# Experimental and Theoretical Studies of 2- (naphthalen-1-yl (piperidin-1-yl) methyl)phenol Compound

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(Received on 5th March 2020, accepted in revised form 13th July 2020)

**Summary:** The 2- (naphthalen-1-yl (piperidin-1-yl) methyl) phenol compound is an alkylaminophenol compound and has been experimentally synthesized by the Petasis reaction. In this study Structural analysis was carried out by FT-IR, NMR, UV-Vis spectroscopy. The high antioxidant value of the compound showed that it could be a potential biologically active drug. Theoretical data support all experimental analysis of the new compound. Comparisons were made by double method. For this purpose, DFT (B3LYP) and HF methods have been used with 6-311G ++ (d, p) set. Also, the compound's electronic and structural properties (bond lengths, bond angles and dihedral angles), the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies, electrostatic potential (MEP), vibrational frequencies, Mulliken atomic charges, excitation energies, and oscillator strengths were calculated. As a result; the theoretical and experimental values were found to be compatible.

**Keywords:** Alkylaminophenol, B3LYP, HOMO-LUMO.

## Introduction

Alkilaminofenol compounds are frequently used in chemotherapy due to its anticancer and antioxidant activities[1–3]. The variety of cancer types needs the presence of new drugs to be used in treatment. Alkylaminophenols, often used for the treatment of bone cancer, are synthesised by the Petasis reaction (Boronic Mannich Reaction) [4–6]. Nicos Petasis first used the Petasis reaction in 1993 as a practical method for the synthesis of naftifine, an antifungal agent[7,8]. The reaction takes place by the removal of boric acid from the boronate complex formed by the boronic acid added to the medium after the amine and carbonyl compounds form iminium ion[9,10]. Although there are many studies on the synthesis of alkylaminophenols in the literature[6,9–17], studies on quantum chemical calculations of these compounds are limited[18]. Therefore, the study; It was carried out in two separate sections. In the first part, a new alkylaminophenol was synthesized. In the second part; Quantum chemical calculations of the compound were carried out in DFT (B3LYP) and HF method in 6-311 ++ G (d, p) set. TD-SCF method was used in the UV-Vis calculations.

## Experimental

### *Materials and Measurement*

The chemicals used for synthesis were used immediately without any extra purification. UV-1700 PharmaSpect UV/ vis spectrophotometer; PerkinElmer 100 FT-IR spectrometry and Agilent 600MHz NMR spectrometers were applied to the analysis

### *Synthesis*

The synthesis was carried out according to the methods in the literature[19].

### *2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol*

Yield 0.238 g (75%), Orange solid, mp 123-124 $^{o}$C. $^{1}$H NMR (600 MHz, $CDCl_3$): δ(ppm) = 1.46-1.63 (m, 7H, piperidine); 2.48 (s, 3H, piperidine); 5.60 (s, 1H, methine ); 6.66 (t, *J* = 7.2, 1H, Ar); 6.92 (t, *J* = 7.2, 2H, Ar); 7.14 (t, *J* = 7.2, 1H, Ar); 7.45 ( t, *J* = 7.8, 1H, Ar); 7.52 (t, *J* = 7.2, 1H, Ar); 7.60 (s, 1H, Ar); 7.79 (d, *J* = 7.8, 2H, Ar); 7.89 (d, *J* = 7.8, 1H, Ar); 8.38 (d, *J* = 8.4, 1H, Ar); 12.84 (s, 1H, Ar-O<u>H</u>).$^{13}$C NMR ($CDCl_3$, 150 MHz): δ, ppm: 24.1 (piperidine); 26.2 (piperidine); 68.3 (piperidine); 117.1 (Aliphatic C); 119.0 (1-benzene); 125.5 (1-benzene); 125.9 (1-benzene); 126.2 (1-benzene); 128.2 (1-naphthalene); 129.0 (1-naphthalene) 129.2 (1-naphthalene); 132.2 (1-naphthalene); 133.9 (1-naphthalene); 135.8 (1-naphthalene); 157.6 (1-benzene). FT-IR: ν($cm^{-1}$): 3752 (Ar-OH), 3200 (Ar-H in-plane), 2958, 2939, 2851 and 2809 (C-H, aliphatic), 1607, 1600, 1586 (C=C, aromatic), 1474, 1455, 1403 (C-H, aliphatic), 1356 (O-H, bending), 1250 (C-O, aromatic), 975, 873, 787 (C-H, aliphatic, out of plane bending).

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*Antioxidant Activity*

The test process of the antioxidant activity was performed via 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging activity with small modifications in 96-well microplate [20]. DPPH was dissolved in methanol at 0.004% concentration. Test compounds were dissolved in Dimethyl Sulfoxide (DMSO). Concentrations were 1.25, 2.5, 5, and 10 mg/ml, respectively. Each well contained a solution of 200 µl DPPH-methanol. 10 µl of serial concentration of each test compound and controls were added separately into each well. Ascorbic acid (11.8 mM), Butylated hydroxytoluene (60 mM) and DMSO were also used as controls. Then, for 30 minutes, the microplates were incubated in the dark at room temperature. After incubation, the absorbance of test compounds' antioxidant activity was measured at 517 nm by the microplate reader. All tests were made in triplicate. The determination of the DPPH-free radical scavenging activity was performed by using the following equation:

Inhibition of DPPH % = [(AbsControl - AbsSample) / AbsControl] x 100

where AbsControl refers to the absorbance of the DPPH-methanol solution and AbsSample refers to the absorbance of test compounds/controls blended with DPPH-methanol solution, separately.

Table-1: DPPH free radical scavenging activity.

| Samples | DPPH% | Samples | DPPH% |
|---|---|---|---|
| **Control** | **0** | **1,25** | **17.05 ± 0.03** |
| **Ascorbic acid** | **70.68 ± 0.03** | **2,5** | **19.35 ± 0.03** |
| **BHT** | **68.64 ± 0.01** | **5** | **34.26 ± 0.03** |
| **DMSO** | **5.56 ± 0.03** | **10** | **40.70 ± 0.02** |

Antioxidants neutralise radicals in diseases such as cancer, which form free radicals in the body. Antioxidant capacity of the alkylaminophenol compound was seen increased by concentration (Table-1). This study is consist of two-part.

In the first part of the study, a synthesis and structural analysis of the compound was completed experimentally. In the second part of the study, experimental results were compared to theoretical data.

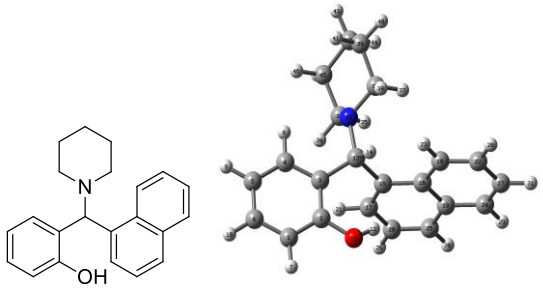
*Computational method*

All calculations of the new compound were carried out with the Gaussian 09W package program, which has many methods and basic set options. In the visualisation of the molecule, GaussView 5.0.9 package program was used. All calculations include the B3LYP function at the DFT level and Hartree Fock method. 6-311++G (d, p) set is used in calculations[21–25]. Geometric, electronic and spectroscopic parameters of the molecule were calculated. Regression analyses were performed with using $^{13}$C-NMR and $^{1}$H-NMR chemical shift values. IR harmonic vibration frequency values were determined and scaled values were reached by multiplying the scale factors. Theoretical IR spectra were created using vibration frequency values and compared with experimental spectra. The geometric properties of the molecule (bond length, angle), electronegativity (χ), total energy, atomic charges, dipole moment (µ), chemical hardness (η) and softness (S), ionisation potential (I), energy difference (ΔE) properties were calculated. In addition, surface shapes such as molecular electron potential (MEP), surface maps (electron potential and electron density potential), total density have been determined. UV-vis calculations for the compound were performed using theory TD-DFT.

**Resuls and Discussion**

*Molecular geometry*

B3LYP, HF theories are calculated at 6-311++ G (d, p) basis set.The optimised Fig is shown in Fig 1. The bond length, bond angles and dihedral angles of the compound are compared in Table-2.




(a) (b)

Fig. 1: (a) Molecular structure of alkylaminophenol compound.
(b) Optimized molecular structure of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol by DFT/B3LYP/6-311++G(d,p)

Table-2: Selected geometric parameters of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol.

| Bond length ($A^0$) | Experimental Bond length | B3LYP | HF | Bond angles($^0$) | Experimental Bond Angles | B3LYP | HF |
|---|---|---|---|---|---|---|---|
| C13-C3 | 1.54 | 1.537 | 1.535 | N32-C13-C3 | | 112.0 | 111.9 |
| C13-H14 | 1.10 | 1.093 | 1.080 | N32-C13-C15 | | 113.5 | 114.3 |
| C3-C2 | 1.37 | 1.409 | 1.397 | C3-C13-H14 | 109.5 | 104.7 | 104.1 |
| C3-C4 | | 1.398 | 1.388 | C15-C13-H14 | | 107.7 | 107.3 |
| C4-C5 | | 1.393 | 1.386 | C3-C4-C5 | | 122.0 | 121.8 |
| C5-C6 | | 1.393 | 1.383 | C4-C5-C6 | | 119.6 | 119.6 |
| C6-C1 | | 1.390 | 1.382 | C6-C1-C2 | | 120.4 | 120.2 |
| C4-H8 | | 1.082 | 1.071 | C1-C2-C3 | | 120.9 | 121.0 |
| C5-H9 | | 1.084 | 1.075 | C2-O11-H12 | 104.5 | 110.1 | 111.4 |
| C6-H10 | | 1.084 | 1.075 | C15-C16-C19 | | 118.9 | 119.0 |
| C1-H7 | | 1.084 | 1.075 | C16-C19-C25 | | 119.7 | 119.9 |
| C2-O11 | 1.43 | 1.372 | 1.358 | C25-C20-C17 | | 120.5 | 120.0 |
| O11-H12 | 0.96 | 0.966 | 0.942 | C17-C15-C16 | | 118.6 | 118.3 |
| C13-C15 | | 1.545 | 1.544 | C19-C16-C18 | | 117.3 | 117.2 |
| C15-C16 | | 1.440 | 1.439 | C16-C19-C24 | | 119.6 | 119.8 |
| C16-C19 | | 1.438 | 1.414 | C19-C24-C27 | | 121.2 | 121.1 |
| C16-C18 | | 1.424 | 1.424 | C24-C27-C22 | | 119.6 | 119.5 |
| C19-C24 | | 1.420 | 1.420 | C27-C22-C18 | | 120.6 | 120.6 |
| C24-C27 | | 1.372 | 1.356 | C22-C18-C16 | | 121.6 | 121.5 |
| C27-C22 | | 1.412 | 1.413 | N32-C36-C39 | | 110.9 | 110.8 |
| C22-C18 | | 1.375 | 1.412 | C36-C39-C42 | | 111.1 | 110.9 |
| C18-H23 | | 1.081 | 1.070 | C39-C42-C45 | | 110.1 | 109.9 |
| C22-H28 | | 1.084 | 1.075 | C42-C45-C33 | | 111.0 | 111.2 |
| C27-H31 | | 1.084 | 1.075 | C33-N32-C36 | | 112.0 | 112.1 |
| C25-H30 | | 1.084 | 1.075 | C4-C3-C13 | | 121.8 | 122.5 |
| C20-H26 | | 1.084 | 1.075 | C2-C3-C13 | | 120.5 | 119.8 |
| C17-H21 | | 1.084 | 1.074 | C13-C15-C17 | | 119.3 | 119.7 |
| N32-C13 | 1.47 | 1.477 | 1.464 | C13-C15-C16 | | 122.1 | 121.8 |
| N32-C36 | | 1.465 | 1.454 | C15-C17-H21 | | 119.0 | 119.4 |
| N32-C33 | | 1.466 | 1.455 | C15-C16-C18 | | 123.8 | 123.6 |
| C33-C45 | | 1.532 | 1.527 | C16-C18-H23 | | 119.9 | 120.1 |
| C45-C42 | | 1.532 | 1.527 | N32-C33-H34 | | 108.9 | 109.2 |
| C42-C39 | | 1.532 | 1.527 | N32-C36-H38 | | 108.3 | 108.6 |
| C39-C36 | | 1.532 | 1.526 | Dihedral Angles | | | |
| C33-H34 | | 1.092 | 1.082 | N32-C13-C3-C2 | | -176.5 | -168.3 |
| C33-H35 | | 1.104 | 1.094 | N32-C13-C15-C17 | | -87.4 | -90.9 |
| C36-H37 | | 1.105 | 1.094 | C4-C3-C2-O11 | | -176.6 | -176.6 |
| C36-H38 | | 1.094 | 1.084 | C1-C2-O11-H12 | | 158.3 | 144.1 |
| C39-H40 | | 1.095 | 1.087 | C15-C16-C18-C22 | | 179.3 | 179.2 |
| C39-H41 | | 1.095 | 1.087 | C19-C16-C18-H23 | | -178.8 | -178.9 |
| C42-H43 | | 1.094 | 1.086 | C25-C19-C24-C27 | | -178.6 | -178.5 |
| C42-H44 | | 1.098 | 1.089 | C16-C15-C17-H21 | | -179.9 | -178.0 |
| C45-H46 | | 1.096 | 1.087 | N32-C33-C45-H47 | | 178.2 | 177.8 |
| C45-H47 | | 1.095 | 1.087 | N32-C36-C39-H40 | | -178.2 | -178.3 |

Experimental and calculated structural properties are given in Table-2. While the O-H bond length for the hydroxyl group was experimentally 0.96 Å, it was calculated as 0.966 Å by the B3LYP method and 0.942 by the HF method. While N32-C13 bond lengths were found 1.47 experimentally, it was calculated as 1.477 Å by B3LYP method and 1.464 by HF method. Similarly, while C = C bond length was experimentally 1.37 Å, theoretically C24 = C27 1,372 Å (B3LYP) and 1.356 Å (HF) were calculated. C3-C13-H14; C2-O11-H12 angles are experimental as 109.5 and 104.5, and used theoretically, calculated as 104.7 °, 110.1 ° (B3LYP) and 104.1, 111.4 (HF). As a result; It can be said that there is a good agreement between experimental bond length and bond angle and calculated values.

*IR spectra*

Vibration spectroscopy (FT-IR) is one of the most common methods used for functional groups and bond structures of compounds. While obtaining IR spectra, there are various differences between experimental and theoretical calculations. This difference can be corrected by a scaling factor. 6- 311 ++ G (d, p) 4000-1700 cm-1 region 0.958[26] and 1700-0 cm-1 region 0.978[27] multiplier of the molecule can be scaled. The IR spectra given in Fig 2 were obtained using experimental and quantum mechanical calculations. The frequencies and vibration bands calculated for the compound are given in Table-3.

The vibration band experimentally observed at 3752 cm-1 was theoretically calculated as 3824 cm-1 (B3LYP) and 3974 cm-1 (HF). Similarly, the aromatic vibration of = C-H was observed at 3200 cm-1 was theoretically calculated as 3080 cm-1 (B3LYP) and 3216 cm-1 (HF). Experimentally, C = C aromatic vibration bands were observed in 1607, 1600, 1586 cm-1, These values was theoretically calculated as 1619, 1611, 1594 cm-1 (B3LYP) and 1778, 1751, 1742 cm-1 (HF). The assignments of all other stress, torsion, and vibration bands are given in Table-3.

Table-3: Significant vibrational frequencies ($cm^{-1}$) in the FT-IR spectrum.

| Vibrational modes (υ) | Exp* | B3LYP | | HF | |
|---|---|---|---|---|---|
| | | unscaled | scaled | unscaled | scaled |
| Ar-OH | 3752 | 3749 | 3824 | 4150 | 3974 |
| =C-H (aromatic ) | 3200 | 3213 | 3080 | 3359 | 3216 |
| CH (aliphatic) | 2958 | 3081 | 2950 | 3239 | 3103 |
| | 2939 | 3064 | 2935 | 3206 | 3078 |
| | 2851 | 3057 | 2927 | 3201 | 3069 |
| | 2809 | 3052 | 2919 | 3193 | 3060 |
| C=C (aromatic) | 1607 | 1658 | 1619 | 1814 | 1741 |
| | 1600 | 1648 | 1611 | 1795 | 1715 |
| | 1586 | 1634 | 1594 | 1782 | 1707 |
| $CH_2$ (aliphatic) | 1474 | 1514 | 1478 | 1644 | 1610 |
| | 1455 | 1497 | 1463 | 1639 | 1601 |
| | 1403 | 1494 | 1455 | 1629 | 1593 |
| OH bending | 1356 | 1486 | 1447 | 1436 | 1399 |
| C-O (aromatic) | 1250 | 1359 | 1330 | 1372 | 1346 |
| C-H(aliphatic, out-of-plane bending) | 975 | 1333 | 1306 | 1269 | 1241 |
| | 873 | 979 | 954 | 996 | 977 |
| | 787 | 930 | 907 | 888 | 871 |

Scaled factor: 0,958 for 4000-1700 $cm^{-1}$; 0,978 for 1700-400 $cm^{-1}$
Exp*= Experimental

*NMR spectra*

In this study, 1 H-NMR and 13C-NMR of the 2- (naphthalen-1-yl (piperidin-1-yl) methyl) phenol compound was first optimized to calculate the chemical shift values. The chemical shift values were created in $CHCl_3$ using the GIAO NMR approach in the HF and in the B3LYP methods by using the 6-311G ++ (d, p) basic set…" (Table-4.)[28–30]. Chemical shifts of 13C-NMR and 1H-NMR were compared experimentally and theoretically. It was found that there is a match between the experimentally obtained and theoretically calculated values of the molecule examined in $CHCl_3$ solvent medium.

Table-4: Selected Experimental and calculated 1H and 13C NMR chemical shifts (ppm).

| Atoms | Experimental | B3LYP | HF |
|---|---|---|---|
| | | $CHCl_3$ | $CHCl_3$ |
| C13H | 5.60 | 5.92 | 5.72 |
| O11H | 12.84 | 3.84 | 2.81 |
| C4H | 7.14 | 8.20 | 8.57 |
| C5H | 6.92 | 7.38 | 7.64 |
| C7H | 6.66 | 6.95 | 7.45 |
| C17H | 7.45 | 7.49 | 7.66 |
| C20H | 7.52 | 7.69 | 7.88 |
| C25H | 7.60 | 8.12 | 8.57 |
| C22H | 7.89 | 7.77 | 8.25 |
| C18H | 8.38 | 8.74 | 8.99 |
| C13 | 117.1 | 67.4 | 61.6 |
| C3 | 119.0 | 135.7 | 143.2 |
| C2 | 157.2 | 160.8 | 163.8 |
| C1 | 125.9 | 121.0 | 128.0 |
| C16 | 129.2 | 139.3 | 145.8 |
| C33 | 26.2 | 49.8 | 48.8 |

The C13H peak, which is one of the characteristic peaks of the compound, has been experimentally seen at 5.60 ppm, while it was found to be 5.92 in the calculations with the B3LYP method and 5.72 ppm in the calculations with the HF method. Another specific peak, the O11H peak, had a shift value at 12.84 experimentally, and this value was calculated as 3.84 and 2.81 theoretically. In alkylaminopheol compounds, the OH peak is normally not within the expected slip range. Intramolecular hydrogen bonds and chemical structure cause OH peak to be observed in a range of 12.00-13.00 ppm.

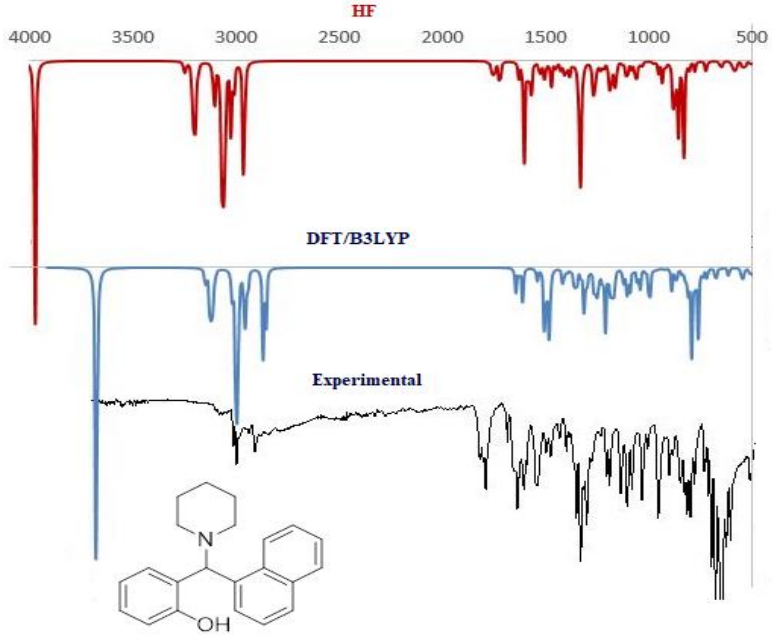



Fig. 2: Theoretical (HF red, B3LYP blue) and experimental (black) and IR spectra of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol.

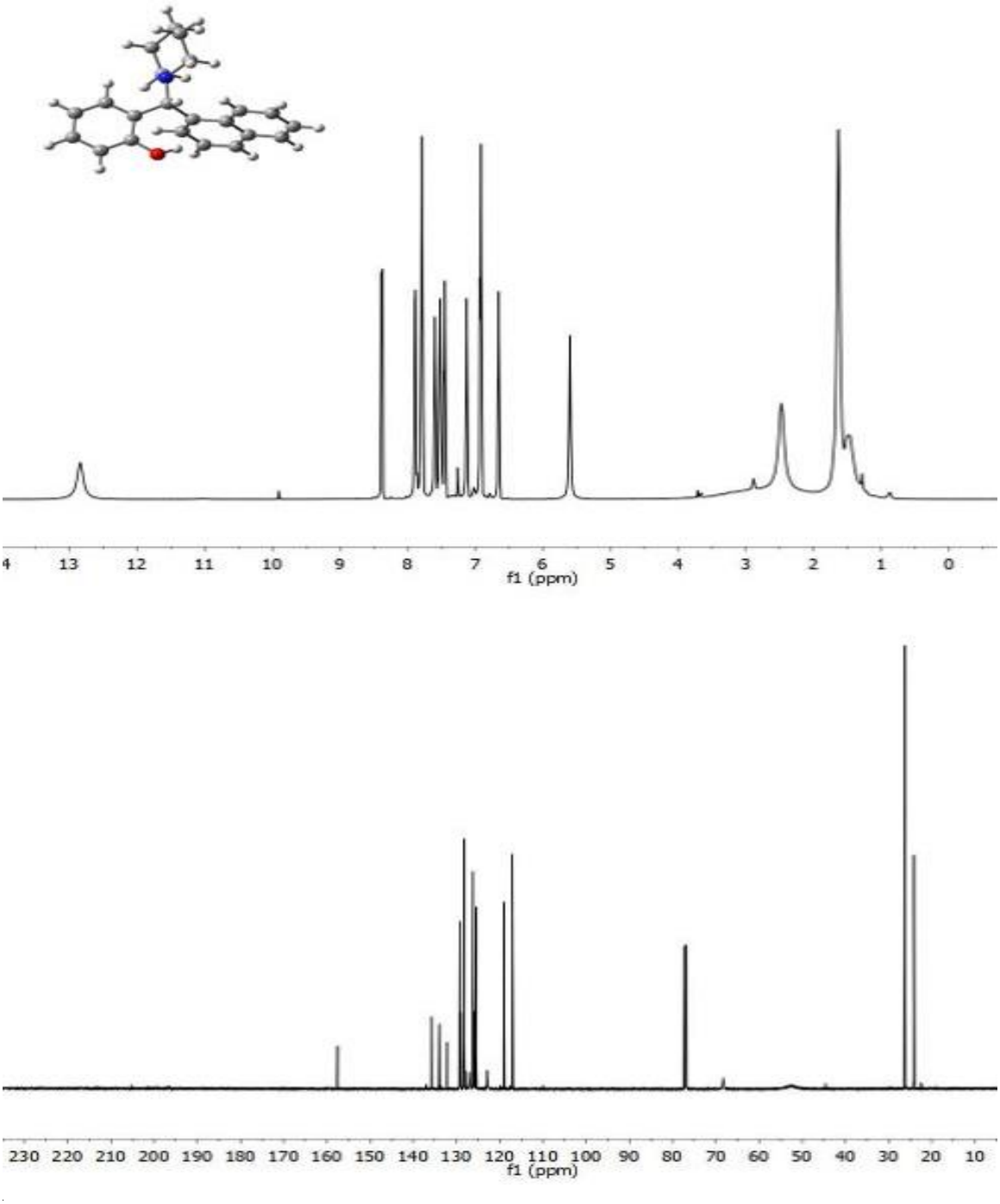



Fig. 3: Experimental $^{1}$H-NMR and $^{13}$C-NMR spectra of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol.

Table-5: Experimental and calculated electronic transitions, oscillator strengths and their assignments for 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol.

| **Experimental values** | | **B3LYP calculated values** | | | |
|---|---|---|---|---|---|
| **$\lambda_{max}$(nm)** | **absorbans** | **$\lambda_{max}$(nm)** | **Excitation energy(eV)** | **$f_{(oscillator\ strength)}$** | **Transitions** |
| **224** | **1.672** | **302.4** | **4.100** | **0.0168** | **HOMO-1 - LUMO ($\pi$–$\pi$*)** |
| **285** | **0.234** | **339.4** | **3.653** | **0.0692** | **HOMO - LUMO (n-$\pi$*)** |

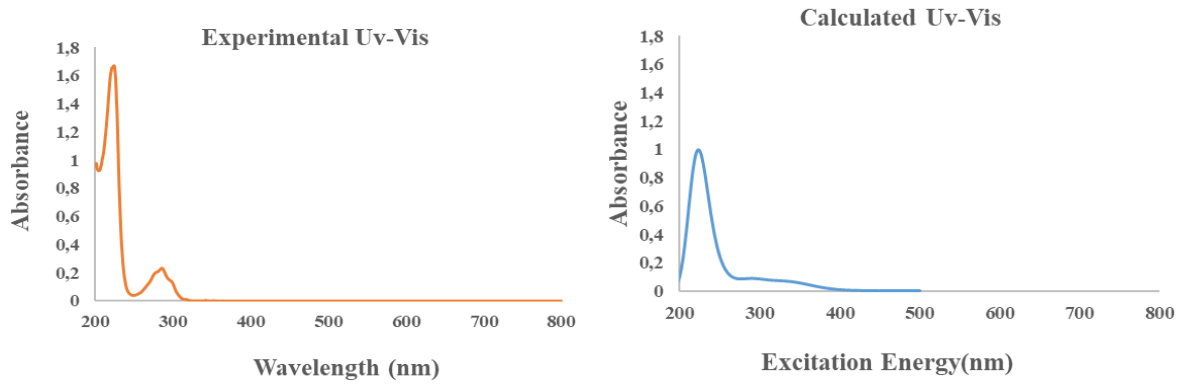



Fig. 4: a) Experimental UV-vis absorption spectra of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol
b) Uv-Vis spectrum drawn by TD-DFT- B3LYP / 6-311 ++ G (d, p) method.

*UV-Vis spectra*

Uv-Vis spectra of the alkylaminophenol compound were taken in ethanol. Experimental absorption wavelengths were observed at 285 and 224 nm. The excitation energies of the absorption spectroscopy of the molecule, the wavelengths (λ) to which they absorb the maximum absorption, oscillator strength (f) were calculated using the TD-SCF method in ethanol solvent medium. In saturated compounds with heteroatom (C = C) π–π * (224); The n-π * (285 nm) transitions that are effective in unsaturated systems with heteroatoms carrying non-bonding electrons are significant in our alkylaminophenol compound. In this case; From HOMO-1 to LUMO π–π *; corresponding n-π * transitions are seen in HOMO-LUMO.

*Mulliken charge*

Mulliken charge distribution is the most common of population analysis methods. It is based on obtaining molecular orbitals with linear combination of atomic orbitals. However, this distribution does not fully reflect the electronegativity of each element. Therefore, it is used to make some qualitative estimates rather than quantitatively estimate experimental results. Mulliken density analysis was performed with B3LYP and HF / 6-311G ++ (d, p) methods

B3LYP and HF methods, which are given in Table-6. Mulliken charge in the B3LYP method is between -0.701 and 0.701, The atomic charge analysis of alkylaminophenol showed the $C_1$, O11, $C_{13}$,$C_{15}$ atoms a maximum negative charges, The $N_1$ and $C_3$ atoms have positive charges of 0.335 and 0.701 a.u., respectively. Mulliken charge in the HF method is between-0.620 ve 0.620. The atomic charge analysis of alkylaminophenol showed the C1, O11, C13,C15 atoms a maximum negative charges, The $N_1$ and $C_3$ atoms have positive charges of 0.502 and 0.568 a.u., respectively.

Table-6: Mulliken and natural population charges of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol.

| Atoms | Mulliken(B3LYP) | Mulliken(HF) |
|---|---|---|
| C1 | -0.230 | -0.359 |
| C2 | -0.656 | -0.509 |
| C3 | 0.701 | 0.568 |
| C4 | 0.238 | 0.143 |
| C5 | -0.509 | -0.490 |
| C6 | -0.262 | -0.445 |
| O11 | -0.251 | -0.340 |
| C13 | -0.029 | -0.140 |
| C15 | -0.079 | -0.011 |
| C16 | 0.0 | -0.021 |
| C17 | -0.233 | -0.276 |
| C18 | -0.103 | -0.278 |
| C19 | 0.202 | 0.322 |
| C20 | -0.330 | -0.351 |
| C22 | -0.304 | -0.354 |
| C27 | -0.519 | -0.520 |
| C24 | -0.005 | -0.062 |
| N32 | 0.335 | 0.520 |
| C33 | -0.356 | -0.293 |
| C36 | -0.205 | -0.170 |
| C39 | -0.369 | -0.455 |
| C45 | -0.405 | -0.575 |
| C42 | -0.345 | -0.377 |

The data obtained has an important role in the quantum mechanical studies of the molecule, such as dipole moment, chemical reactivity, and electronic properties.

*Frontier molecular orbitals (FMOs)*

The molecular reactivity (FMO) of a molecule is important in defining its optical and electrical properties, and in defining the absorption of light. According to the molecular orbital theory; all molecules have HOMO (Highest occupied molecular orbital) and LUMO (Lowest Unoccupied molecular orbital). The frontier molecular orbital (HOMO and LUMO) shapes of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol were determined using DFT/B3LYP and HF methods with 6-311++G(d,p) basis sets. The HOMO and LUMO orbitals for this molecule are given in Fig 4.The calculated HOMO and LUMO energies of 2-

(naphthalen-1-yl (piperidin-1-yl) methyl) phenol were -5.939 and -1.689 eV, respectively, so the energy difference was 4.25 eV.some physicochemical parametres were calculated by these equations: hardness, $\eta = (IA) / 2 = 2.125$, electronegativity, $\chi = (I-A) / 2 = 3.814$, softness S = 1.0625 and electrophilicity index $\omega = \chi^2 / 2\eta = 3.422$ where A (-ELUMO) and I (-EHOMO) are electron affinity and ionization potential. The same procedures were applied in the HF method. All data were shown in Table-7. These parameters were used to understand toxicity in terms of reactivity. In terms of reaction, theoretical toxicity is dtermined using the electrophilicity index.

*Molecular electrostatic potential (MEP)*

MEP surface describes the charge distribution in the molecule. Molecular electrostatic potential (MEP) is used to investigate the chemical reactivity of a molecule. Surfaces of the optimized electronic structures were drawn using the B3LYP and HF / 6 - 311 ++ G (d, p) sets in Fig 5. The colour code of this map ranges from -4.310 $e^{-2}$ and +4.310$e^{-2}$ a.u. and -4.785 $e^{-2}$ and +4.785 $e^{-2}$ a.u. Where blue shows the strongest attraction and red indicates repulsion. From MEP surface, the negative potential area is on the oxygen atom of the hydroxyl group while positive potential areas are on the phenyl hydrogen atoms. These results provide information about the region where the compounds may have inter-molecular interactions, especially with biological molecules.

Table-7: HOMO and LUMO energies, the energy gap (ΔE), absolute electronegativity (χ) chemical hardness (η), softness (S) and electrophilicity index (ω) of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol using B3LYP/6-311++G(d,p) and HF/6-311++G(d,p) levels

| Global reactivity descriptors | B3LYP/6-311++G(d,p) | HF/6-311++G(d,p) |
|---|---|---|
| E(HOMO, eV) | -5.939 | -8.094 |
| E(LUMO, eV) | -1.689 | 0.010 |
| ΔE(eV) | 4.250 | 8.104 |
| χ | 3.814 | 4.042 |
| η | 2.125 | 4.052 |
| s | 1.063 | 2.026 |
| ω | 3.423 | 4.032 |

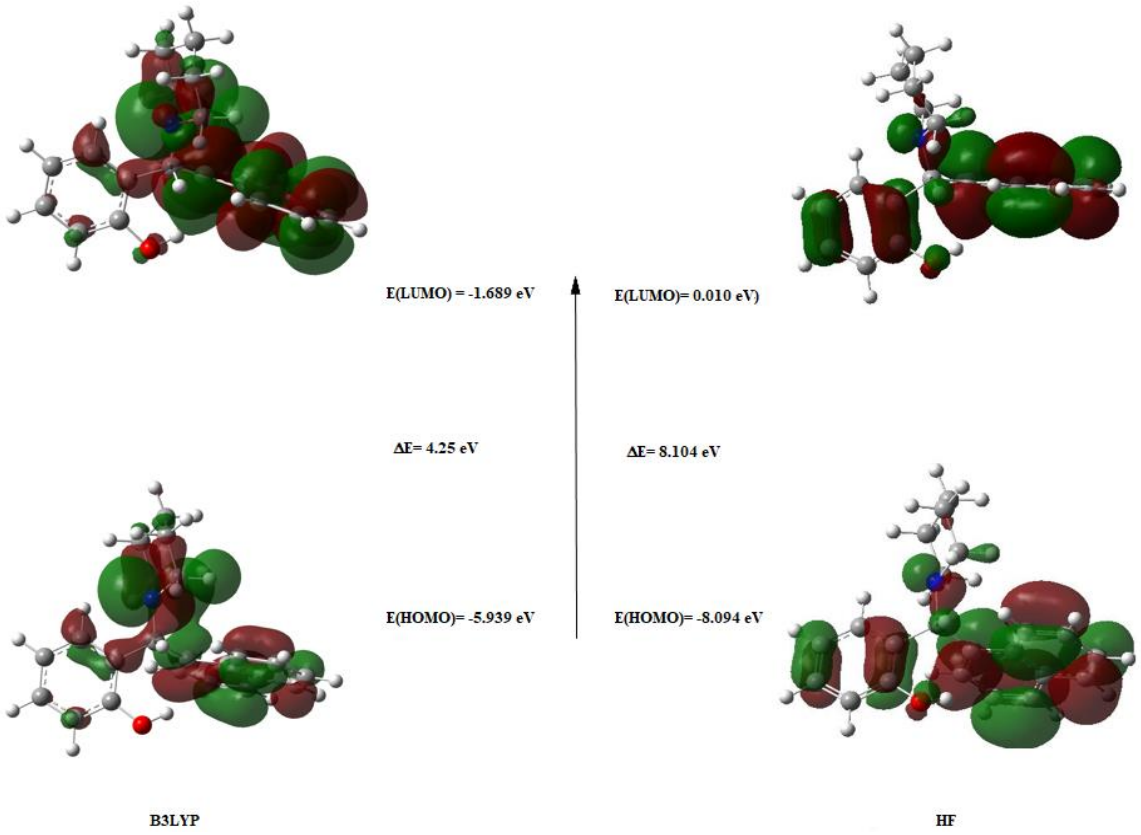



Fig. 5: HOMO and LUMO orbitals of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol with the energy gap.

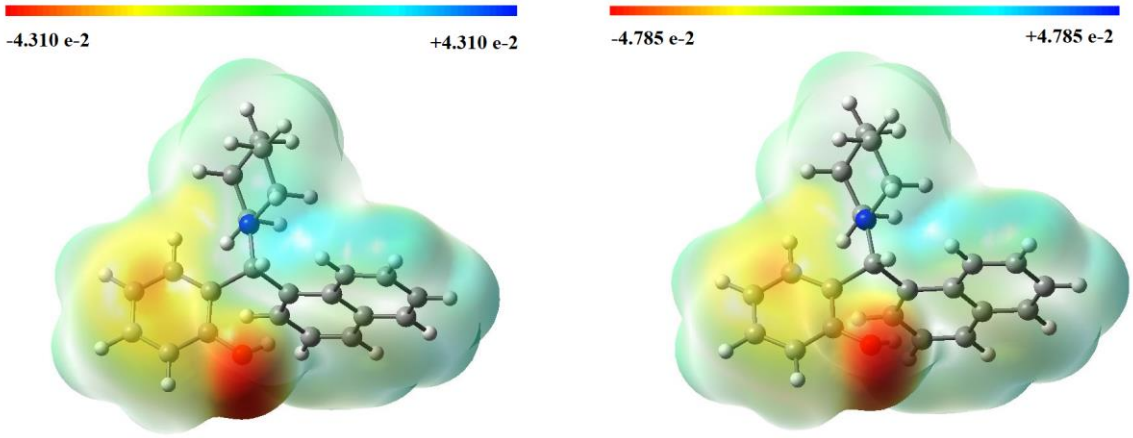



Fig. 6: The total electron density mapped with molecular electrostatic potential surface of 2-(naphthalen-1-yl(piperidin-1-yl)methyl)phenol with B3LYP and HF methods.

## Conclusions

In this study, for the first time, alkylaminophenol derivative 2- (azepan-1-yl (naphthalen-1-yl) methyl) phenol compound was synthesized with very high efficiency. Structural analysis of the compound was carried out experimentally with FT-IR, NMR, UV-vis. Because of quantum chemical calculations of alkylaminophenol are limited in the literature, the physicochemical parameters of the compound were examined in comparison with the DFT/B3LYP and HF methods using (6-311 ++ G (d, p) basis set. Electrical, magnetic and vibration properties of the molecule were obtained about information. It was observed that the theoretical and experimental data were compatible. The high electronegativity of some atomic group caused a slight deviation in the values. Because, when high electronegativity is combined with other factors, it has been observed that it affects the correlation between experimental and theoretical results. As a result; a potential drug active compound was synthesised, and all electronic properties of the compound were examined by quantum chemical calculations.

## Acknowledgements

This study was supported with KUAP(F)-2016/5 project by Bursa Uludag University Scientific Research Projects Unit

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