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Comparative analysis of nonlinear optical properties in santalin A and santalin B: a density functional theory approach

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Abstract: This study investigates the non-linear optical (NLO) properties of Santalin A and Santalin B using density functional theory (DFT) at the B3LYP/6-311G+(d,p) level of theory, marking the first computational exploration of these properties for Santalin compounds. The comparative analysis reveals distinct differences in the physicochemical and electronic properties of the two compounds, influencing their potential applications. Santalin A, characterized by a tightly bound highest occupied molecular orbital (HOMO), a larger band gap, and higher ionization potential, exhibits greater stability, making it suitable for applications requiring resistance to electronic changes, such as insulation or semiconductor roles. Its higher dipole moment (7.04) and polarizability ($8.01 \times 10^{-40} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$) suggest it could be more effective in advanced NLO applications, such as optical switching and second-harmonic generation. In contrast, Santalin B demonstrates higher reactivity with a less negative HOMO (−4.701 eV), a smaller band gap (2.040 eV), and greater electron affinity (2.66), indicating its potential for applications requiring enhanced conductivity, electron transfer, and flexibility, such as in organic electronics. Both compounds show notable NLO responses; Santalin A and B both exhibit remarkable nonlinear optical (NLO) properties, with Santalin A showing a higher dipole moment (7.0477 Debye vs. 6.53 Debye), greater anisotropic polarizability ($48.55 \times 10^{-39} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$ vs. $37.12 \times 10^{-39} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$), and slightly stronger hyperpolarizability ($1.13 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$ vs. $1.06 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$). Both molecules have similar second-order hyperpolarizabilities (γ), with Santalin A at $-6.66753 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$ and Santalin B at $-6.76983 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$, highlighting their potential for advanced NLO

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applications. However, Santalin A exhibits slightly more pronounced properties. The findings emphasize the importance of tailoring material selection based on specific application needs, with Santalin A being more suited for stability-driven contexts and Santalin B excelling in environments that demand high reactivity and conductivity.

Keywords: nonlinear optical (NLO) properties; Santalin A; Santalin B; density functional theory (DFT)

1 Introduction

For more than a century, natural products chemists have been interested in the pigments present in red sandalwood (*Pterocarpus santalinus*) and kindred red woods, dating back to the first report by Pelletier. Despite extensive research, it wasn't until 1954 that two pure compounds, Santalin and santarubin, were successfully isolated by Robertson and Whalley. The initial structural suggestions for these coloring compounds emerged from their study, which involved questioning degradative processes. Commercial samples of barwood and camwood were also found to contain Santalin, the main pigment from red sandalwood. On the other hand, Santarubin was only detected in barwood and camwood. The 'anhydrobenzopyranol' structure of both pigments was firmly established during this research.¹ However, the use of red sandalwood is somewhat limited, as the colors produced are not lightfast and are sensitive to alkalis. The coloring matter, Santalin, found in the wood has been isolated and analyzed by various chemists. Different formulas have been proposed to represent its composition. Notably, Pelletier first analyzed Santalin and assigned it the formula $C_{16}H_{16}O_5$. Subsequently, Bolley suggested it was $C_{27}H_{26}O_9$, while Weyermann and Hiffely found it to be $C_{15}H_{14}O_5$. Lastly, Franchimont and Sicherer proposed the formula $C_{17}H_{16}O_6$.² Santalin possesses excellent chromatic characteristics and contains bioactive chemicals recognized for their stability,³ anti-inflammatory, antioxidant,³ anticancer, antimicrobial, and antidiabetic properties.^{4–7} Santalin A and Santalin B are both red pigments found in red sandalwood. The main difference between them is that Santalin B has an additional methoxy group compared to Santalin A. This means that Santalin B is a more methylated form of Santalin A. Specifically, Santalin B has a methyl group attached in a position where Santalin A has a free hydroxyl group.⁸ Santalin A is identified as 9,10,12-tri-O-methylSantalin,⁹ while Santalin B is known as 9,10,12,4'-tetra-O-methylSantalin,⁹ which has an additional methoxy group at the 4' position. Both molecules have a similar core structure, but the extra methoxy group in Santalin B slightly changes its chemical properties.¹⁰

There has been some controversy regarding the natural occurrence and stability of Santalin A and Santalin B. While both pigments are reported to be present in red sandalwood (*P. santalinus*), some studies suggest that Santalin B may not be a truly naturally occurring compound but rather an artifact formed during extraction or processing. The presence of the additional methoxy group in Santalin B raises questions about whether it is a direct biosynthetic product of the plant or if it results from methylation reactions occurring under certain conditions, such as solvent interactions or enzymatic modifications post-harvest. Furthermore, the stability of these pigments is another debated aspect. Santalin A and Santalin B are known to be sensitive to light, heat, and pH variations, which can lead to degradation or structural modifications over time. Some researchers argue that the reported differences in the composition of these pigments across various studies may be due to their instability rather than genuine variability in their natural occurrence. This instability complicates their use in natural dye applications and pharmacological studies, as their color and bioactive properties may change depending on environmental factors. Furthermore, the potential nonlinear optical (NLO) properties of Santalin A and Santalin B have attracted interest due to their conjugated structures and extended π -electron systems. These structural features are key factors in molecules exhibiting NLO behavior, as they enable strong electron delocalization, which is essential for second- and third-order nonlinear optical effects such as second-harmonic generation (SHG), third-harmonic generation (THG), and two-photon absorption (TPA). Given their polyphenolic nature and presence of methoxy groups, Santalin A and B could exhibit enhanced hyperpolarizability, which is a crucial parameter in determining NLO efficiency. The additional methoxy group in Santalin B could further influence its electron-donating capacity, potentially leading to differences in its optical responses. However, the extent of their NLO properties remains largely unexplored and would require detailed computational and experimental investigations, including density functional theory (DFT) calculations and Z-scan techniques, to quantify their nonlinear susceptibilities. This study investigates the structural properties, stability, and NLO behavior of Santalin A and Santalin B using DFT/6311G+(d,p) level of theory. By analyzing their molecular geometry, electronic structure, and environmental stability depending upon the conformational analysis of optimization, frontier molecular orbitals, global descriptive parameters, and molecular electrostatic potential map, we aim to clarify the controversies surrounding their stability and degradation. Additionally, key NLO parameters such as dipole moment (μ), electrophilicity index (ω), polarizability (α), and hyperpolarizability (β) will be computed to assess their potential applications in photonic and optoelectronic devices.¹¹ This work provides fundamental insights into their chemical behavior and optical properties, contributing to their broader applicability in scientific and industrial fields.

2 Computational methodology

In this study, the 3D structures of Santalin A and Santalin B were obtained from PubChem: Santalin A (PubChem ID 5490179) and Santalin B (PubChem ID 5490285).¹² The Santalin structures were optimized using the Gaussian09 program,^{11–13} applying the Lee-Yang-Parr correlation functional (B3LYP) and the 6-311G(d,p) basis set with Gauss view.¹⁴ As a visual interface, through these quantum computational calculations, we investigated these compounds' structural geometry, frontier molecular orbitals, and electronic properties. The HOMO, or the highest occupied molecular orbital, and LUMO, or the lowest unoccupied molecular orbital, along with key properties such as the electrophilic index (ω), hardness (η), softness (S), electronegativity (χ), ionization potential (IP), and electron affinity (EA). Additionally, nonlinear optical calculations such as polarizability, hyperpolarizability, and second-order hyperpolarizability.^{15–19}

3 Result and discussion

This study presents a detailed investigation of the molecular structural properties of Santalin A and Santalin B and the molecular structure is displayed in Figure 1. The physicochemical properties of both compounds including molecular structure, solubility, hydrogen bonding were tabulated in Table 1.^{1,9} The geometry of Santalin A and B was optimized using the DFT/B3LYP/6-311G(d,p) method. The optimized structures are shown in Figure 2. Bond angles, bond lengths, and Mulliken charge parameters were also calculated and are provided in the Supplementary Material.

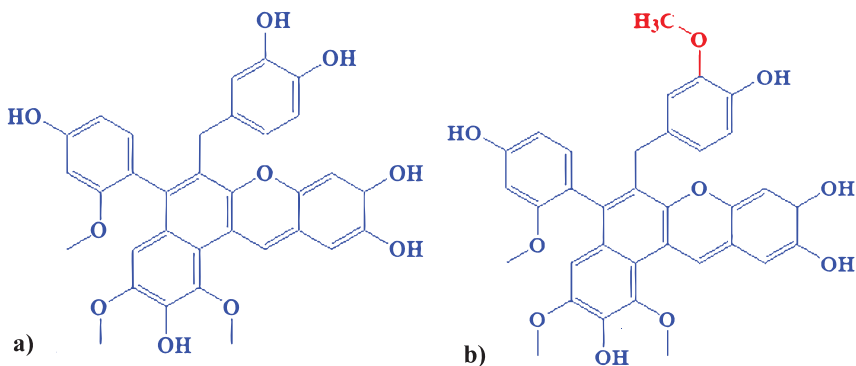


Figure 1: Two-dimensional structure of (a) santalin A and (b) santalin B.

Table 1: Showing the physicochemical properties of santalin A and santalin B.

Parameters	Santalin A	Santalin B
Formula	C ₃₃ H ₂₆ O ₁₀	C ₃₄ H ₂₈ O ₁₀
Molecular weight	582.55 g/mol	596.58 g/mol
Num. heavy atoms	43	44
Num. arom. heavy atoms	30	30
Fraction Csp ³	0.12	0.15
Num. rotatable bonds	6	7
Num. H-bond acceptors	10	10
Num. H-bond donors	5	4
Molar refractivity	161.98	166.44
TPSA	159.05 Å ²	148.05 Å ²
Water solubility		
Log S (ESOL)	−5.90	−6.11
Solubility	7.39 mg/mL; 1.27 mol/L	4.59 mol/L
Class	Moderately soluble	Poorly soluble
Log S (Ali)	6.72	−6.83
Solubility	1.11 mg/mL; 1.90 mol/L	8.79 mol/L
Class	Poorly soluble	Poorly soluble
Log S (SILICOS-IT)	−9.63	−10.31
Solubility	1.36 mg/mL; 2.34 mol/L	2.89e-08 mg/mL; 4.84e-11 mol/L
Class	Poorly soluble	Insoluble

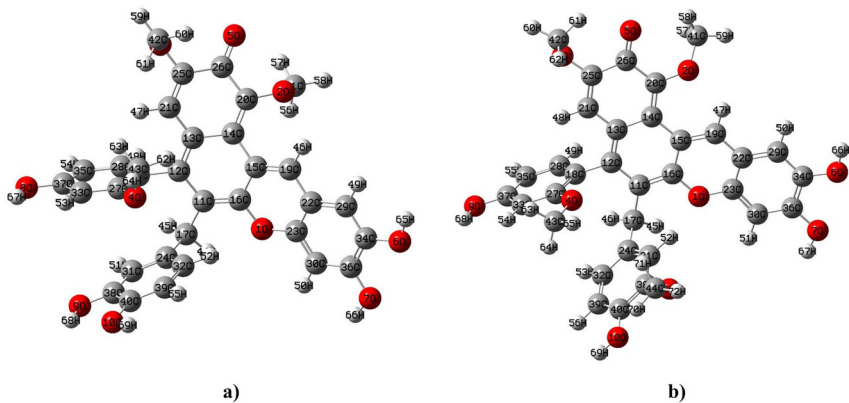


Figure 2: The optimized geometry of (a) santalin A and (b) santalin B using the DFT/B3LYP/6-311G(d,p) level of theory.

Santalin B has a slightly higher molecular weight (596.58 g/mol) than Santalin A (582.55 g/mol) due to additional atoms, contributing to the marginally larger size and potential effects on physical properties. Both compounds have a similar number of heavy atoms (43 in Santalin A, 44 in Santalin B) and share 30 aromatic heavy atoms, indicating comparable aromaticity and electronic stability. Santalin B exhibits slightly greater molecular flexibility, with a higher fraction of sp^3 carbons (0.15 vs. 0.12) and more rotatable bonds (7 vs. 6). Both compounds have 10 hydrogen bond acceptors, but Santalin A has one more donor (5 vs. 4), potentially influencing interactions in polar environments. The higher molar refractivity of Santalin B (166.44 vs. 161.98) suggests a slightly larger molecular volume, while Santalin A has a higher Topological Polar Surface Area (TPSA) ($159.05 \text{ \AA}^2$ vs. $148.05 \text{ \AA}^2$), indicating more exposed polar functional groups. Both compounds are poorly soluble in water, but Santalin A shows slightly better solubility across different models, with Log *S* (ESOL) values classifying it as moderately soluble (−5.90) while Santalin B is poorly soluble (−6.11). Log *S* (SILICOS-IT) further differentiates them, categorizing Santalin A as poorly soluble (−9.63) and Santalin B as insoluble (−10.31), highlighting Santalin B's even lower solubility in certain models.²⁰

3.1 ^{13}C NMR

The chemical structures of Santalin A and B, derived from the theoretical calculation of ^{13}C NMR spectra, are shown in Figure 2(a and b), along with their corresponding ^{13}C NMR spectra (c and d). The primary structural difference between the two is the presence of a methoxy group ($-\text{OCH}_3$) at C-6 in Santalin B, which is absent in Santalin A. This modification likely influences the electronic environment and chemical shifts of adjacent carbons, especially those in the aromatic system. Both molecules contain sp^2 hybridized carbons in the aromatic rings in the 100–160 ppm region, as well as oxygenated carbons, which include methoxy ($-\text{OCH}_3$) and hydroxyl ($-\text{OH}$) substituted carbon peaks in the 50–60 ppm range.²¹ Significant downfield shifts (>160 ppm) indicate carbonyl or phenolic groups, which are deshielded due to electron-withdrawing effects. Although both spectra are highly similar, confirming that Santalin A and B share a common core structure, the presence of an additional methoxy carbon resonance (~ 56 ppm) shown in Figure 3d corresponds to the extra $-\text{OCH}_3$ group in Santalin B. The deshielding of adjacent carbons suggests that electron donation from the methoxy group alters the conjugation in the system.²²

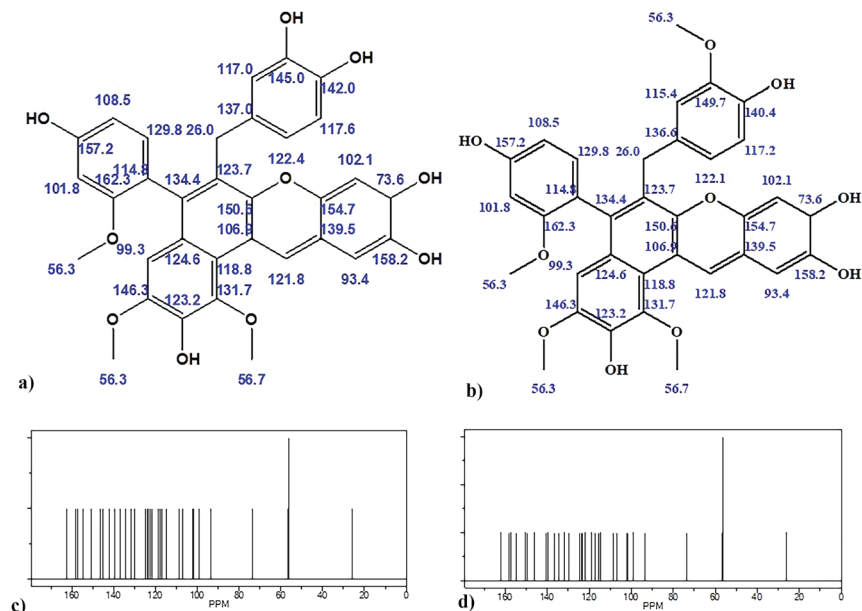


Figure 3: The molecular structures of (a) santalin A (b) santalin A along with their corresponding ^{13}C NMR spectra in (c and d).

3.2 ^1H NMR

The ^1H NMR spectra of Santalin A and Santalin B, depicted in Figure 4 and obtained from computational calculations, reveal characteristic aromatic proton signals between 6.0 and 8.0 ppm, indicating their polyphenolic nature. Both compounds exhibit deshielded hydroxyl ($-\text{OH}$) protons at approximately 5.0 and 15.0 ppm, suggesting strong intramolecular hydrogen bonding. The presence of methoxy ($-\text{OCH}_3$) groups is observed around 3.73 ppm in both spectra, with Santalin B showing an additional methoxy signal, distinguishing it from Santalin A.²³ The subtle shifts in the aromatic region reflect electronic differences due to variations in substitution patterns. Overall, the spectra confirm structural similarity, with Santalin B possessing an extra methoxy group that leads to slight chemical shift variations.

3.3 Frontier molecular orbitals

The Frontier molecular orbitals, the HOMO, LUMO, and the bandgap of Santalin A and Santalin B, along with their related molecular orbitals are showed in Figure 5.

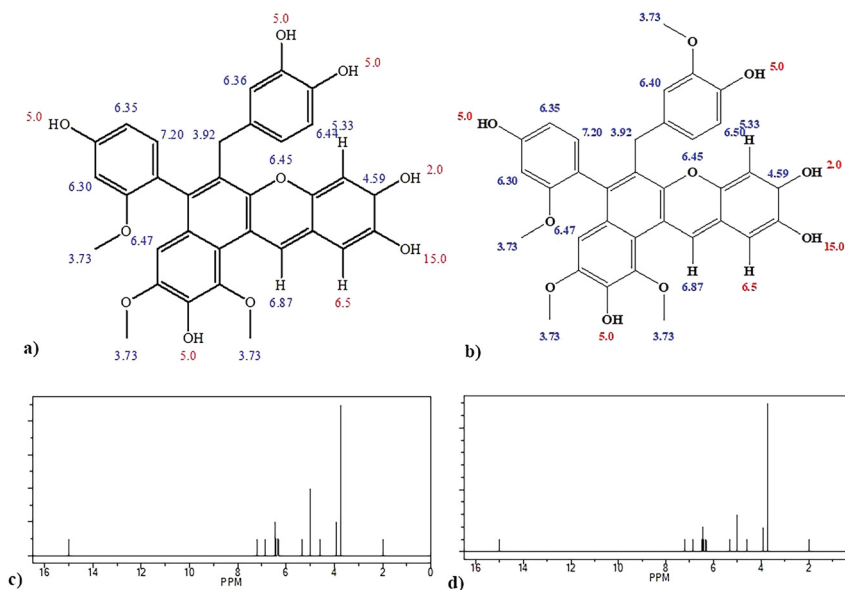


Figure 4: Molecular structure of (a) santalin (b) santalin B A with proton chemical shifts labeled. ^1H NMR spectrum of (c) santalin A. (d) Santalin B.

These properties provide valuable insights into the electronic properties of the compounds, which can influence their behavior in various applications, such as their reactivity, photophysical properties, and electronic conductivity. The comparison of the frontier molecular orbitals (FMOs) of Santalin A and Santalin B provides key insights into their electronic properties and potential behavior in various applications. For Santalin A, the HOMO is located at -6.57 eV, which is more negative than the HOMO of Santalin B at -4.7 eV. This suggests that the electrons in Santalin A are more tightly bound, making it more stable and less prone to excitation or chemical reactions compared to Santalin B. On the other hand, the higher HOMO value for Santalin B indicates that its electrons are less tightly bound, which could allow for easier excitation to higher energy states or facilitate chemical reactions more readily than Santalin A. When considering the LUMO, Santalin A has a value of 0.68 eV, while Santalin B has a much lower LUMO value of -2.6 eV. The less negative LUMO of Santalin A suggests that it has a greater tendency to accept electrons than Santalin B, which is more stable in its unoccupied state due to the more negative LUMO. This suggests that Santalin A might be more reactive toward electron-accepting interactions, while Santalin B is less likely to engage in such processes, reflecting its stability. Further, the bandgap between the HOMO and LUMO reveals a significant

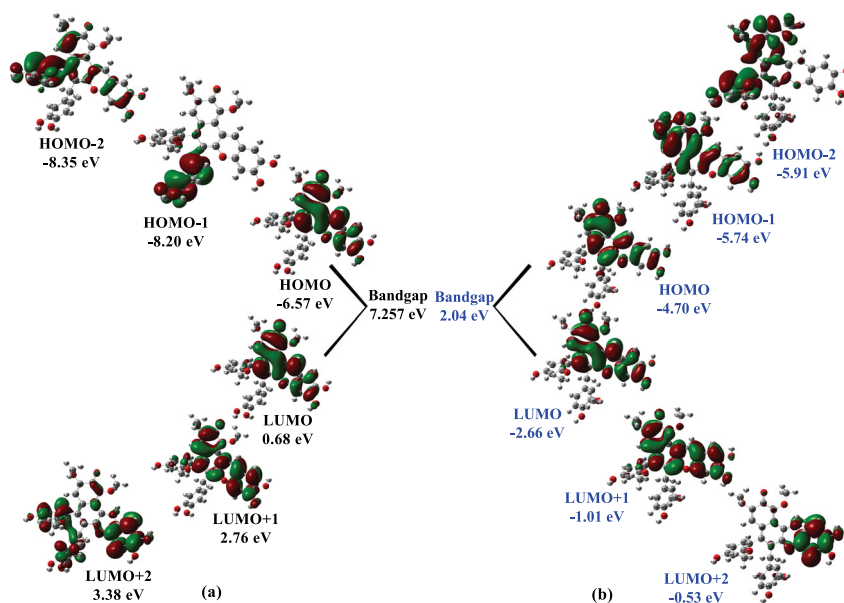


Figure 5: HOMO, LUMO and band gap of (a) santalin A and (b) santalin B.

contrast in their electronic conductivity properties. Santalin A has a large bandgap of 7.25 eV, which may limit its conductivity and make it behave more like an insulator or semiconductor in certain conditions. In contrast, Santalin B has a much smaller bandgap of 2.04 eV, indicating that it may have better electronic conductivity due to the lower energy need to stimulate electrons to move from the HOMO to the LUMO. This difference suggests that Santalin B might be more suitable for applications that require better electron mobility or conductivity. Overall, Santalin A demonstrates greater stability with a more tightly bound electron configuration and a larger bandgap, Santalin B has a higher reactivity due to its less tightly bound HOMO and lower LUMO, along with better potential for electronic conductivity. These properties suggest that Santalin A may be more appropriate for stability-driven applications, while Santalin B could be better suited for applications requiring enhanced electron transfer.

Beyond the HOMO and LUMO, additional orbitals such as HOMO-1, HOMO-2, LUMO+1, and LUMO+2 are also relevant. The HOMO-1 and HOMO-2 values for Santalin A are more negative than those for Santalin B, suggesting that the additional occupied molecular orbitals in Santalin A are farther from the Fermi level and may contribute to its more stable electronic configuration. On the other hand, the LUMO+1 and LUMO+2 values for Santalin A are also more positive than those of

Santalin B, further indicating that Santalin A may be more capable of accepting electrons at higher energy levels compared to Santalin B.

3.4 Molecular electrostatic potential map

MESP map provides a three-dimensional visualization of the charge distribution within a molecule, highlighting regions of both positive and negative potential. This representation is crucial for understanding and predicting chemical reactivity, as it allows for the identification of molecular polarity. The map uses color coding to differentiate between regions: red represents electron-rich, negative areas that attract electrophiles, while blue denotes electron-deficient, positive regions that are more likely to interact with nucleophiles. Green indicates regions with a neutral potential. MESP maps are especially valuable for studying drug-target interactions and assessing molecular properties. The scale of surface potential follows this order: red < orange < yellow < green < blue.¹¹

The MESP maps for Santalin A and Santalin B are shown in Figure 6. Typically, regions with a negative electrostatic potential (red) highlight electron-rich sites that are prone to attract electrophiles, while positive regions (blue) indicate electron-deficient areas that tend to attract nucleophiles. Notably, Santalin A and Santalin B display contrasting characteristics in these regions. For Santalin A, electron-deficient (blue) regions surround the 20th carbon atom, indicating a tendency to attract nucleophiles. Meanwhile, the 12th, 15th, and 19th carbon atoms are more likely to interact with electrophiles. In contrast, for Santalin B, electron-rich (red) regions are present around the 20th carbon atom, making it susceptible to attracting

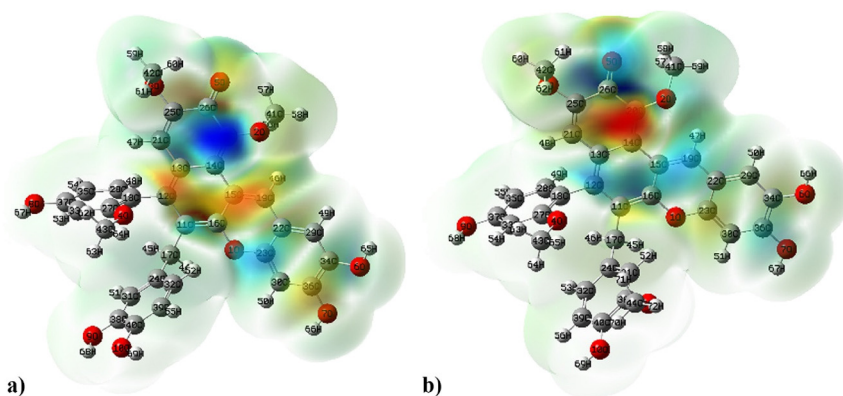


Figure 6: Molecular electrostatic potential map of (a) santalin A and (b) santalin B.

electrophiles. The 12th, 15th, and 19th carbon atoms in Santalin B are more likely to interact with nucleophiles.

3.5 Global descriptive parameters

Global descriptive parameters are used to examine several key electronic properties, including IP, EA, η , χ , S , μ , and ω of Santalin A and Santalin B. The HOMO and LUMO energy values are used for the global descriptors calculation, and the calculation as follows according to Koopman theorem.^{24,25}

$$\text{IP} \approx -E_{\text{HOMO}}$$

$$\text{EA} \approx -E_{\text{LUMO}}$$

$$\eta \approx (\text{IP} - \text{EA})/2$$

$$\chi \approx (\text{IP} + \text{EA})/2$$

$$S \approx 1/2\eta$$

$$\mu \approx -\chi$$

$$\omega \approx \mu^2/2\eta$$

The global reactivity descriptors calculated using the B3LYP/6-311++G(d,p) method show significant differences between Santalin A and Santalin B. For Santalin A, the HOMO and LUMO energies were -6.57 eV and -0.68 eV, respectively, leading to an IP of 6.57 eV, EA of -0.68 eV, and ΔE of 5.89 eV. The derived η was 3.625 eV, S was 0.138 eV⁻¹, χ was 2.948 eV, and μ was -2.948 eV. The ω was found to be 1.198 eV. In contrast, Santalin B had a HOMO of -4.70 eV and LUMO of -2.60 eV, resulting in a smaller ΔE of 2.10 eV, indicating higher reactivity. The IP and EA values were 4.70 eV and 2.60 eV, respectively, leading to $\eta = 1.05$ eV, $S = 0.476$ eV⁻¹, $\chi = 3.65$ eV, $\mu = -3.65$ eV, and $\omega = 6.34$ eV. These results clearly indicate that Santalin B is more electrophilic, softer, and more reactive than Santalin A, which is relatively stable and less chemically active.

Upon recalculating the same descriptors using the CAM-B3LYP/6-311++G(d,p) method, subtle yet important shifts were observed, particularly in electron affinity and chemical potential. For Santalin A, the HOMO shifted to -6.83 eV and the LUMO to -1.44 eV, yielding a new ΔE of 5.39 eV, slightly narrower than before. The updated descriptors were: IP = 6.83 eV, EA = 1.44 eV, $\eta = 2.695$ eV, $S = 0.186$ eV⁻¹, $\chi = 4.135$ eV, $\mu = -4.135$ eV, and $\omega = 3.173$ eV. For Santalin B, HOMO = -6.20 eV, LUMO = -2.91 eV, $\Delta E = 3.29$ eV, IP = 6.20 eV, EA = 2.91 eV, $\eta = 1.645$ eV, $S = 0.304$ eV⁻¹, $\chi = 4.555$ eV,

$\mu = -4.555$ eV, and $\omega = 6.303$ eV. Compared to B3LYP, the CAM-B3LYP results show enhanced electrophilic character in both molecules, especially Santalin B, whose higher EA, χ , and ω values confirm its strong electron-accepting ability. Overall, the CAM-B3LYP functional, which better accounts for long-range charge transfer effects, reinforces the reactive and electrophilic nature of Santalin B and supports its potential for interactions in charge-sensitive environments.

3.6 Nonlinear optical property

Nonlinear optical materials exhibit a response to incident electromagnetic fields that is not proportional to the applied field strength, leading to the generation of new optical frequencies and other fundamental phenomena. The nonlinear polarization $P(t)$ in a material can be expressed as a power series expansion in terms of the applied electric field $E(t)$ as follows:

$$P = P_0 + \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \dots \dots \dots$$

where E is the electric field's intensity and $\chi^{(n)}$ is the bulk medium's n th-order nonlinear susceptibility tensor. The linear optical response is governed by $\chi^{(1)}$, influencing properties such as dispersion and refractive index. The second order term $\chi^{(2)}$ enables processes like SHG, sum-frequency, and difference-frequency generation, while the third-order term $\chi^{(3)}$ facilitates third harmonic generation (THG), the Kerr effect, and self-focusing. For SHG, the induced nonlinear polarization is expressed as:

$$P^2(2\omega) = \varepsilon_0 \chi^2 E^2(\omega)$$

resulting in output light at twice the incident frequency. Similarly, THG follows:

$$P^3(3\omega) = \varepsilon_0 \chi^3 E^3(\omega)$$

leading to a frequency tripling effect. The third-order susceptibility also affects the nonlinear refractive index, given by:

$$n = n_0 + n_2 I$$

where n_0 represents the linear refractive index, n_2 denotes the nonlinear refractive index coefficient, and stands for optical intensity. Tensors can be used to express the polarizability and hyperpolarizability of NLO. As seen below, the linear polarizability tensor α is a 3*3 matrix with nine components.

$$\alpha_{ij} = \begin{bmatrix} \alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{yx} & \alpha_{yy} & \alpha_{yz} \\ \alpha_{zx} & \alpha_{zy} & \alpha_{zz} \end{bmatrix},$$

$$\beta = \begin{bmatrix} \beta_{xxx} & \beta_{xxy} & \beta_{xxz} \\ \beta_{xyx} & \beta_{xyy} & \beta_{xyz} \\ \beta_{xzx} & \beta_{xzy} & \beta_{xzz} \\ \beta_{yxx} & \beta_{yxy} & \beta_{yxz} \\ \beta_{yyx} & \beta_{yyy} & \beta_{yyz} \\ \beta_{yzx} & \beta_{yzy} & \beta_{yzz} \\ \beta_{zxx} & \beta_{zxy} & \beta_{zxz} \\ \beta_{zyx} & \beta_{zyy} & \beta_{zyz} \\ \beta_{zzx} & \beta_{zzy} & \beta_{zzz} \end{bmatrix}$$

γ_{ijkl} is a fourth-rank tensor, it has **81** elements (3^4), but due to intrinsic and symmetry-related constraints, the number of independent components is significantly reduced for most materials. The typical representation of the γ tensor in matrix form is:

$$\gamma = \begin{bmatrix} \gamma_{xxxx} & \gamma_{xxxy} & \gamma_{xxxz} & \gamma_{xxyx} & \gamma_{xxyy} & \gamma_{xxyz} & \cdots \\ \gamma_{xyxx} & \gamma_{xyxy} & \gamma_{xyxz} & \gamma_{xyyx} & \gamma_{xyyy} & \gamma_{xyyz} & \cdots \\ \gamma_{xzxx} & \gamma_{xzyx} & \gamma_{xzzz} & \gamma_{xzyx} & \gamma_{xzzy} & \gamma_{xzyz} & \cdots \\ \gamma_{yxxx} & \gamma_{yxxy} & \gamma_{yxxz} & \gamma_{yxyx} & \gamma_{yxyy} & \gamma_{yxyz} & \cdots \\ \gamma_{yyxx} & \gamma_{yyxy} & \gamma_{yyxz} & \gamma_{yyyx} & \gamma_{yyyy} & \gamma_{yyyz} & \cdots \\ \gamma_{yzxx} & \gamma_{yzyx} & \gamma_{yzzz} & \gamma_{yzyx} & \gamma_{yzyy} & \gamma_{yzyz} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

The γ (gamma) tensor, or second hyperpolarizability tensor, plays a fundamental role in governing third-order nonlinear optical processes, including third-harmonic generation (THG), self-focusing, and self-phase modulation. It determines the strength of the optical Kerr effect,²⁶ which is crucial for ultrafast optical switching and photonic applications, enabling high-speed data transmission and optical signal processing. Additionally, the γ tensor influences nonlinear refractive index changes, which are essential for laser pulse shaping, mode-locking techniques, and the development of advanced laser systems.

Theoretical calculations make it simple to comprehend the nonlinear optical behavior of NLO molecules. Intramolecular charge transport and hyperpolarizability are essential for explaining how molecular structure influences the NLO properties of these compounds (Table 2). Consequently, establishing a theoretical correlation between molecular structure and NLO properties may enable the design and synthesis of new NLO materials. The asymmetric electronic distribution in the ground or excited states is improved by the electron cloud's interaction with an external electric field, thereby increasing the optical nonlinearity of the system. The parameters involved in this study include the μ , α , β , and γ . The total static dipole μ ,

Table 2: Global descriptive parameters of santalin A, santalin B using DFT/B3LYP/6311G(d,p) and DFT/CAM-B3LYP/6311G(d,p).

	Level of theory	HOMO	LUMO	ΔE	IP	EA	η	χ	s	μ	ω
Santalin A	DFT/B3LYP/6311G(d,p)	-6.58	0.68	7.25	6.58	-0.68	3.6	2.94	0.13	-2.94	1.19
	DFT/CAM-B3LYP/6311G(d,p)	-5.87	-1.69	4.17	5.87	1.69	2.08	3.78	0.23	-3.78	3.43
Santalin B	DFT/B3LYP/6311G(d,p)	-4.70	-2.6	2.07	4.70	2.6	1.02	3.68	0.49	-3.68	6.64
	DFT/CAM-B3LYP/6311G(d,p)	-6.02	-1.5	4.50	6.02	1.5	2.25	3.76	0.22	-3.76	3.14

average polarizability (α), anisotropy of polarizability ($\Delta\alpha$), total first hyperpolarizability (β_{tot}), and average second-order hyperpolarizability (γ) are defined using their respective x , y , and z components, calculated based on specific relations.^{27,28}

$$\begin{aligned}\mu &= (\mu_x^2 + \mu_y^2 + \mu_z^2)^{\frac{1}{2}} \\ \alpha &= 1/3 (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \\ \Delta\alpha &= 1/\sqrt{2} [(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{xx} - \alpha_{zz})^2 + (\alpha_{yy} - \alpha_{zz})^2 + 6(\alpha_{xy}^2 + \alpha_{xz}^2 + \alpha_{yz}^2)] \\ \beta_{\text{tot}} &= [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})^2]^{\frac{1}{2}} \\ \gamma &= 1/5 (\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2\gamma_{xxyy} + 2\gamma_{xxzz} + 2\gamma_{yyzz})\end{aligned}$$

The nonlinear optical behavior of NLO of Santalin A and Santalin B is showed in Table 3. Santalin A and Santalin B both exhibit notable nonlinear optical (NLO) properties, but with some differences in their behavior. Santalin A has a slightly higher total dipole moment (7.0477 Debye) compared to Santalin B (6.53 Debye), indicating a stronger overall charge separation in Santalin A. Both molecules show anisotropic polarizability, with Santalin A having a higher change in polarizability ($48.55 \times 10^{-39} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$) than Santalin B ($37.12 \times 10^{-39} \text{ C}^2 \text{ m}^2 \text{ J}^{-1}$), suggesting Santalin A may interact more strongly with electric fields, particularly along the x and z axes. Regarding hyperpolarizability, Santalin A's total hyperpolarizability ($1.13 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$) is slightly higher than Santalin B's ($1.06 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$), indicating that Santalin A might offer a stronger response to intense electric fields, making it more suitable for applications in optical switching and second-harmonic generation. Both molecules exhibit similar second-order hyperpolarizabilities (γ), with Santalin A at $-6.66753 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$ and Santalin B at $-6.76983 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$, emphasizing their potential for advanced NLO applications. Overall, while both compounds show strong potential for NLO technologies, Santalin A appears to have slightly more pronounced properties in terms of dipole moment, polarizability, and hyperpolarizability.

A comparison of B3LYP and CAM-B3LYP results (Table 3) reveals notable differences in the computed nonlinear optical (NLO) properties of Santalin A and B. The dipole moments increase significantly when using the long-range corrected CAM-B3LYP functional – rising from 7.04 D to 7.84 D for Santalin A and from 6.53 D to 14.00 D for Santalin B – suggesting improved charge separation under CAM-B3LYP. The mean polarizability (α_{tot}) in atomic units shows slight variations, with Santalin B displaying higher values at CAM-B3LYP (−253.70 a.u.) compared to B3LYP (−241.35

Table 3: Dipole moments and polarizabilities of santalin A, santalin B using DFT/B3LYP/6311G(d,p) and DFT/CAM-B3LYP/6311G(d,p).

Dipole moment				Polarizability					
A	A	B	B	A	A	B	B		
B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP	B3LYP	CAM-B3LYP		
μ_x	0.34	-1.674	0.46	9.5441	α_{xx}	-227.71	-218.1529	-223.35	-259.399
μ_y	-6.40	-7.2558	-6.5	10.2164	α_{xy}	3.74	-5.2017	35.72	-12.4267
μ_z	2.92	-2.4683	0.41	-0.7752	α_{yy}	-267.83	-256.7805	-255.52	-258.978
					α_{xz}	-17.68	-16.1177	-13.77	-24.0517
					α_{yz}	-10.64	11.3667	-2.65	2.6806
					α_{zz}	-233.21	-234.9143	-245.19	-242.724
					α_{tot}	-242.92	-236.616	-241.35	-253.7
μ_{tot}	7.04	7.844	6.53	14.0024	$\Delta\alpha$	48.55	48.55	37.12	37.12
					$8.01 \times 10^{-40} C^2 m^2 J^{-1}$	$7.20 \times 10^{-40} C^2 m^2 J^{-1}$	$6.21 \times 10^{-40} C^2 m^2 J^{-1}$	$7.39 \times 10^{-40} C^2 m^2 J^{-1}$	$7.39 \times 10^{-40} C^2 m^2 J^{-1}$
					$7.20 \text{ \AA}^3$	$7.20 \text{ \AA}^3$	$7.20 \text{ \AA}^3$	$5.50 \text{ \AA}^3$	$5.50 \text{ \AA}^3$
									$3.83 \text{ \AA}^3$
Urea									
Hyper polarizability				Second hyper polarizability					
A	A	B	B	A	A	B	B		
	CAM		CAM		CAM		CAM		
β_{xxx}	-36.35	19.84	-43.12	394.64	γ_{xxx}	-15,620.81	-15,940.25	-16,181.98	-19,010.84
β_{xxy}	95.79	71.80	-19.54	132.84	γ_{yyy}	-14,264.40	-13,067.59	-14,288.16	-12,704.79
β_{xyy}	-15.83	-23.97	9.93	151.32	γ_{zzz}	-1,861.90	-2,099.93	-2,814.88	-1,873.98
β_{yyy}	-326.02	-295.94	-262.46	372.48	γ_{xxy}	-5,407.55	-5,034.34	-4,377.60	-5,822.92
β_{xxz}	117.72	-112.26	99.40	-42.61	γ_{xxz}	-3,133.51	-3,298.53	-3,283.49	-3,240.32
β_{xyz}	9.920	20.30	44.78	-3.04	γ_{yyz}	-2,318.03	-2,205.29	-2,839.18	-2,537.62
β_{yyz}	52.21	-49.11	-26.06	1.1954					
β_{zzz}	-10.77	9.19	10.02	40.63					

Table 3: (continued)

	Hyper polarizability			Second hyper polarizability		
	A	A CAM	B CAM	A	A CAM	B CAM
β_{yz}	-37.60	-54.33	-37.60			
β_{zz}	51.44	-53.69	-22.79			
β_{tot}	$1.13 \times 10^{-50} C^3$	$1.13 \times 10^{-50} C^3$	$1.06 \times 10^{-50} C^3$	$-6.66 \times 10^{-61} C^4$	$-6.50776 \times 10^{-61} C^4$	$-6.76 \times 10^{-61} C^4$
	$10^{-50} C^3 m^3 J^{-2}$	$m^3 J^{-2}$	$m^3 J^{-2}$	$10^{-61} C^4 m^4 J^{-3}$	$m^4 J^{-3}$	$m^4 J^{-3}$
	$3.05 \times 10^{-30} e.s.u$	$3.05 \times 10^{-30} e.s.u$	$2.85 \times 10^{-30} e.s.u$			
	Urea		$0.3728 \times 10^{-30} e.s.u$			
				Urea		$0.746 \times 10^{-36} e.s.u$
				para-nitroaniline (PNA)		$1.323-2.646 \times 10^{-30} e.s.u$
				DAST((4-N,N-dimethylamino-4'-		$1.5 \times 10^{-27} e.s.u$
				N'-methyl-stilbazolium tosylate)		

a.u.). The first-order hyperpolarizability (β) has no change $1.13 \times 10^{-30} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$ for Santalin A but the value changed from $1.06 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$ to $2.56 \times 10^{-50} \text{ C}^3 \text{ m}^3 \text{ J}^{-2}$ for Santalin B, indicating an enhancement in NLO response with CAM-B3LYP. Additionally, the second-order hyperpolarizability (γ) shows an increase from $-6.76 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$ to $-7.08231 \times 10^{-61} \text{ C}^4 \text{ m}^4 \text{ J}^{-3}$ for Santalin B, emphasizing CAM-B3LYP's better capacity to capture high-order electron cloud distortions. These comparisons affirm that CAM-B3LYP predicts stronger NLO activity than B3LYP, particularly in Santalin B, highlighting its potential as a superior NLO chromophore.

4 Conclusions

The comparative analysis of Santalin A and Santalin B highlights several significant differences in their physicochemical and electronic properties, which influence their potential applications in NLO materials. Santalin A ($\text{C}_{33}\text{H}_{26}\text{O}_{10}$) and Santalin B ($\text{C}_{34}\text{H}_{28}\text{O}_{10}$) differ by one carbon and two hydrogen atoms, giving Santalin B a higher molecular weight (596.58 g/mol vs. 582.55 g/mol). Both have similar structures, with Santalin A containing 43 heavy atoms and Santalin B 44, including 30 aromatic heavy atoms each, indicating comparable aromaticity. Santalin B has slightly greater flexibility, with a higher sp^3 carbon fraction (0.15 vs. 0.12) and more rotatable bonds (7 vs. 6). Both have 10 hydrogen bond acceptors, but Santalin A has one more donor (5 vs. 4), influencing interactions in polar environments. This trait, particularly in the oxygenated carbon regions, where the additional $-\text{OCH}_3$ group in Santalin B causes deshielding of adjacent carbons, altering conjugation, while subtle shifts in the aromatic region of the ^1H NMR spectra indicate electronic differences due to variations in substitution patterns, confirming their structural similarity with slight chemical shift variations. The optimized structures and frontier molecular orbitals of Santalin A and B highlight their distinct stability and reactivity, with Santalin A exhibiting greater stability due to its tightly bound electrons and larger bandgap, while Santalin B shows higher reactivity and better electronic conductivity, making it more suitable for applications requiring enhanced electron transfer. Notably from MESP maps, Santalin B exhibits a more pronounced electron-rich region, suggesting a higher tendency to attract electrophiles, while Santalin A shows stronger electron-deficient areas, making it more reactive toward nucleophiles, indicating that Santalin B may be better suited for electrophilic interactions, whereas Santalin A is more favorable for nucleophilic interactions. Santalin A, with a higher ionization potential (6.57 eV) and hardness (3.62 eV), is more stable and resistant to electronic changes, while Santalin B, with a lower IP (4.70 eV), higher electron affinity (2.66 eV), and greater electrophilicity ($\omega = 6.64$), is more reactive and prone to electron-accepting interactions.

Though both compounds Santalin A and B exhibit comparable nonlinear optical properties, Santalin A (7.0477×10^{-29} C m) has a slightly higher dipole moment than Santalin B (6.53×10^{-29} C m), indicating stronger charge separation in Santalin A, this may again resulted in marginally higher total hyperpolarizability (1.13×10^{-50} C³ m³ J⁻²) than Santalin B (1.06×10^{-50} C³ m³ J⁻²). However, Santalin B (-6.76983×10^{-61} C⁴ m⁴ J⁻³) has a slightly higher second-order hyperpolarizability than Santalin A (-6.66753×10^{-61} C⁴ m⁴ J⁻³), making it marginally better for second-order NLO applications. Even with CAM-B3LYP calculations, Santalin B shows a notably higher dipole moment (14.00 D), first hyperpolarizability (2.56×10^{-50} C³ m³ J⁻²), and second-order hyperpolarizability (-7.08231×10^{-61} C⁴ m⁴ J⁻³) compared to Santalin A, confirming its strong potential as an efficient nonlinear optical material. The second-order hyperpolarizability (γ) is a key metric for evaluating nonlinear optical (NLO) materials. Benchmark compounds like urea ($\gamma = 0.746 \times 10^{-36}$ e.s.u), para-nitroaniline (PNA) ($1.323-2.646 \times 10^{-30}$ e.s.u),²⁹ and DAST ($\approx 1.5 \times 10^{-27}$ e.s.u)³⁰ are well-studied for their NLO performance. In comparison, Santalin A and B show dramatically higher theoretical γ values. Santalin A yields $\gamma \approx -1.044 \times 10^4$ e.s.u (B3LYP/CAM-B3LYP), while Santalin B ranges from -1.084 to -1.136×10^4 e.s.u, exceeding DAST by over 30 orders of magnitude. These exceptionally large values likely result from strong π -conjugation and charge transfer characteristics. Although computational, the results strongly suggest that Santalin A and B merit experimental investigation. If stable, they could serve as promising candidates for advanced NLO applications in photonic devices and optical modulators. The superior second-order NLO properties may be attributed to the additional $-\text{OCH}_3$ group, which contributes to greater electron delocalization and influences charge distribution across the molecule with a narrow band gap and lower IP.

This structural modification enhances its ability to polarize under an applied electric field, leading to a higher second-order hyperpolarizability. The presence of electron-donating groups in conjugated systems typically increases nonlinear optical (NLO) properties by stabilizing charge-separated states, which is evident in Santalin B.

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