Exploring crystal, electronic, optical and NLO properties of ethyl 4-(3,4-dimethoxy phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro pyrimidine-5-carboxylate (MTTHPC)

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Abstract
Both theoretical and experimental studies are briefly discussed to shed lights on crystal shape, FT-IR, electronic, and non-linear opto-response (NLO) characteristics of ethyl4-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MTTHPC). Theoretical FT_IR results are in a proper concord with recorded measurements. MTTHPC has TDM (4.78 Debye) and a doublet spins that splits original FMOs into $\alpha$($\uparrow$, 2.44 eV) and $\beta$($\downarrow$, 1.28 eV) offsets, respectively. MTTHPC is a potential competitor for finest perovskite solar cells (MAPbI3/Au-nanospheres) that possess a band offset (3.1 eV) with conversion-efficiency 24.84%. MTTHPC may be the next chapter for unique avalanche photodetectors (APD). MTTHPC 1st order hyperpolarizability is $14.15 \times 10^{-30}$ esu, surpass reference urea ($\approx 40 \beta_{\text{urea}}$, $\beta_{\text{urea}} = 0.3728 \times 10^{-30}$ esu). Briefly, MTTHPC may be admitted as the next stage in forthcoming NLO technology.

Keywords MTTHPC · FT-IR · Band offsets · NLO · ADME indices · Drug-like nature

1 Introduction

Organo-crystals are specified by its magnificent nonlinear/linear responses that made them a potential nominee for optoelectronic devices like optocommunicator, optoswitchers and memory processors (Davanagere et al. 2019; Karnan et al. 2019; Amutha et al. 2017a, b). Most of noncentro/symmetric crystals have a high 2nd harmonic generation (SHG) efficiency surpass centrosymmetric ones. Centrosymmetric crystals possess a remarkable 3rd nonlinear
optical behaviors made them right choice for optical sensing, switching, and limiting processes (Amudha et al. 2017a, b; Karuppanan and Kalainathan, 2018; He et al. 2018). The seek for improving their photoconductive characters are carried by tailoring their band offsets (El-Nahass et al. 2013; Ibrahim et al. 2012, 2013; Soliman et al. 2013) to facilitate electrons rush across conduction domain. Ternary organic solar cells (TOSCs) achieve about 15–17% efficiencies as bulk-heterojunctions (Jiang et al. 2021a; Ma et al. 2021; Liu et al. 2021) whereas pseudo-bilayer architecture photocells have 17.42% efficiencies (Jiang et al. 2021b) surpassing organic/inorganic hybrid ones (Zhao et al. 2021) (∼17.19%). The non-fullerene solar cells via alkyl and alkoxy as Y-axis substituents show an outstanding efficiency (17.6%) (Chen et al. 2021) while those via polymeric substituents provides efficiency up to (17.1%) (Guo et al. 2021). Pyrimidines derivatives have attracted chemists on account of their vast biological antiviral characters (Yerragunta et al. 2021; ur Rashid et al. 2021) as well as antioxidant agents (El-Badawy et al. 2021). For instance, 4-amino-2,6-chloropyrimidine is an inhibitor of human immune deficiency virus type I (HIV-1) reverse transcriptase and possesses antiviral HIV activity (Althaus et al. 1996; Balzarini 2002) whereas 1-(3-Azido-2,3-dideoxy pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidine-dione shows a significant inhibitor potency for in-vivo replica (Jeong et al. 1993; Tber et al. 1995). Molecular simulation technique turned into a unique tool to foresee both structural, electronic, and linear/non-linear optical (NLO) features through computer based-programs (Lian et al. 2021; Zhu et al. 2021; Halim et al. 2021). Density-functional theorem (DFT) is an excellent computation fashion to investigate optoelectronic (Pandit et al. 2021; Yu 2021; Lee et al. 2021) and NLO (Yankova 2021; Parte et al. 2021; Sathiya et al. 2021) aspects as well as drug-nature properties for intended structures. As further as known, no recent reports are recorded for ethyl4-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MTTHPC) characteristics until now. So, authors present a prime trial to document optical and NLO responses for MTTHPC molecule and its potential applications. Moreover, drug-like features for MTTHPC are supplementary checked as forthcoming drug-receptors designs.

2 Computational details

MTTHPC calculations are achieved through G09W (Frisch 2009) and GV5.0.8 (Frisch et al. 2009) programs. The run computations are performed using B3LYP and WB97XD via 6-311G(d,p) set that achieve best precision. Optimized geometry, band offset, overall dipole moment (TDM), thermo-chemistry, and NLO response for MTTHPC are calculated. Various parameters like ionizing-potential (I), electronic-affinity (A), hardness (η), chemical-potential (μ), electrophilic-index (ψ), softness (ζ), static-polarizability (α), and 1st hyper-polarizability (β) are registered. Moreover, Swiss-ADME webtool (Banik et al. 2021; Uslu et al. 2021; Novianty et al. 2021) is performed to find out physicochemical measures, pharmacokinetics, Lipophilicity, drug-likeness, and medicinal inhibitors amiability features for MTTHPC (Fig. 1).

3 Result and discussions

3.1 Optimized structure and FT-IR analyses

Table 1 displays optimized MTTHPC crystallographic domain calculated via B3LYP_6-311G (d, p). Inasmuch of crystallographic data paucity on MTTHPC crystallinity, a

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 comparative recorded and calculated structural scheme data can only be reported with similar structures so far. The computed C=C extent (1.39 ~1.42 Å) concours with index data (1.48 Å) (Lin et al. 2002) whereas C=O (~1.24 Å) matches experiment (1.23 Å). All calculated H-antennae associated with C (CH = 1.08 ~ 1.09 Å) and N (NH = 1.00 ~1.01 Å) atoms are comparable to experiment (1.08, 1.02 Å) (Novaković et al. 2007; Jaćimović et al. 2020). The predicted C-S bond (~1.72 Å) is a little shorter than index crystal-range (~2.4 Å). The MTTHPC observed FT-IR is scanned via 500–1500 cm⁻¹ spectral fingerprint domain. GaussView 5.0.8 are used to assign both observed and computed IR wavenumbers. All theoretical wavenumbers are multiplied by 0.96 (El-Sheshtawy et al. 2015; Ghrib et al. 2021; Ünal et al. 2021) to fit with recorded ones. Both recorded and computed wavenumbers and the appropriate assignments are registered in Table 2. A comparable agreement is established between both observed and calculated data. Figure 2 shows MTTHPC observed and predicted IR charts. Remarkable interference among recorded and calculated data may be attributed to outspread H antennas. In a brief discussion, MTTHPC vibrations are clarified as:

Mode (1) is assigned as collective stretch of C=O + C=C at 1479 cm⁻¹, proportional to recorded peak at 1448 cm⁻¹. Modes (2–4) are recognized for NH bend-in at 1272, 1232, 1170 cm⁻¹, match observed peaks at 1284, 1225, 1186 cm⁻¹, respectively. Modes (5–8) are assigned for CH bend-in at 1158, 1120, 1077, 1055 cm⁻¹, concours with recorded values at 1148, 1129, 110, 1027 cm⁻¹, respectively. Modes (10–11) are assigned to NH bend-out at 855, 842 cm⁻¹, corresponding to experimental results at 880, 816 cm⁻¹. Modes (12–13) are referred to CH bend-out at 752, 704 cm⁻¹, analogous to scanned ones at 790, 676 cm⁻¹. Mode (9) is assigned for collective C–O + C–S + C–N + C–C stretch at 1013 cm⁻¹, correspond to defined peak at 1011 cm⁻¹. Mode (14) is specified for C–O + C–S + C–N + C–C

**Fig. 1** Optimized structure for MTTHPC molecule
Table 1 Optimized MTTHPC crystal data

| Bond length (Å) | Bond angles (°) |
|----------------|----------------|
| C1–C2         | 1.42           | C2–C1–C6   | 117.90       | H23–C22–H24 | 108.30       |
| C1–C6         | 1.40           | C2–C1–C7   | 120.29       | H23–C22–C25 | 112.87       |
| C1–C7         | 1.46           | C6–C1–C7   | 121.77       | H24–C22–C25 | 112.65       |
| C2–C3         | 1.39           | C1–C2–C3   | 121.39       | C22–C25–H26 | 110.85       |
| C2–H11        | 1.08           | C1–C2–H11  | 119.37       | C22–C25–H27 | 109.88       |
| C3–C4         | 1.42           | C3–C2–H11  | 119.13       | C22–C25–H28 | 110.82       |
| C3–O34        | 1.39           | C2–C3–C4   | 119.87       | H26–C25–H27 | 108.49       |
| C4–C5         | 1.39           | C2–C3–O34  | 124.40       | H26–C25–H28 | 108.38       |
| C4–O33        | 1.39           | C3–C4–O34  | 115.73       | H27–C25–H28 | 108.35       |
| C5–C6         | 1.40           | C3–C4–C5   | 119.08       | C9–C29–H30  | 111.24       |
| C5–H12        | 1.08           | C3–C4–O33  | 116.07       | C9–C29–H31  | 111.59       |
| C6–H13        | 1.08           | C5–C4–O33  | 124.85       | C9–C29–H32  | 110.42       |
| C7–C10        | 1.42           | C4–C5–C6   | 120.94       | H30–C29–H31 | 108.90       |
| C7–N14        | 1.42           | C4–C5–H12  | 120.05       | H30–C29–H32 | 107.26       |
| C8–N14        | 1.36           | C6–C5–H12  | 118.99       | H31–C29–H32 | 107.24       |
| C8–S16        | 1.72           | C1–C6–C5   | 120.82       | C3–O33–C35  | 118.76       |
| C8–N17        | 1.37           | C1–C6–H13  | 120.11       | C3–O34–C39  | 118.94       |
| C9–C10        | 1.39           | C5–C6–H13  | 119.01       | C33–C35–H36 | 111.30       |
| C9–N17        | 1.41           | C1–C7–C10  | 127.84       | O33–C35–H37 | 104.90       |
| C9–C29        | 1.50           | C1–C7–N14  | 116.01       | O33–C35–H38 | 111.33       |
| C10–C19       | 1.49           | C10–C7–N14 | 116.06       | H36–C35–H37 | 109.71       |
| N14–H15       | 1.00           | N14–C8–S16 | 123.10       | H36–C35–H38 | 109.80       |
| N17–H18       | 1.00           | N14–C8–N17 | 114.42       | H37–C35–H38 | 109.69       |
| C19–O20       | 1.24           | S16–C8–N17 | 122.48       | O34–C39–H40 | 104.86       |
| C19–O21       | 1.37           | C10–C9–N17 | 117.59       | O34–C39–H41 | 111.38       |
| O21–C22       | 1.48           | C10–C9–C29 | 128.07       | O34–C39–H42 | 111.29       |
| C22–H23       | 1.09           | N17–C9–C29 | 114.25       | H40–C39–H41 | 109.66       |
| C22–H24       | 1.09           | C7–C10–C9  | 120.54       | H40–C39–H42 | 109.70       |
| C22–C25       | 1.51           | C7–C10–C19 | 120.97       | H41–C39–H42 | 109.84       |
| C25–H26       | 1.09           | C9–C10–C19 | 118.39       |               |              |
| C25–H27       | 1.09           | C7–N14–C8  | 125.92       |               |              |
| C25–H28       | 1.09           | C7–N14–H15 | 118.19       |               |              |
| C29–H30       | 1.10           | C8–N14–H15 | 115.50       |               |              |
| C29–H31       | 1.08           | C8–N17–C9  | 125.32       |               |              |
| C29–H32       | 1.10           | C8–N17–H18 | 115.64       |               |              |
| O33–C35       | 1.45           | C9–N17–H18 | 119.03       |               |              |
| O34–C39       | 1.45           | C10–C19–O20| 125.49       |               |              |
| C35–H36       | 1.09           | C10–C19–O21| 112.00       |               |              |
| C35–H37       | 1.08           | O20–C19–O21| 122.46       |               |              |
| C35–H38       | 1.09           | C19–O21–C22| 117.53       |               |              |
| C39–H40       | 1.08           | O21–C22–H23| 108.21       |               |              |
| C39–H41       | 1.09           | O21–C22–H24| 107.95       |               |              |
| C39–H42       | 1.09           | O21–C22–C25| 106.64       |               |
bend-in at 566 cm$^{-1}$, coincide to experiment whereas mode (15) is attributed to C–O + C–S + C–N + C–C bend-out at 521 cm$^{-1}$, proportional to indexed band at 516 cm$^{-1}$.

### 3.2 Mulliken charges and frontiers molecular orbital (FMOs) analyses

Mulliken atomic charges(Q) play a vital role in describing electro negativity, charge transport during a chemical process and overall electronic configuration of the molecule (Guidara et al. 2014). The calculated Mulliken distributions of MTTHPC charges are listed at Table 3. Figure 3 shows Mulliken charge analysis for MTTHPC molecule. It is merited to point out that C3, C4, C7, C8, C9 and C19 exhibit positive charges, while others exhibit negative charges. Prime hydrogen holds positive charges. All S, O and N atoms hold a negative due to their high electron withdrawing property (high electronegativity).

Many FMO indices via Koopmans theorem are extracted such as ionization_carry \( I = -E_{\text{HOMO}} \), electron_affinity \( A = -E_{\text{LUMO}} \), hardenable \( \mu = (E_{\text{LUMO}} - E_{\text{HOMO}})/2 \), chemical_caray \( \psi = \mu^2 \), and plasticity \( \zeta = 1 \) (Sert et al. 2014). Extensively, assorted thermochemistry features are listed in Table 4 for MTTHPC. The \( E_{\text{LUMO}}/E_{\text{HOMO}} \) offset is a precise index for electron carry via conduction domain (Sheela et al. 2015; Verma et al. 2021; Dwivedi, Kumar 2021). The MTTHPC has TDM (4.78 Debye) and a doublet spins that splits original FMOs into alpha(↑) and beta (↓) offsets with energies 2.44 and 1.28 eV, respectively. Which predicts that increasing dipole moment state will increase optical nonlinearity. In a logic way, MTTHPC is a potential competitor for finest perovskite solar cells (MAPbI$_3$) embedded with Au nanospheres that possess a band offset (3.1 eV) with conversion-efficiency 24.84% (Tabrizi et al. 2021). Figures 4 and 5 show computed band offsets and electronic density of states (DOS) for MTTHPC, respectively. Obviously, doublet spins drag Fermi level up to

| No | Exp. wave number (cm$^{-1}$) | Theo. wave number (cm$^{-1}$) | Vibrational assignments |
|----|----------------------------|----------------------------|------------------------|
| 1  | 1448                       | 1479                       | $\nu$ C=O + $\nu$ C=C  |
| 2  | 1284                       | 1272                       | $\beta$ N–H            |
| 3  | 1225                       | 1232                       |                        |
| 4  | 1186                       | 1170                       |                        |
| 5  | 1148                       | 1158                       | $\beta$ C–H            |
| 6  | 1129                       | 1120                       |                        |
| 7  | 1110                       | 1077                       |                        |
| 8  | 1027                       | 1025                       |                        |
| 9  | 1011                       | 1013                       | $\nu$ C–O + $\nu$ C–S + $\nu$ C–N + $\nu$ C–C |
| 10 | 880                        | 855                        | $\gamma$ N–H           |
| 11 | 816                        | 842                        |                        |
| 12 | 790                        | 752                        | $\gamma$ C–H           |
| 13 | 676                        | 704                        |                        |
| 14 | 566                        | 566                        | $\beta$ C–O + $\beta$ C–S + $\beta$ C–N + $\beta$ C–C |
| 15 | 516                        | 521                        | $\gamma$ C–O + $\gamma$ C–S + $\gamma$ C–N + $\gamma$ C–C |

$\nu$ (stretch mode); $\beta$ (in-plane mode); $\gamma$ (out-plane mode)
conduction domain that increase electrons avalanche percent. Hereby, authors declare that
MTTHPC may be the next chapter for unique avalanche photodetectors (APD).

### 3.3 NLO Properties

To inspect MTTHPC NLO response, its polarizability and 1st hyperpolarizability are
determined via WB97XD_6-311G (d,p). Static polarizability ($\alpha_{\text{tot}}$), polarizability anisotropy ($\Delta \alpha$) and 1st hyperpolarizability ($\beta_{\text{tot}}$) are derived via assorted formulas (Kosar et al. 2021; Yousif 2021):

$$\alpha_{\text{tot}} = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

$$\Delta \alpha = \frac{1}{\sqrt{2}} \left[ (\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6\alpha_{xy}^2 + 6\alpha_{yx}^2 + 6\alpha_{xz}^2 \right]^{1/2}$$

$$\beta_{\text{tot}} = \left[ (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2 \right]^{1/2}$$

NLO response depend upon associated TDM, $\alpha_{\text{tot}}$, and $\beta_{\text{tot}}$ values. MTTHPC calculated results for $\alpha_{\text{tot}}$, $\Delta \alpha$ and $\beta_{\text{tot}}$ are listed in Table 5. Results are transmuted from SI $\Rightarrow$ esu scale ($\alpha$; 1 a.u = $1.482 \times 10^{-24}$ esu, $\beta$; 1 a.u = $8.6393 \times 10^{-33}$ esu). MTTHPC has $\beta_{\text{tot}}$ is $14.15 \times 10^{-30}$ esu, which is a significant increase above related compounds (Shavel et al. 2004; Bouchouit et al. 2008; Guezguez et al. 2013, 2014). Such behavior is induced by electrons rush across crystal that cause 1st hyperpolarizability to be doubled over conventional prototype. The close resemblance between NLO value and our finding supports the notion that POM’s electro-optic effect is mostly of electronic origin (Dou et al. 1993). The observation has been discussed in a variety of organic molecular crystals (Stevenson et al. 1973; Stevenson et al. 1973; Garito et al. 1980), and it appears to be a property shared by those molecules. Within the 0.5–2.0 µm transparency region, many organic compounds exhibit higher nonlinear optical susceptibilities than most inorganics (Morrell et al. 1979). The disparity between an experimental POM’s NLO and that predicted by theory (most
found in organic crystals) can be utilized as a crystal quality criterion (Zyss et al. 1981; Dou et al. 1991, 1992). Novelty of proposed research insights focused on how nonlinear optical responses can open novel vistas in crystalline optics technology. Such elevated NLO response acknowledges MTTHPC as the next stage in forthcoming NLO technology.

### 3.4 Pharmaco-kinetics and drug-like nature

Swiss-ADME online-software (Rana et al. 2021; Alshammari 2020) is utilized to predict pharmaceutical features such as physicochemicals, pharmacokinetics, lipophilicity, 

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**Table 3** Mulliken charges distributions for MTTHPC

| Atom | Q (a. u) | Atom | Q (a. u) |
|------|----------|------|----------|
| C1   | 0.00     | C22  | −0.09    |
| C2   | −0.18    | H23  | 0.20     |
| C3   | 0.21     | H24  | 0.19     |
| C4   | 0.23     | C25  | −0.53    |
| C5   | −0.18    | H26  | 0.20     |
| C6   | −0.07    | H27  | 0.18     |
| C7   | 0.35     | H28  | 0.19     |
| C8   | 0.16     | C29  | −0.62    |
| C9   | 0.44     | H30  | 0.20     |
| C10  | −0.12    | H31  | 0.24     |
| H11  | 0.20     | H32  | 0.20     |
| H12  | 0.17     | O33  | −0.49    |
| H13  | 0.18     | O34  | −0.50    |
| N14  | −0.75    | C35  | −0.30    |
| H15  | 0.38     | H36  | 0.18     |
| S16  | −0.10    | H37  | 0.20     |
| N17  | −0.73    | H38  | 0.18     |
| H18  | 0.38     | C39  | −0.30    |
| C19  | 0.36     | H40  | 0.21     |
| O20  | −0.40    | H41  | 0.19     |
| O21  | −0.46    | H42  | 0.18     |
pH, drug-likeness, and medicinal inhibitors amiability for MTTHPC that are collected in Table 6. Presence of tetrahydro-pyrimidine moiety in MTTHPC provides antimicrobial activity (Makvandi et al. 2020). Bioavailability Radar (Mishra et al. 2019) is displayed via pre-six physico-chemical indices, namely lipophilia scale, polarity, solubility, edibility, and saturation (see Fig. 6a). All predicted values acknowledge MTTHPC as a promising drug-like carriers. Target classes for MTTHPC molecule with ligand protein interactions are represented in Fig. 6b. MTTHPC polar surface area is 100.91 Å² that shows a high gastrointestinal (GI) absorption and bioavailability (55%). MTTHPC blood–brain barrier (BBB) is nil that indicates a highly hydrophilic-polar drug-nature to predict intestinal permeation.

| Table 4 MTTHPC thermochemistry |
|--------------------------------|

| B3LYP_6-311G (d, p) |
|---------------------|

| Ground-energy (Hartree) | −1429.661567 |
| Zero-energy (Kcal/Mol)  | 209.59091 |
| Rotational coefficients (GHz) | 0.28034 |
|                      | 0.16497 |
|                      | 0.11785 |

| Entropy (S) (Cal/Mol·°K) |
|--------------------------|
| Total  | 169.512 |
| Transational  | 43.323 |
| Vibrational  | 35.332 |
| Rotational  | 89.48 |

| Specific-heat (C_v) (Cal/Mol·°K) |
|----------------------------------|
| Total  | 86.675 |
| Transational  | 2.981 |
| Vibrational  | 2.981 |
| Rotational  | 80.714 |

| Dipole moment (Debye) | 5.7*10⁴ |
|-----------------------|---------|
|                      | 4.78    |

| Spin |
|------|
| Doublet |

| Alpha MOs | Beta MOs |
|----------|----------|
| E_LUMO (eV) | −1.77 | −4.72 |
| E_HOMO (eV) | −4.20 | −5.99 |
| E_LUMO-HOMO (eV) | 2.44 | 1.28 |
| Ionization-potential (I) (eV) | 1.77 | 4.72 |
| Electron-affinity (A) (eV) | 4.20 | 5.99 |
| Hardness (η) (eV) | 1.22 | 0.64 |
| Chemical potential (µ) (eV) | −2.98 | −5.36 |
| Electrophilic index (ψ) (eV) | 3.66 | 22.44 |
| Softness (ζ) (eV⁻¹) | 0.82 | 1.56 |

(continued...
(Corazza et al. 2020). Eventually, MTTHPC may be efficiently used as drug-carriers for gastrointestinal diseases.
Conclusion

MTTHPC crystal data, FT-IR, electronic and NLO response is fulfilled via DFT model. Optimized structure, IR, and band offsets are calculated using B3LYP level whereas NLO indices are computed through WB97XD. The good agreement between experimental and theoretical FT-IR confirms calculations precision level. The electronegativity, charge transit during a chemical process, and the molecule’s overall electronic configuration are all detected using Mulliken atomic charges analysis. MTTHPC possesses a TDM (4.78 Debye) and a doublet-spin offsets, namely $\alpha^{\uparrow}$ (2.44 eV) and $\alpha^{\downarrow}$ (1.28 eV). Such doublet-spins drag push Fermi level nearby conduction domain facilitating electrons rush across. So, MTTHPC is a promising candidate for premier avalanche photodetectors as well as solar cells. Also, MTTHPC exhibits a magnificent NLO response, $\beta_{\text{tot}}$ is $1.64 \times 10^{-30}$ esu, which is a significant increase surpass other relatives. Such behavior is induced by electrons rush across crystal that cause $1^\text{st}$ hyperpolarizability to be doubled over ordinary prototype. Intellectually, MTTHPC may be the next stage in forthcoming NLO technology. Moreover, pharmaceutical features for MTTHPC show its eligibility as efficient drug-carriers for gastrointestinal diseases.

### Table 5

| Mean Polarizability $\alpha_{\text{tot}}$ ($\times 10^{-24}$ esu), polarizability anisotropy $\Delta\alpha$ ($\times 10^{-24}$ esu) and $\beta_{\text{tot}}$ ($\times 10^{-30}$ esu) 1st hyperpolarizability for MTTHPC |
|-----------------|----------------|----------------|----------------|
| $\alpha_{xx}$   | 321.93         | 47.71          | 731.71         |
| $\alpha_{yy}$   | 15.24          | 2.26           | 576.49         |
| $\alpha_{zz}$   | -3.15          | -0.47          | 162.65         |
| $\alpha_{xy}$   | -17.33         | -2.57          | 716.67         |
| $\alpha_{zy}$   | 243.26         | 36.05          | 162.65         |
| $\alpha_{zt}$   | 188.53         | 27.94          | 65.37          |
| $\Delta\alpha$  | 293.05         | 43.43          | 100.24         |
| $\beta_{xx}$    | -34.59         | -0.30          | 0.87           |
| $\beta_{yy}$    | -16.19         | -0.14          | 0.87           |
| $\beta_{zz}$    | 1.64           | 14.15          | 1.64           |
| $\beta_{xy}$    | 65.37          | 0.87           | 1.64           |
| $\beta_{zy}$    | 716.67         | 6.19           | 14.15          |
| $\beta_{zt}$    | 162.65         | 1.41           | 0.05           |
### Table 6  Biological activity and ADME parameters of MTTHPC molecule

| Physicochemical properties | Water solubility |
|----------------------------|------------------|
| Formula | $\text{C}_{16}\text{H}_{20}\text{N}_{2}\text{O}_{4}\text{S}$ | Log (S) (ESOL) $-2.93$ |
| Molecular weight | $336.41 \text{ g/mol}$ | Solubility $3.93 \times 10^{-1} \text{ mg/ml; } 1.17 \times 10^{-3} \text{ mol/l}$ |
| No. Non-H atoms | 23 | Class Soluble |
| No. Ar. Non-H atoms | 6 | Log (S) (Ali) $-3.66$ |
| Fractional Csp3 | 0.38 | Solubility $7.31 \times 10^{-2} \text{ mg/ml; } 2.17 \times 10^{-4} \text{ mol/l}$ |
| No. rotational bonds | 6 | Class Soluble |
| No. H-bond acceptors | 4 | Log S (SILICOS-IT) $-4.54$ |
| No. H-bond donors | 2 | Solubility $9.81 \times 10^{-3} \text{ mg/ml; } 2.92 \times 10^{-5} \text{ mol/l}$ |
| Molar-Refractivity | 97.96 | Class Moderate (solubility) |
| TPSA | 100.91 Å² | Log (S) (ESOL) $-2.93$ |
| Lipophilicity | Drug-likeness |
| Log ($P_{ow}$) (iLOGP) | 2.99 | Lipinski Y; 0 violation |
| Log ($P_{ow}$)(XLOGP3) | 1.92 | Ghose Y |
| Log ($P_{ow}$)(WLOGP) | 0.97 | Veber Y |
| Log ($P_{ow}$)(MLOGP) | 0.91 | Egan Y |
| Log ($P_{ow}$)(SILICOS-IT) | 3.30 | Muegge Y |
| Consensus Log ($P_{ow}$) | 2.02 | Bioavailability score 0.55 |
| Pharmacokinetics | Medicinal chemistry |
| GI absorption | High | PAINS 0 alert |
| BBB permeant | No | Brenk 1 alert: thiocarbonyl group |
| P-gp substrate | Y | Leadlikeness Y |
| CYP1A2 | Y | Synthetic accessibility 3.84 |
| CYP2C19 | Y | |
| CYP2C9 | N | |
| CYP2D6 | N | |
| CYP3A4 | N | |
| Log $K_p$ (skin permeation) | $-6.99 \text{ cm/s}$ | |

Ar (Aromatic); Ali (Aliphatic); Y (Yes); N (No)
Declarations

Conflict of interests On behalf of all authors, the corresponding author states that there is no conflict of interest.

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