Novel Synthesis of \( \text{NE,N'E-4,4'-sulfonylbis(N-(substituted-}
\text{dichlorobenzylidene) anilines derivative their application}
\text{biological and DFT studies} \)

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Abstract. The structure of synthesized compounds has been established on the basis of their
spectral (FT-IR, \textsuperscript{1}H&\textsuperscript{13}C NMR and Mass) data. The purity of the compounds was confirmed by
TLC. The compounds 1-3 were evaluated for their \textit{in vitro} activity against several microbes.
Compound 1-3 exhibited potent antibacterial activity with the reference standard ciprofloxacin and
fluconazol. In the ground-state, compounds 1-3 molecular geometries were determined using the
DFT based on B3LYP/6-31G (d,p) and compared to the experimental results. In addition,
compounds 1-3, MEP maps and molecular frontier orbitals were performed, and the results
obtained were compatible with the electronic properties.

Keywords: Schiff base, azomethine, in vitro activity, NLO, DFT.

1. Introduction

The common structural feature of these compounds is the azomethine group with a general
formula \( \text{RN=CH-R'} \), where \( R \) and \( R' \) are alkyl, aryl, cyclo alkyl or heterocyclic groups which may be
variously substituted. These compounds are also known as anils, imines or azomethines [1-4]. Schiff
bases that contain aryl substituents are substantially more stable than alkyl substituents. Schiff bases
of aliphatic aldehydes are relatively unstable and readily polymerizable, while those of aromatic
aldehydes have effective conjugation and stability [5]. The formation is generally driven to the
completion by separation of the product or removal of water or both. Many Schiff bases can be
hydrolysed back to their aldehydes or ketones and amines by aqueous acid or base [6]. Schiff bases
were reported to possess antibacterial, antifungal and antitumor activities. Several researchers have
studied the synthesis, characterization and structure-activity relationship of Schiff bases [7]. Some of
the Schiff base complexes containing N and O donor atoms are effective stereo specific catalysts for
oxidation [8], reduction [9], hydrolysis [10], biological activities [11,12], and other organic and
inorganic transformations. These organic transformations are environmentally friendly and hence they
are highly desirable for the treatment of waste water which contains toxic organic pollutants. Aniline
one such pollutant, is used in the manufacturing of dyes, polymers, which includes rubber, herbicides,
pesticides, fungicides, and pharmaceuticals, is released into environment from these industries.
Aniline is also found in the effluents of petroleum refinery plants. Aniline containing chemicals find
wider applications in various arenas. Because of its toxic and unmanageable nature it is considered to
be an increasing threat to both the environment and human health. Therefore, aniline has aroused great
attention and is classified as a persistent organic pollutant. So there is an urgent need to develop
efficient and economical methods to remove this pollutant from wastewater. The presence of both
hard nitrogen or oxygen and soft sulphur donor atoms in the backbones, makes the ligands readily
coordinate with a wide range of transition metal ions yielding stable and intensely coloured metal complexes, some of which have been shown to exhibit interesting physical and chemical properties and potentially useful biological activities [13].

Based on these studies, we have taken up the compounds for synthesis and evaluated for antibacterial activity. The structural assignment of the products was based on their IR, NMR and Mass spectral data and DFT studies. The title compounds were screened for their antibacterial and antifungal activity.

2. Experimental section

2.1 Materials and physical measurements

Analytical reagent (AR) grade chemicals were obtained commercially and used without purification, 1,4-Dioxane, 4,4'-sulfonyldianiline, Substituted- chloroaldehyde and CH₃COOH. Elemental analyses were carried out on VARIOMICRO V2.2.0 CHN analyser. The ¹H and ¹³C NMR spectrum of the synthesized compounds 1-3 in CDCl₃ was recorded on a Bruker Avance 400 MHz NMR spectrometer. The ¹H and ¹³C NMR were referred, respectively to TMS as an internal standard and the central line of CDCl₃. High-resolution mass spectra (HRMS) were recorded using electro spray ionization on a Bruker Maxis machine. The reactions were carried out with freshly distilled solvents.

2.2 Synthesis of Acetanilide and 4,4-diacetamidodiphenyl-14c sulfoxide [14]

The sequence of reaction used to synthesize DDS-14c is outlined in Scheme 1.

General procedure Acetanilide (phenyl-¹⁴C) (II):
Acetanilide (phenyl-¹⁴C) (II) was synthesized from 2.19g(16.90 mmol) of uniformly carbon-14 labelled aniline hydrochloride (I) with a specific activity of 156.4 pCi/ mmole, according to; the method of Searle and cupery as described by murray and Williams. They yield was 2.17 g of white crystalline II (95.0%) m.p 105-112°C, with a specific radioactivity of 151.6 pCi / mmole. Thin layer chromatography (tlc) (appendix-system A) detected II with an estimate radiochemical purity of >98.5%; no I (< 0.1%) was detected.

2.2.1. General procedure 4,4-diacetamidodiphenyl-14c sulfoxide(III)

4,4-diacetamidodiphenyl-14c sulfoxide(III) was synthesized from II using a modification of the procedure described by sugasawa and sakurai for non radioactive preparation of III. To slurry of 2.17 g (16.05 mmoles) of II (151.6 pCi/ mmole) in 30ml of carbon disulfide was added with stirring 0.58ml (8.05 mmoles) of thionyl chloride and then 4.43 g (33.2 mole) of aluminium chloride in small portions. The reaction mixture, which darkened very quickly, was refluxed for 3 days while still warm, the reaction solvent was decanted from the reaction flask leaving a black residue. This residue was cooled to 30°C and decomposed with 40ml of 2N HCl yielding a suspension of tan solids. The solids were collected by filtration to yield 2.09g pf tan crystalline III (82.3% yield) m.p 260-263°C, with a specific radioactivity of 293.7 pCi /mmoles. TLC (appendix-system A) detected III with an estimated radiochemical purity of >94.3%; II was detected as a radiochemical impurity in the amount of <0.5%. The chemical purity of III was estimated as 93.5% by ultraviolet analysis in methanol = 270; E ∞ = 32100).

2.3. Synthesis of N₂,N'民办-sulfonylbis(N-(substituted-dichlorobenzylidene) anilines derivative

0.1 mole of 4,4'-sulfonyldianiline (0.21 g, 1 mmol) was added to substituted-dichlorobenzaldehyde (0.22 g, 2 mmol) were taken and mixed in 1,4-Dioxane (25 mL) added two drops of glacial acetic acid. The resultant mixture was string for 4 hrs and cooled. The precipitates were poured into crushed ice. Solids thus obtained were filtered and washed several times with water, followed by ethanol and then dried in a vacuum. The crude products were crystallized in ethanol (Scheme-1).
2.3.1. **NE,N'E-4,4'-sulfonylbis(N-(2,3-dichlorobenzylidene)aniline) (1):**

MF: C_{26}H_{16}Cl_{2}N_{2}O_{2}S. m.p. 198-202 °C. Yield: 75 %. Mol. Wt.: 562.29. Light yellow color solid. Elemental analysis (%) anal. found: C, 55.41; H, 2.77; N, 4.83; calcld: C, 55.54; H, 2.87; N, 4.98%. FT-IR (KBr), ν cm⁻¹ 1699 cm⁻¹ (S=O), 1605 cm⁻¹ (C=N), 3112 cm⁻¹ (Aromatic C-H). 1H NMR (400 MHz, CDCl₃): 7.12-8.27 ppm (Ar-protons), 8.59 (C=N, proton). 13C NMR (100MHz, CDCl₃) δ: 123.43-139.69 ppm (Ar-C), 149.36 ppm (C=N), 188.15 ppm (S=O). MS-ESI (m/z): 563.51 [M+H].

2.3.2. **NE,N'E-4,4'-sulfonylbis(N-(2,6-dichlorobenzylidene)aniline) (2):**

MF: C_{26}H_{14}Cl_{2}N_{2}O_{2}S. m.p. 211-214 °C. Yield: 79 %. Mol. Wt.: 631.18. Light yellow color solid. Elemental analysis (%) anal. found: C, 49.32; H, 2.20; N, 4.32; calcld: C, 49.47; H, 2.24; N, 4.44%. FT-IR (KBr), ν cm⁻¹ 1693 cm⁻¹ (S=O), 1603 cm⁻¹ (C=N), 3118 cm⁻¹ (Aromatic C-H). 1H NMR (400 MHz, CDCl₃): 7.24-8.19 ppm (Ar-protons), 8.53 (C=N, proton). 13C NMR (100MHz, CDCl₃) δ: 123.29-138.25 ppm (Ar-C), 147.70 ppm (C=N), 189.95 ppm (S=O). MS-ESI (m/z): 632.41 [M+H].

2.3.3. **NE,N'E-4,4'-sulfonylbis(N-(3,4-dichlorobenzylidene)aniline) (3):**

MF: C_{26}H_{13}Cl_{7}N_{2}O_{2}S. m.p. 201-205 °C. Yield: 81 %. Mol. Wt.: 661.53. Light yellow color solid. Elemental analysis (%) anal. found: C, 44.87; H, 1.90; N, 4.16; calcld: C, 44.91; H, 1.97; N, 4.21%. FT-IR (KBr), ν cm⁻¹ 1702 cm⁻¹ (S=O), 1601 cm⁻¹ (C=N), 3111 cm⁻¹ (Aromatic C-H). 1H NMR (400 MHz, CDCl₃): 7.22-8.30 ppm (Ar-protons), 8.49 (C=N, proton). 13C NMR (100MHz, CDCl₃) δ: 123.95-137.57 ppm (Ar-C), 147.73 ppm (C=N), 188.39 ppm (S=O). MS-ESI (m/z): 660.99 [M+H].

2.4. **In vitro antimicrobial activity**

The synthesized compounds were screened for their antibacterial activity using *Staphylococcus aureus* and *E. coli*. Control experiment was carried out under similar condition by using ciprofloxacin as standard. The inhibition zone measure in mm showed that Compound 1-3 were more active than other compounds tested against the above microbes. The antifungal activity was tested against the fungal species *Aspergillus niger* and *Candida albicans* at 100 μg concentration.

2.5. **Computational details**

The Molecular Geometry of compound 1-3 was designed with a hybrid functional B3LYP/6-31G(d, p) basis set using the DFT process. All calculations were performed with software package.
Gaussian 09W. The bond parameters, optimized structure, calculations for NLO, HOMO–LUMO, and MEP were tested at the same stage of theory and plotted using the Gauss view method.

3. Results and Discussion

Schiff base from \( NE,N'EE-4,4'-sulfonylbis(N-(substituted-dichlorobenzylidene) anilines \) derivative were synthesized. Thin layer chromatography was performed on pre-coated silica gel-G, glass plates using chloroform: ethanol (9:1) solvent systems to ascertain the purity of these compounds. The compounds gave single spots. The structure of synthesized compounds was confirmed by infrared spectroscopy, \(^1\)H NMR spectroscopy and mass spectroscopy. Infrared spectroscopy showed the characteristic absorption bands of \( C=\text{N} \) stretching and \( S=\text{O} \) vibration of these compounds. The \(^1\)H NMR spectra of the synthesized compounds show chemical shifts, which are characteristics of the anticipated structure of compounds.

3.1. In vitro antimicrobial activity of compounds 1-3

Antibacterial screening of newly synthesized compounds was carried out against \( E. \text{coli}, S. \text{aureus} \) and antifungal activity against \( C. \text{albicans} \) and \( A. \text{niger} \) according to cup-plate method. The synthesized compounds have found to be better antimicrobial activity than parent compound. All the synthesized compounds have shown mild to good activity against the pathogenic bacteria and fungi. Compounds 1-3 have shown to be more potent than ciprofloxacin and compounds 1-3 are more potent than fluconazol and other were near about equipotent in antibacterial and antifungal activity. The present studies are model for application of structure based \( NE,N'EE-4,4'-sulfonylbis(N-(substituted-dichlorobenzylidene) anilines \) in development of novel molecules.

3.2. Computational studies of compounds 1-3

The DFT computations are done at the B3LYP/6-31G basis set level on a private computer using a Gaussian 03W program package. The optimized molecular geometry structure is showcased in Fig 1. The Frontier molecular orbital analysis, Mulliken atomic charges and Molecular electrostatic potential analysis (MEP) are also obtained from the optimized structure. The geometry optimization of compounds 1-3 were determined at B3LYP level theory with 6-311+G(d,p) basis set and are accordance with the atom numbering scheme of the molecule shown in (Fig. 1).

![Fig. 1 (a) Optimized structures (b) Numbering pattern of compounds 1-3](image-url)

Fig. 1 (a) Optimized structures (b) Numbering pattern of compounds 1-3
3.2.1. HOMO-LUMO Energies

The Frontier molecular orbital interpretation of organic molecule is HOMO–LUMO which explains the last word charge transfer interface among the molecule. HOMO-LUMO analysis clearly predicts the energy gap. The calculations are at the B3LYP level with a 6-31G (d,p) basis set using DFT method. HOMO-LUMO molecular orbital are given an insight into the more reactivity of the molecule and an active site can be established by the distribution of frontier molecular orbital. HOMO tends to give the electrons and LUMO has free area to accept the electrons. HOMO is ionization potential energy and LUMO is an electron affinity. Frontier molecular orbital pictures of the compounds 1-3 are given in Fig 2. The HOMO-LUMO energy distinction between the levels corresponds to the electronic transition absorption of the molecule. The energy gap difference between the molecules of HOMO-LUMO calculation are presented in Table 1. The difference of the charge separation between the HOMO and LUMO of those structures play important role in the ICT. Furthermore, the difference on the values of ΔE of compounds 1-3 was observed, which has different substituent at 15α and 1α- sites of the phenyl core significantly change the ΔE value.

Table 1 Calculated energy values (eV) of compounds 1-3 in gas phase

|                  | 1            | 2            | 3            |
|------------------|--------------|--------------|--------------|
| $E_{\text{HOMO}}$ | -7.08276     | -7.00113     | -7.17364     |
| $E_{\text{LUMO}}$ | -0.69113     | -0.29496     | -0.74800     |
| $E_{\text{LUMO-HOMO}}$ | 6.39163     | 6.70617      | 6.42564      |
| Electronegativity | -3.886945    | -3.648045    | -3.96082     |
| Hardness         | 3.195815     | 3.353085     | 3.21282      |
| Electrophilicity index | 2.363769716 | 1.984475837 | 2.441483661 |
| Softness         | 0.156454613 | 0.149116411 | 0.155626521 |

Fig. 2 HOMO and LUMO molecular orbitals in gas phase of compounds 1-3
Chemical hardness is related to the stability and reactivity of a chemical system, it measures the resistance to change in the electron distribution or charge transfer. In this sense, chemical hardness corresponds to the gap between the HOMO and LUMO. The larger the HOMO–LUMO energy gap, the molecule becomes harder, more stable and less reactive.

The results of chemical hardness and electronic chemical potential of compounds 1-3 showed that compound 2 is harder and less reactive than compound 1 and 3. Electrophilicity index measures the propensity or capacity of a species to accept electrons. When comparing the values of electrophilicity in compounds 1-3, the electrophilicity value indicates that compound 3 is a stronger nucleophile than the other compounds. Table 1 shows that compound 3 is the strongest nucleophile whereas compound 2 is the strongest electrophile.

### Mulliken atomic charge analysis

Charge distribution in the phenyldiazenyl compounds are done by using the B3LYP/6-31G(d,p) basis set and the population analysis data information are listed in Table 2. The calculation of atomic charges plays an important role in the application of quantum mechanical calculations to molecular systems. The compounds 1-3 shows that the positive charges in a molecule are C6, C7, C9, C9a & S13; and high negative charges in a molecule are N8, O14, O15, N18a.

### Table 2 Mulliken atomic charges of compounds 1-3

| Atom 1 | Atom 2 | Atom 3 |
|--------|--------|--------|
| C1     | C1     | C1     |
| -0.123 | -0.130 | -0.102 |
| C2     | C11'   | C2     |
| -0.086 | -0.032 | -0.098 |
| C3     | C2     | C12'   |
| -0.057 | -0.064 | -0.026 |
| C4     | C3     | C3     |
| -0.092 | -0.071 | -0.086 |
| C4'    | C4     | C13'   |
| 0.022  | -0.071 | 0.031  |
| C5     | C5     | C4     |
| -0.133 | -0.149 | -0.071 |
| C15'   | C5'    | C5     |
| 0.069  | 0.010  | -0.088 |
| C6     | C6     | C6     |
| 0.135  | 0.142  | 0.086  |
| C7     | C7     | C7     |
| 0.106  | 0.079  | 0.119  |
| N8     | N8     | N8     |
| -0.456 | -0.441 | -0.470 |
| C9     | C9     | C9     |
| 0.237  | 0.241  | 0.243  |
| C10    | C10    | C10    |
| -0.093 | -0.088 | -0.092 |
| C10'   | C10'   | C10'   |
| -0.088 | -0.090 | -0.088 |
| C11    | C11    | C11    |
| -0.092 | -0.088 | -0.093 |
| C11'   | C11'   | C11'   |
| -0.088 | -0.092 | -0.087 |
| C12    | C12    | C12    |
| -0.170 | -0.169 | -0.170 |
| S13    | S13    | S13    |
| 1.137  | 1.138  | 1.138  |
| O14    | O14    | O14    |
| -0.559 | -0.550 | -0.559 |
| O15    | O15    | O15    |
| -0.557 | -0.560 | -0.556 |
| C1a    | C1a    | C1a    |
| -0.087 | -0.149 | -0.075 |
| C2a    | C11a   | C2a    |
| -0.085 | 0.010  | -0.095 |
| C3a    | C2a    | C2a    |
| -0.057 | -0.071 | 0.027  |
| C4a    | C3a    | C3a    |
| -0.098 | -0.071 | -0.085 |
| C4a'   | C4a    | C3a    |
| 0.022  | -0.069 | 0.031  |
| C5a    | C5a    | C4a    |
| -0.142 | -0.130 | -0.073 |
| C5a'   | C5a    | C5a    |
| -0.035 | 0.032  | -0.114 |
| C6a    | C6a    | C6a    |
| 0.097  | 0.192  | 0.084  |
| C7a    | C7a    | C7a    |
| 0.115  | 0.079  | 0.118  |
| N8a    | N8a    | N8a    |
| -0.479 | -0.441 | -0.474 |
| C9a    | C9a    | C9a    |
| 0.246  | 0.241  | 0.243  |
| C10a   | C10a   | C10a   |
| -0.092 | -0.088 | -0.092 |
| C10a'  | C10a'  | C10a'  |
| -0.088 | -0.090 | -0.088 |
| C11a   | C11a   | C11a   |
| -0.093 | -0.087 | -0.092 |
| C11a'  | C11a'  | C11a'  |
| -0.087 | -0.093 | 0.088  |
| C12a   | C12a   | C12a   |
| -0.169 | -0.169 | 0.170  |
The positive regions are related to nucleophilic reactivity. The negative regions are located around the nitrogen and oxygen atoms which are related to electrophilic reactivity. These data clearly show that compounds 1-3 are the most reactive towards substitution reactions.

3.2.3. Molecular electrostatic potential analysis

The MEP analysis proceeds with the study of the electron density and is the exceptionally visual method that pictures out the polarity of the molecule and hydrogen bonding interactions. MEP Surface potential is calculated by the DFT method. Molecular electrostatic potential is a useful descriptor used to visualize the electrophilic or nucleophilic reactive sites of molecular system, and to display the electrostatic potential regions in terms of color grading. The negative regions are located around the (O14) and (S13) atoms. As shown in (Fig. 3), the negative and positive potential sites are around the electronegative atoms and the hydrogen atoms, respectively, while the remaining species are surrounded by zero potential. As we conclude from this our title molecules are ready to involve both electrophilic and nucleophilic substitution reactions. MEP of the nitrogen atom N8, N8a shown by red and yellow color appearing below on top of the molecular plane of N8 and N8a atoms. Blue color exhibit the surface of the molecule's most preferred site for the attraction, while the red color region one reveals that the best site for repulsion within the molecule. Green color region predominates to corresponding halfway potential between the molecules and is illustrated at two regions of red and blue in phenylidiazeyl compounds.

![MEP diagram of compounds 1-3](image)

**Fig.3 MEP diagram of compounds 1-3**

3.2.4. NLO analysis

Organic materials with commutable NLO responses are sought for optoelectronic applications such as molecular-scale memory devices with multiple storage and nondestructive reading capacity. A large variety of NLO switches exhibiting large changes in the hyperpolarizability (β), the molecular second-order NLO response.

**Table 4** Dipole moment, polarisability of compounds 1-3

| Parameter | Dipolemoment (Debye) | 1 | 2 | 3 |
|-----------|----------------------|---|---|---|
| μx        | 2.2567               | 0.0068 | 1.0408 |
| μy        | -4.3620              | 6.6697 | -2.5624 |
| μz        | 1.3940               | -1.7645 | -1.7226 |
| μtotal    | 5.1052               | 6.8992 | 3.2583 |

| Parameter | Polarisability (a.u) | 10^23 | 10^24 |
|-----------|----------------------|-------|-------|
| αxx       | 31.8842              | 65.5792 | 5.9969 |
| αyx       | -35.9754             | -45.3129 | -28.4747 |
| αxz       | 4.0912               | -20.2663 | 22.4778 |
| αyz       | 23.0379              | -0.0330 | 9.9441 |
| αxy       | 33.3444              | -0.0985 | -18.3082 |
| αyz       | 5.2000               | -1.7091 | -3.9035 |
| αo (esu)  | 3.55 x10^-23        | 6.48 | 2.81 |
| Δα (esu)  | 1.18 x10^-24        | 7.22 | 6.0 |
Some quantum chemical descriptors which are dipole moment (μ), the polarizability (α), the anisotropy of the polarizability (Δα) and hyperpolarizability (β) have been used for explaining the NLO properties in many computational studies. In this context, the design of NLO switches, that is, molecules computed for their hyperpolarizability by alternate their substitution at 8 and 8a-sites in phenyl core. NLO properties increase with increasing the polarizability, anisotropy of the polarizability and hyperpolarizability. Dipole moment, which is used to study the intermolecular interactions, is a reflector of the molecular charge distribution. It can be used as descriptor to depict the charge movement across the molecule. The dipole moment of the compounds 1-3 were calculated and decreasing goes up like 3 > 2 > 1 with the maximum contribution along y-axis (Table 4). The calculated polarizability (α), is in the range of 1.18-7.22×10^{-23} respectively for the compounds 1-3. According to (Table 5), all the molecules have greater hyperpolarisability values than urea. Therefore, NLO properties of our compounds are better than urea. Results from (Table 5), the general decreasing ranking of NLO properties should be as follows: 3 > 2 > 1. With results in hand, molecule 3 is the best candidate for NLO properties. The hyperpolarizability β is dominated by the longitudinal components of β_{yyy}, β_{xxx} and β_{zzz}. Large values of particular components of the polarizability and hyperpolarizability indicate on a substantial delocalization of charges in these directions.

| Parameter | Hyperpolarisability (a.u) |
|-----------|--------------------------|
|          | 1            | 2            | 3            |
| β_{xxx}  | 432.4178     | 1.0403       | 231.0587     |
| β_{yyy}  | -192.2103    | 181.7299     | -205.1380    |
| β_{zzz}  | -5.6108      | 12.9729      | 4.4169       |
| β_{xyy}  | -87.8223     | -0.0015      | 41.3990      |
| β_{xxy}  | -23.7163     | 330.8225     | 209.2646     |
| β_{xzy}  | 110.1737     | -91.7276     | -115.2182    |
| β_{xz}   | 30.1485      | -0.1918      | 22.6035      |
| β_{yz}   | -3.4740      | -10.2103     | -3.5340      |
| β_{zy}   | -14.5751     | -6.7900      | 28.1439      |
| β_{xy}   | -50.0683     | 0.3062       | 28.1439      |
| β_0 (esu) | 5.25         | 4.62         | 4.57         |

4. Conclusion

In conclusion a novel NE,N’E-4,4’-sulfonylbis(N-(substituted-dichlorobenzylidene) anilines (1-3) was synthesized and their structure was confirmed by 1H & 13C NMR, and HR-MS spectroscopy. The synthesized compounds have found to be better antimicrobial activity than parent compound. All the synthesised compounds have shown mild to good activity against the pathogenic bacteria and fungi. Compounds 1-3 have shown to be more potent than ciprofloxacin and compounds 1-3 are more potent than fluconazol and other were near about equipotent in antibacterial and antifungal activity. The molecular hyperpolarizability of the 1-3 is 1.73-4.20 × 10^{-30} esu and is about 10 times greater than the standard urea value (β of urea is 0.3728 × 10^{-30}esu). Hence the 1-3 can be used as a potential NLO material.

Competing interests
The authors declare that they have no challenging interests.

Authors' contributions
All authors read and sanctioned the final manuscript.

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