131.63, 129.19, 122.67, 121.46, 119.68, 119.30, 112.80, 56.31. UV: 286 (n- $\pi^*$ ), 360 ( $\pi$ - $\pi^*$ ). Elemental analysis (C, H, N)%: Found (Calculated): 64.20(64.25), 4.59(4.62), 5.35(5.33).

**II** (5-chloro-N-[(4-chloro)phenyl]salicylaldimine) =  $\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}$ , Molecular weight: 266.12 g/mol, Yield 83.27%, IR ( $\text{cm}^{-1}$ ): 3073 (O-H), 1610 (C=N), 1558-1442 (C=C), 1275 (C-O).  $^1\text{H}$  NMR (ppm): 12.70 (s, 1H, OH), 8.90 (s, 1H, C=N), 7.70-6.90 (m, 5H, C-H<sub>Ar</sub>).  $^{13}\text{C}$  NMR (ppm): 162.85, 159.33, 147.49, 133.48, 131.42, 129.96, 129.02, 123.78, 123.19, 119.20, 115.68. UV: 262 (n- $\pi^*$ ), 351 ( $\pi$ - $\pi^*$ ). Elemental analysis (C, H, N)%: Found (Calculated): 58.65(58.67), 3.40(3.41), 5.24(5.26).

**III** (5-chloro-N-[(2-methyl-5-chloro)phenyl]salicylaldimine) =  $\text{C}_{14}\text{H}_{11}\text{Cl}_2\text{NO}$ , Molecular weight: 280.15 g/mol, Yield 96.54%, IR ( $\text{cm}^{-1}$ ): 2980-2450 (O-H), 1618 (C=N), 1557-1479 (C=C), 1282 (C-O).  $^1\text{H}$  NMR (ppm): 12.90 (s, 1H, OH), 8.85 (s, 1H, C=N), 7.76-6.90 (m, 6H, C-H<sub>Ar</sub>), 2.20 (s, 3H, C-H<sub>methyl</sub>).  $^{13}\text{C}$  NMR (ppm): 163.25, 159.54, 148.59, 133.57, 132.52, 131.67, 131.49, 127.02, 123.16, 121.21, 119.17, 118.59, 17.73. UV: 263 (n- $\pi^*$ ), 353 ( $\pi$ - $\pi^*$ ). Elemental analysis (C, H, N) %: Found (Calculated): 59.99(60.02), 3.96(3.97), 5.00(5.00).

The salicylaldimines were obtained in good yields as solids. They were stable in air and the colours ranged from light – deep yellow. They were soluble in most organic solvents but insoluble in water.

The IR spectra data of each of the compounds confirmed the formation of the azomethine bonds  $\nu(-\text{HC}=\text{N})$ . All the spectra displayed the azomethine absorption bands at 1618-1610  $\text{cm}^{-1}$ . The spectra exhibited the phenolic stretching  $\nu(\text{C}-\text{O})$  vibrations at 1282-1254  $\text{cm}^{-1}$  and the hydroxyl (O-H) absorption bands at 3073-2447  $\text{cm}^{-1}$ . The compounds displayed the aromatic (C=C) bands in the range 1592-1442  $\text{cm}^{-1}$  [17, 23-29].

The  $^1\text{H}$  NMR spectra of the salicylaldimines displayed a singlet signal at  $\delta$  13.90-12.70 ppm which was attributed to the phenolic -OH protons [18, 27, 29-33]. All the salicylaldimines displayed a singlet signal at  $\delta$  8.91-8.85 ppm assigned to the azomethine (-HC=N) protons [15, 27, 30, 31, 33-36] which further confirmed the formation of the salicylaldimines. The aromatic protons appeared as multiplets at  $\delta$  7.70-6.90 ppm [15, 30, 31, 35]. A sharp singlet signal assigned to the protons of methoxy and methyl groups appeared at  $\delta$  3.81 and 2.20 ppm in the spectra of compounds I and III respectively [11, 35-37]. The  $^{13}\text{C}$  NMR spectra of the compounds were consistent with the  $^1\text{H}$  NMR. The spectra displayed the azomethine carbon peaks in the range 163.25-161.75 ppm and the aromatic carbons around 160.12-112.80 ppm. The spectra of compounds I and III displayed the carbons of the methoxy and methyl groups at  $\delta$  56.31 and 17.73 ppm respectively [11, 15, 27, 33, 35-37]. The UV spectra of the compounds displayed two absorption peaks around 286-262 and 351-360 nm which were attributed to n- $\pi^*$  of the azomethines and  $\pi$ - $\pi^*$  of the aromatic rings in the compounds.

## 3.2 Computational Studies

### 3.2.1 Theoretical IR Spectra

The theoretical IR vibrational frequency values of the salicylaldimines (Table 1) were in agreement with the experimental values. The azomethine ( $-\text{HC}=\text{N}$ ) absorption bands of the compounds **I**, **II** and **III** appeared at 1678, 1697, and 1681  $\text{cm}^{-1}$  respectively. These bands were experimentally observed at 1615, 1610 and 1618  $\text{cm}^{-1}$  respectively. The phenolic ( $\text{C}-\text{O}$ ) stretching vibrations of the compounds appeared around 1335-1334  $\text{cm}^{-1}$  in the theoretical data while the experimental values were observed around 1282-1254  $\text{cm}^{-1}$ . The theoretical  $\nu(\text{O}-\text{H})$  stretching vibrations in the compounds appeared around 3195-3080  $\text{cm}^{-1}$  while the experimental stretching vibrations were observed around 3073-2447  $\text{cm}^{-1}$ . The aromatic ( $\text{C}=\text{C}$ ) absorption bands appeared in the range 1646-1401  $\text{cm}^{-1}$  theoretically. However, these bands were observed around 1592-1442  $\text{cm}^{-1}$  experimentally.

### 3.2.2 Theoretical NMR spectra

The theoretical chemical shifts of the salicylaldimines (Table 2) were in good agreement with the experimental values. The data obtained revealed that the aromatic hydrogen in **I**: H6, H11, H15, H12, H10, H13, H17 appeared at 8.01, 8.15, 8.17, 7.83, 7.76, 8.08, 8.32 ppm respectively in the theoretical spectrum, these appeared in the range 7.70-6.90 ppm in the experimental study. The hydrogen of the azomethine ( $-\text{HC}=\text{N}$ ) and  $-\text{OH}$  groups appeared at 10.31 ppm and 14.69 ppm respectively in the theoretical calculations while they were experimentally observed at 8.91 ppm and 13.90 ppm respectively. The chemical shift of the three hydrogen in the  $-\text{OCH}_3$  group were observed at 4.80 ppm in the theoretical calculations and at 3.81 ppm in the experimental spectrum. The aromatic carbon in **I** appeared in the range 156.12-113.69 ppm, these were observed experimentally in the range 160.12-112.80 ppm. Moreover, the carbon in the azomethine and  $-\text{OCH}_3$  groups appeared at 158.83 ppm and 52.28 ppm respectively in the theoretical calculations, these were experimentally observed at 161.75 ppm and 56.31 ppm respectively. However in **II**, the hydrogen in the aromatic ring: H6, H11, H10, H13, H17, H14, H1 appeared at 8.04, 8.26, 8.25, 8.25, 7.81, 7.92, 7.81 ppm respectively in the theoretical calculations. These were experimentally reported in the range 7.70-6.90 ppm. The hydrogen of the azomethine ( $-\text{HC}=\text{N}$ )

and  $-\text{OH}$  groups were observed at 9.11 ppm and 13.55 ppm respectively in the theoretical spectrum while they were reported in the experimental study at 8.90 ppm and 12.70 ppm respectively. The aromatic carbon in **II** appeared in the range 155.97-114.10 ppm in the theoretical data, these appeared experimentally in the range 159.33-115.68 ppm. The azomethine carbon appeared at 160.30 ppm theoretically and at 162.85 ppm in the experimental spectrum. Nevertheless, the aromatic hydrogen in **III**: H6, H11, H13, H14, H8, H1 appeared at 8.15, 8.25, 8.17, 7.93, 8.08, 7.86 ppm respectively in the theoretical spectrum, these appeared in the range 7.76-6.90 ppm in the experimental study. The hydrogen of the azomethine ( $-\text{HC}=\text{N}$ ) and  $-\text{OH}$  groups appeared at 9.25 ppm and 14.33 ppm respectively in the theoretical calculations while they were experimentally observed at 8.85 ppm and 12.90 ppm respectively. The chemical shift of the three hydrogen in the  $-\text{CH}_3$  group were observed at 3.20 ppm in the theoretical calculations and at 2.23 ppm in the experimental spectrum. The aromatic carbon in **III** appeared in the range 156.20-113.88 ppm in the theoretical data, these appeared experimentally in the range 159.54-118.59 ppm. The carbon in the azomethine and  $-\text{CH}_3$  groups appeared at 155.68 ppm and 20.00 ppm respectively in the theoretical calculations while they were experimentally observed at 163.25 ppm and 17.73 ppm respectively.

### 3.2.3 Theoretical electronic spectra

The theoretical electronic spectra data of the compounds were comparable to the experimental values. The agreement between the theoretical and experimental electronic spectra data corroborated the suggested structures. The theoretical spectrum of compound **I** showed four absorption bands at 239, 250, 268, 345 nm, these bands were related to the promotion of electrons from HOMO-2  $\rightarrow$  LUMO, HOMO-3  $\rightarrow$  LUMO, HOMO  $\rightarrow$  LUMO+1, HOMO  $\rightarrow$  LUMO respectively. However, compound **II** displayed five absorption bands at 251, 262, 288, 317, 375 nm. These bands were obtained when electrons were promoted from HOMO  $\rightarrow$  LUMO+2, HOMO  $\rightarrow$  LUMO+1, HOMO-2  $\rightarrow$  LUMO, HOMO-1  $\rightarrow$  LUMO and HOMO  $\rightarrow$  LUMO respectively. Furthermore, compound **III** exhibited three absorption bands at 240, 246, 260 nm, these bands were related to the promotion of electrons from HOMO  $\rightarrow$  LUMO+1, HOMO-4  $\rightarrow$  LUMO, HOMO-3  $\rightarrow$  LUMO respectively.

Table 1. Theoretical IR data of the salicylaldimines

Compounds	IR (cm <sup>-1</sup> )				UV-Vis (nm)
	OH	C=N	C=C	C-O	
I	3081	1678	1646-1401	1335	236, 247, 265, 290, 318, 344
II	3195	1697	1646-1440	1334	242, 244, 258, 316
III	3162	1681	1641-1426	1335	240, 246, 260, 292, 319, 344

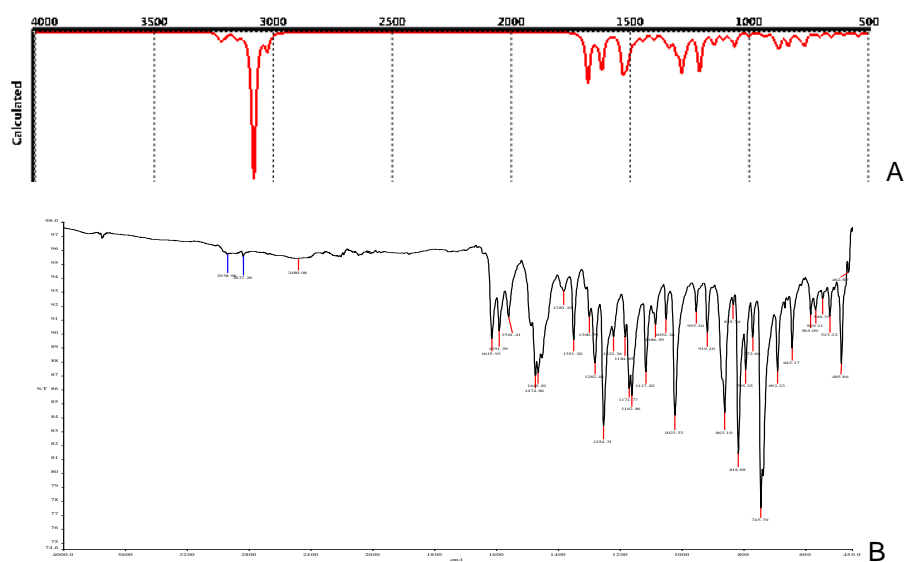


Fig. 1. IR spectra of compound I, theoretical (A) and experimental (B)

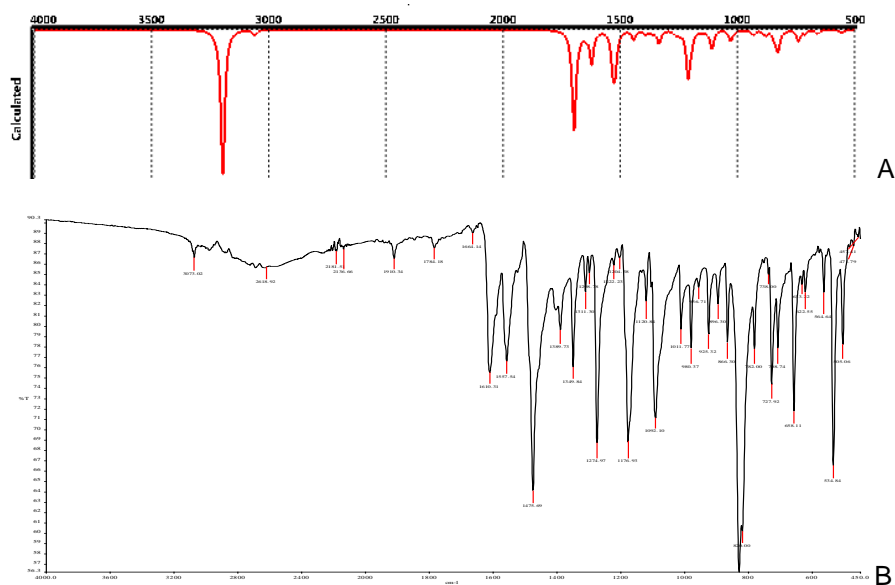
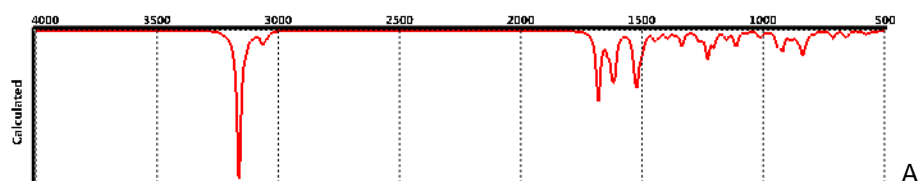


Fig. 2. IR spectra of compound II, theoretical (A) and experimental (B)



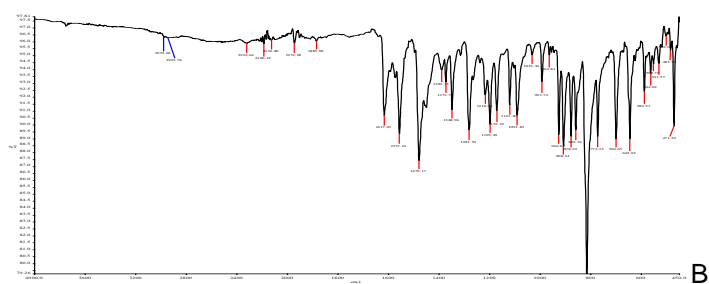


Fig. 3. IR spectra of compound III, theoretical (A) and experimental (B)

Table 2. Theoretical NMR data of the salicylaldimines

Positions of H & C	$\delta$ (ppm)		
	I	II	III
H1	4.80	7.81	7.86
C1	126.78	127.64	127.81
H2	-	-	-
C2	127.39	127.85	127.75
H3	4.80	-	3.20
C3	116.68	115.07	116.01
H4	10.31	9.11	9.25
C4	156.12	155.97	156.20
H5	4.80	-	3.20
C5	113.69	114.10	113.98
H6	8.01	8.04	8.15
C6	127.62	129.33	129.19
H7	-	-	3.20
C7	158.83	160.30	155.68
H8	-	-	8.08
C8	130.79	145.84	144.71
H9	14.69	13.55	-
C9	147.64	115.96	113.88
H10	7.76	8.25	-
C10	106.39	123.97	137.75
H11	8.15	8.26	8.25
C11	121.95	134.95	121.76
H12	7.83	-	-
C12	116.17	123.97	126.50
H13	-	8.25	-
C13	125.87	115.96	127.83
H14	-	7.92	-
C14	52.48	-	20.00
H15	-	-	-
C15	-	-	-
H16	-	-	-
C16	-	-	-
H17	-	-	-
C17	-	-	-

Table 3. The HOMO, LUMO and Energy gap of the salicylaldimines

	I	II	III
HOMO	-5.7	-6.2	-6.1
LUMO	-1.8	-1.9	-2.1
ENERGY GAPS	3.9	4.3	4.0

**Table 4. The total antioxidant capacity of the salicylaldimines**

Compounds	TAC $\mu\text{g}$ per AA
I	0.65
II	0.69
III	0.79

Key: AA = ascorbic acid

### 3.2.4 Frontier molecular orbitals

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are also called the frontier molecular orbitals. They determine the way molecules interact with other species. The HOMO is the orbital energy that donates electron, since it is the orbital of highest energy containing electrons. Conversely, the LUMO is the orbital of lowest energy. The energy gap between the HOMO and LUMO is expected to play significant roles in the intra- and inter- charge transfers according to the frontier molecular orbital theory [20, 38, 39]. The energy band gaps between the HOMO and LUMO is more important in considering electronic transitions than individual orbital component of a molecule. Since the difference between the LUMO and HOMO shows the reactivities and stabilities of molecules in chemical reactions, thus, the lower the energy gap, the more reactive and less stable the molecule. Therefore, Fig. 1 shows the proposed structures, optimized structures, HOMO and LUMO of the synthesized salicylaldimines. The calculated energy band gaps (Table 3) for the compounds I, II and III are 3.9, 4.3 and 4.0 eV respectively. This shows that compound I is expected to be more reactive than compounds II and III. Thus, the chemical stability of the compounds could be ordered as  $\text{II} > \text{III} > \text{I}$ .

### 3.3 Total Antioxidant Capacity

The results of the total antioxidant capacities (TAC) of the synthesized salicylaldimines are presented in Table 5. The results showed that all the synthesized compounds displayed antioxidant capacities. This indicated that they have the ability to inhibit or limit the harm caused by free radicals. Antioxidants function by freely donating electrons to free radicals without changing into electron-scavenging substances themselves [40, 41]. They are chemicals that avert or reduce the harm caused by free radicals and can also be called free radical scavengers [42-44]. Free radicals are molecules that have one or more unpaired electrons. They are unstable and very reactive molecules because of

the unpaired electrons. In order to be stable, free radicals either donate or accept electrons from another molecules which then become free radicals [43, 45]. These new free radicals will either donate or accept electrons from another molecules, thereby, initiating chain reactions. If free radicals are too many in a biological system, they can overwhelm the cells' usual defenses. Thus, causing harms to the cells which eventually lead to many diseases [41, 42]. However, when there are antioxidants in the cells, they donate electrons to the free radicals, thereby, stabilizing them and stopping the chain reactions [46].

The observed differences in the TAC of the compounds are due to the presence of different substituents on the compounds and probably the positions of the substituents. Compound III displayed the highest total antioxidant capacities while compound I exhibited the least capacities. Hence, compound III would be a better free radical scavenger.

## 4. CONCLUSION

A comparison of the experimental and theoretical results showed that the theoretical results were comparable to the experimental values, thus, corroborating the proposed structures. The calculated energy gaps showed that compound I would be more reactive than compounds II and III. The TAC results showed that compound III exhibited the highest antioxidant capacities, which implies that it possesses the highest ability to inhibit or reduce the harm caused by free radicals.

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## COMPETING INTERESTS

Author has declared that no competing interests exist.

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