Theoretical investigation and reconsideration of intramolecular proton-transfer-induced the twisted charge-transfer for the fluorescent sensor to detect the aluminum ion

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Abstract
A Schiff base compound 6-amino-5-(((2-hydroxynaphthalen-1-yl)methylene)amino)-2-mercaptopyrimidin-4-ol (AHM) in acetonitrile solvent is found to show “OFF–ON type” mode upon addition of Al³⁺ ion and successfully applied for selective recognition of Al³⁺ ion. In this work, the reconsideration of excited state intramolecular proton transfer (ESIPT) and twisted intramolecular charge transfer (TICT) has been explored in detail based on density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods. In the absence of Al³⁺, the lone pair electrons are transferred from –C=N to –OH forming a hydrogen-bonding configuration, and AHM shows weak fluorescence. When AHM is coordinated with metal ion, the TICT state is eliminated, and emission is significantly enhanced. Thus, in this paper, the origination of the non-emissive behavior of AHM has been explained in detail. The frontier molecular orbitals (MOs) and hole-electrons are used to analyze the charge distribution, providing strong evidence for the possibility of ESIPT and TICT processes occurring.

Keywords Aluminum sensor · Excited state intramolecular proton transfer · Fluorometric sensor · OFF–ON type · Twisted charge transfer

Introduction
Metal ions are closely related to the basic processes of living systems and human health problems [1–3]. Aluminum is the most abundant metal in the crust, and its elemental elements and compounds are widely used in production and life [4]. In recent years, the utilization of aluminum has been increased to food additives [5, 6], construction [7], medicine, ceramics, cosmetics, and other fields. However, with the widespread use of aluminum and its alloys, the content of aluminum in soil and water gradually increased, resulting in the accumulation of Al³⁺ in food, water, air, etc. In addition, prolonged exposure to high levels of Al³⁺ is toxic to the kidney, liver, brain, and nervous system [8–11]. Moreover, the abnormal concentration of Al³⁺ has adverse effects on the growth of seeds and root systems [12, 13]. Thus, timely monitoring of Al³⁺ levels in humans and the natural environment is needed to prevent the direct effects of Al³⁺ on the biosphere and human health [14]. In the previous report, the detection techniques have been defected because of the lack of coordination and spectrum performance. In recent years, chemical sensors used for monitoring biological and environment-related metal ions have been studied by researchers because of their advantages of simple synthesis route and high selectivity [15–19].

It is found that the closing sensor usually produces low signal output during binding, which can easily interfere with the time separation of similar compounds by time-resolved fluorescence method [20, 21]. Thus, many studies are inclined to the design and application of opening the sensor. Moreover, Al³⁺ is a fluorescence quencher due to its paramagnetism, which could affect the information of “turn-on” fluorescent sensors for its detection [22–24].
addition, selective binding of organic functional groups is one of the rational strategies for designing excellent fluorescent probes. Schiff base derivatives contain strong donor position (imine nitrogen atoms) which could provide a nitrogen-rich oxygen coordination environment [25, 26]. Moreover, Quinoline is also an ideal tool for metal ion fluorescence sensing based on good water solubility, good biocompatibility, and large Stokes shift [27–29]. Generally, the practical chemical sensors mainly rely on various types of fluorescence mechanisms, such as ESIPT [30], photoinduced electron transfer (PET), and ICT mechanisms [31–33].

AHM is a sensor to show turn-on type, which is synthesized by Yadav and Singh [34]. The sensor AHM consists of two parts, named A part and B part, which are connected by a carbon–nitrogen double bond (C=N), as shown in Scheme 1. Moreover, the imine nitrogen atom is able to transfer an electron to the hydroxyl-naphthalene, and the proton on the hydroxyl-naphthalene unit is transferred to the imine nitrogen, resulting in intramolecular hydrogen bond. Schiff bases bearing a C=N structure could easily isomerize and tend to exhibit very weak fluorescence. However, the Schiff base, with π electrons in C=N group, offers a good possibility for chelation with metal ions. Thus, when AHM and Al\(^{3+}\) form the complex, the C=N isomerization is inhibited and the fluorescence performance is enhanced. First, the presence of C=N double bonds may lead to a TICT. It is worth noting that there are two hydroxyl groups in AHM molecule; whether both can induce ESIPT reaction remains to be discussed, which are not considered in the experiment. Meanwhile, the photophysical characteristics of sensor AHM are complicated and the detection mechanism of sensor AHM and Al\(^{3+}\) will be investigated. The charge transfer process is studied by hole-electron analysis and the variation of various parameters. In addition, the possible non-emission channels are studied by relaxation scanning. The detection mechanism of the sensor is analyzed in detail by studying the three-coordination structure between Al\(^{3+}\) and the sensor.

**Computation details**

1. All calculations were accomplished with the Gaussian16 program package [35] by using DFT and TDDFT methods. B3LYP functional [36] and TZVP basis set [37, 38] were selected to serve the calculation. The B3LYP functional is of 20% Hartree–Fock exchange and has a low requirement for lattice point integration. In addition, the polarizable continuum model using the integral equation formalism variant (IEFPCM) was applied with acetonitrile (ACN) as the solvent simulating the experiment environment [39].

2. We optimize the structures of AHM-a, AHM-b, and AHM-c in the \(S_0\) and \(S_1\) states without setting any restrictions on symmetry, bonds, and angles and calculate the IR frequencies in the same calculation level. It is proved that the molecular structures of our optimized AHM-c are at the local lowest point. The only imaginary frequency along with hydrogen bond orientation represents the transition-state structure of ESIPT reaction.

3. The calculated electron spectra are comparable with the experimental value, which show the reliability of the selected theoretical calculation method. Moreover, the charge transfer process is studied by hole-electron analysis [40, 41]. The degree of charge transfer is measured using the value of the centroid distance (D) index, the degree of overlap (\(S_r\)), the width distribution (H), degree of separation (t), hole delocalization index (HDI), and electron delocalization index (EDI), which are introduced by using the Multiwfn program [42, 43]. Among them, D is a measure of charge-transfer length and \(S_r\) is a measure of spatial separation of a hole and electron. H represents the overall average distribution width of electrons and holes and \(t\) measures the separation of the hole from the electron. Additionally, HDI and EDI can measure the degree of orbital delocalization. The smaller the value is, the higher the degree of hole (electron) delocalization is, that is, the more uniform the distribution is. All the formulas are as follows:

\[
D_x = |X_{ele} - X_{hole}| \\
D_y = |Y_{ele} - Y_{hole}| \\
D_z = |Z_{ele} - Z_{hole}|
\]

\[
D_{index} = \sqrt{(D_x)^2 + (D_y)^2 + (D_z)^2}
\]
\[ S_r \text{ index} = \int S_r(r)dr \equiv \int \sqrt{\rho_{\text{hole}}(r)} \rho_{\text{ele}}(r)dr \]

\[ H \text{ index} = (|\sigma_{\text{ele}}| + |\sigma_{\text{hole}}|)/2 \]

\[ t \text{ index} = D \text{ index} - |H.u_{\text{CT}}| \]

\[ \text{HDI} = 100 \times \int \sqrt{\left| \rho_{\text{hole}}(r) \right|^2} dr \]

\[ \text{EDI} = 100 \times \sqrt{\int \left| \rho_{\text{ele}}(r) \right|^2 dr} \]

4. We have used Multiwfn software to study the type of hydrogen bond interaction by applying RDG function. The formula is as follows:

\[ \text{RDG}(r) = \frac{1}{2(3\pi^2)^{1/3}} \frac{\Delta \rho(r)}{\rho(r)^{4/3}} \]

The weak interactions depend on the \( \lambda_2 \) of eigenvalue and the \( \rho \) of electron density in view of Bader’s atoms-in-molecules (AIM) theory. The relationship between them is as follows:

\[ \Omega(r) = \text{Sign}(\lambda_2(r)) \rho(r) \]

### Table 1 Geometrical information of chemical sensor AHM

| AHM  | ∠C3C2N1C4 | ∠C2N1C4C5 | ∠O1H1N1 | O1-H1 | H1-N1 |
|------|------------|------------|---------|-------|-------|
| AHM-a-S0 | 157°       | 177°       | 149°    | 1.01 Å | 1.64 Å |
| AHM-b-S0 | 47°        | 179°       | 148°    | 1.01 Å | 1.63 Å |
| AHM-c-S0 | 138°       | 177°       | 138°    | 1.70 Å | 1.03 Å |
| AHM-d-S0 | 137°       | −12°       | 129°    | 0.97 Å | 2.40 Å |
| AHM-TICT | −179°      | 91°        | 144°    | 0.98 Å | 1.84 Å |
| AHM-c-S1 | 173°       | −179°      | 148°    | 1.58 Å | 1.05 Å |

### Results and discussion

**Geometrical information of fluorescent sensor AHM**

The sensor AHM has been optimized in the S\(_0\) state. The optimized geometric structures are shown in Fig. 1b (referred to AHM-a). In Table 1, the \( z\text{C}_3\text{C}_2\text{N}_1\text{C}_4 \) is 157°, meanwhile, two single bonds, named \( \text{C}_2-\text{N}_1 \) and \( \text{C}_4-\text{C}_5 \), are observed, and the rotation between the single bonds makes the structure of AHM more flexible. Additionally, the distance between \( \text{H}_2-\text{N}_1 \) is 3.66 Å, and there is no intramolecular hydrogen bond between them. However, there is a hydrogen bond between \( \text{H}_1 \) and \( \text{N}_1 \) with a bond length of 1.64 Å and the \( \text{O}_1\text{H}_1\text{N}_1 \) angle of 149°, which prevents the rotation of the intramolecular single bond. Thus, it is not necessary to consider the rotation forces caused by the \( \text{C}_4\text{C}_5 \) deformation. To
in Table 2. As seen in Table 2, the analyzed wavelength and other data are listed for the excitation and emission process of AHM was further analyzed. In order to explore the photophysical properties of the sensor, the electronic exited states (CI) was optimized and given in Fig. 3a and Table 1. The C3C2N1C4 dihedral angle is 173°, which means there is a near planar structure. As listed in Table 2, AHM-c is a bright state lying at 504 nm, which is assigned to HOMO→LUMO (98.1%) transition. The orbitals are plotted in Fig. 2. A total of 0.16 electrons are transferred from the A part to the B part during the excitation, and the charge transfer is not obvious. Moreover, the D index is relatively small, which means that the S0→S1 of AHM-c is a LE state. The geometry in the S1 state is optimized and given in Fig. 3a and Table 1. The C3C2N1C4 dihedral angle is 173°, which means there is a near planar structure in the S1 state. The fluorescence quenching is not caused by planar structure. As listed in Table 2, AHM-c is a bright state in the S1 state, and its oscillator strength is 0.9065. The calculated emission peak is 504 nm, which is consistent with the experimental value (500 nm). As is shown, the HOMO mainly distributes on the A part and C part. According to the hole-electron analysis, the charge transfer amount is relatively small (0.14 e). It is worth noting that the emission intensity observed at 500 nm in the experiment is very weak, so the existence of a non-emission deactivation channel is assumed.

**Excitation and emission process of AHM**

In order to explore the photophysical properties of the sensor, the excitation and emission process of AHM was further analyzed. The calculated wavelengths and other data are listed in Table 2. As seen in Table 2, the S0→S1 transition for AHM-a is predicted at about 403 nm with oscillator strength of 0.7211, and the process is from HOMO to LUMO. For S0→S1 of AHM-a, during the excitation process, the distribution region of the electron does not change significantly, which also means that the excitation of S0→S1 is a local excitation (LE). Here, hole-electron analysis is also used, and only 0.08 electrons are transferred between the A part and B part. In addition, as listed in Table 3, the D index is relatively small, which provides direct evidence for proving that S0→S1 is LE state. The proton transfer reaction, triggered by a strong hydrogen bond between H1 and N1, could generate the new isomer AHM-c (Fig. 1c) which was obtained by the ground state relaxation scanning the distance between H1 and N1. As shown in Table 1, ∠C3C2N1C4 and ∠C2N1C3C5 are 138° and 177°, respectively. As depicted in Fig. 1d, the product AHM-c is more stable than AHM-a. Also, the GSIPT energy barrier from AHM-a to AHM-c is merely 2.4 kcal/mol which indicates that the AHM-c structure is the most likely configuration. Consequently, the excitation and emission process of AHM-c will be further explored.

As is reported in Table 2, the dominant transition of AHM-c is the S0→S1 transition, with the oscillator strength of 0.5271 lying at 410 nm, which is assigned to HOMO→LUMO (98.1%) transition. The orbitals are plotted in Fig. 2. A total of 0.16 electrons are transferred from the A part to the B part during the excitation, and the charge transfer is not obvious. Moreover, the D index is relatively small, which means that the S0→S1 of AHM-c is a LE state. The geometry in the S1 state is optimized and given in Fig. 3a and Table 1. The C3C2N1C4 dihedral angle is 173°, which means there is a near planar structure in the S1 state. The fluorescence quenching is not caused by planar structure. As listed in Table 2, AHM-c is a bright state in the S1 state, and its oscillator strength is 0.9065. The calculated emission peak is 504 nm, which is consistent with the experimental value (500 nm). As is shown, the HOMO mainly distributes on the A part and B part while LUMO mainly distributes on the A part and C=N part. According to the hole-electron analysis, the charge transfer amount is relatively small (0.14 e). It is worth noting that the emission intensity observed at 500 nm in the experiment is very weak, so the existence of a non-emission deactivation channel is assumed.

**Table 2** Excitation and emission energies of the AHM, including the oscillator strength (f) and orbital transition (OT) contributions to the electronic exited states (CI)

| Experiment | Transition | λ (nm/eV) | f | OT | CI (%) |
|------------|------------|-----------|----|-----|--------|
| Absorption | S0→S1     | 403/3.07  | 0.7211 | H→L | 98.3%  |
| Emission   | S0→S1     | 327/3.78  | 0.0406 | H-1→L | 90.3%  |
| AHM-a-S0   | S0→S1     | 315/3.92  | 0.0508 | H-2→L | 85.6%  |
| AHM-b-S0   | S0→S1     | 300/4.12  | 0.0315 | H→L+2 | 5.4%   |
| AHM-c-S0   | S0→S1     | 403/3.07  | 0.5952 | H→L  | 95.4%  |
| AHM-c-S0   | S0→S1     | 339//3.65 | 0.0123 | H-1→L | 90.1%  |
| AHM-c-S0   | S0→S1     | 317/3.91  | 0.0836 | H-2→L | 88.5%  |
| AHM-c-S1   | S0→S1     | 299/4.14  | 0.0178 | H→L+1 | 92.3%  |
| AHM-c-TICT | S0→S1     | 410/3.02  | 0.5271 | H→L  | 98.1%  |
| AHM-c-S1   | S0→S1     | 349/3.55  | 0.0246 | H-1→L | 40.6%  |
| AHM-c-S1   | S0→S1     | 336/3.68  | 0.1087 | H-1→L | 51.3%  |
| AHM-c-S1   | S0→S1     | 308/4.02  | 0.0806 | H-2→L | 42.3%  |
| AHM-c-S1   | S0→S1     | 504/2.45  | 0.9065 | L→H  | 99.4%  |
| AHM-TICT   | S0→S1     | 4016/0.30 | 0.0001 | L→H  | 99.4%  |

**Table 3** The data of the excited states for the sensor AHM, including the centroid distance (D), the degree of overlap (S), the width distribution (H), degree of separation (t), hole delocalization index (HDI), and electron delocalization index (EDI)

|          | D (Å) | S (Å) | H (Å) | t (Å) | HDI  | EDI  |
|----------|-------|-------|-------|-------|------|------|
| AHM-a S0→S1 | 0.63  | 0.73  | 3.45  | -0.86 | 6.31 | 7.42 |
| AHM-a S0→S1 | 1.66  | 0.74  | 3.18  | -2.32 | 6.66 | 7.22 |
| AHM-a S0→S1 | 0.68  | 0.69  | 3.33  | -1.58 | 6.66 | 7.94 |
| AHM-a S0→S1 | 0.72  | 0.71  | 3.26  | -1.77 | 7.06 | 7.93 |
The origination of the non-emissive behavior of AHM

Generally, bending of the C=N double bond may result in the formation of non-luminous isomers. As shown in Fig. 4, the bending degree of AHM-a in the $S_0$ state was studied by relaxing and scanning the dihedral angle of C$_2$N$_1$C$_4$C$_5$. The $\angle$C$_2$N$_1$C$_4$ of AHM-a-$S_0$ (Fig. 4a) and AHM-d-$S_0$ (Fig. 4c) structure are 124° and 122°, respectively. As shown in Fig. 5, the structure of AHM-a in the $S_1$ state was firstly optimized.
and a distorted structure was found. The local HOMO is delocalized through the B part, and LUMO is mainly localized on the C=N and A part, with complete charge separation. Furthermore, a total of 0.40 electrons are transferred from the left moiety to the right moiety during the $S_1 \rightarrow S_0$ excitation by using hole-electron analysis. As listed in Table 1, $\angle C_3C_2N_1C_4$ and $\angle C_2N_1C_4C_5$ are $-179^\circ$ and $91^\circ$, respectively. Moreover, by TDDFT calculation, the oscillator strength is almost zero (0.0001). This indicates that in the $S_1$ state, AHM-a is a typical TICT state and then named as AHM-TICT. However, the bending angle of the $N_1-C_4$ double bond requires the energy of 30.17 kcal/mol. Thus, the TICT state cannot be attained by direct excitation and excited state relaxation from AHM-d-$S_0$.

In order to explore the pathway to the TICT state, the $H_1-N_1$ distance of AHM-c in the $S_1$ state was relaxed-scanned. As shown in Fig. 6, the energy barrier of ESIPT from AHM-c-$S_1$ to the transition state is merely 2.08 kcal/mol.
Moreover, the product produced by ESIPT happens to be AHM-a-S1, also known as AHM-TICT, which indicates that ESIPT triggers the distortion of the structure and spontaneously reaches the TICT state. Due to the higher energy barrier from AHM-a to AHM-d, it is difficult to form AHM-d structure. In the S1 state, AHM-c carries out ESIPT process and further triggers the TICT state.

**IR vibrational spectra and RDG isosurfaces of sensor AHM**

In Fig. S1, the IR spectra of the main hydrogen bonds involved in the S0 and S1 states have been computed. For the AHM, the O1-H1 peak shifts from 3563 cm\(^{-1}\) in the S0 state to 2945 cm\(^{-1}\) in the S1 state. The IR vibrational frequency of O1-H1 bond of AHM has a red shift of 618 cm\(^{-1}\), which indicates that the AHM sensor has a large Stokes shift. It can also be manifested that the intramolecular hydrogen bond in S1 state is much stronger than that in S0 state through the analysis of stretching vibration frequencies.

As shown in the RDG scatter graph of Fig. S2a, the value range of the RDG isosurfaces is set from −0.05 to 0.05. The spike peaks of the AHM complex are observed and located at −0.0408 (Fig. S2b). The interaction type is assigned to hydrogen bond interaction and the more to the left of the peak, the stronger the hydrogen bond is. In the diagram, it can be seen that the part representing the hydrogen bonding interaction in O1-H1−N1 presents a ring in the RDG isosurfaces. There is a strong hydrogen bond interaction between H proton and N receptor in the S1 state.
The photo-physical process of the AHM was clarified. Next, the Al$^{3+}$ detecting mechanism is explored. The reaction sites of hydrogen bonded donor and acceptor and their interactions can be analyzed by electrostatic potential (ESP). As shown in Fig. 7a, the ESP surface of AHM in the S$_0$ state is studied. The yellow ball and the blue ball correspond to the maximum and minimum values of the electrostatic potential, respectively. The most negative site is located near O$_1$ atom, and its value is $-125$ kJ/mol. Thus, the interaction between Al$^{3+}$ and the O$_1$ position should be strong. Then, the complex formed between AHM and Al$^{3+}$ is optimized, shown in Fig. 7b. Detailed geometric parameters are listed in Table 4. In order to ensure the rationality of the configuration in the coordination regions, Mayer bond order analyses [44] of the AHM-Al are conducted through the Multiwfn program. The Mayer bond orders of three bonds (Al-O$_1$, Al-O$_2$, Al-N$_1$) are 0.73, 0.72, and 0.53, respectively. These results indicate that the bonds of the Al-O$_1$, Al-O$_2$, and Al-N$_1$ are the coordinate bond. And the coordinate bond of Al-O$_1$ and Al-O$_2$ is stronger than Al-N$_1$ coordinate bond in the AHM-Al complexes. In order to further explore the influence of other cations on the molecular properties of the probe AHM, the corresponding discussion and explanation are given in the supplementary information.

As listed in Table 4, the structure of AHM-Al in the S$_1$ state is very similar to that in the S$_0$ state. In the S$_1$ state, the flatness of the molecule increases and the non-emitting TICT state is eliminated. Furthermore, the HOMO and LUMO orbitals of the ligand (AHM-a) and the complexes (AHM-Al) are also compared and analyzed. The energy gaps between HOMO and LUMO are found as 3.526 eV and 2.479 eV, respectively, for AHM-a and AHM-Al.

| Table 4 Geometries of the complex (at B3LYP/TZVP theory level) | AHM-Al-S$_0$ | AHM-Al-S$_1$ |
|-----------------------------|----------------|----------------|
| $\angle$C$_2$C$_4$N$_1$C$_4$ | 149$^\circ$    | 153$^\circ$    |
| $\angle$C$_2$N$_1$C$_3$   | $-161^\circ$   | $-169^\circ$   |
| $\angle$N$_1$C$_3$C$_4$   | 19$^\circ$     | 16$^\circ$     |
| Al-O$_1$                  | 1.79 Å (0.73)  | 1.72 Å (0.74)  |
| Al-O$_2$                  | 1.84 Å (0.72)  | 1.77 Å (0.71)  |
| Al-N$_1$                  | 1.95 Å (0.53)  | 1.85 Å (0.55)  |

| Table 5 Excitation and emission energies of the metal-sensor complexes (B3LYP/TZVP) |
|----------------------------------|-------------------|-------------------|-------------------|
| Transition                       | $\lambda$ (nm/eV) | $f$               | OT                |
| AHM-Al-S$_0$                     |                   |                  |                   |
| S$_0$ $\rightarrow$ S$_1$       | 431/2.87          | 1.2638            | H $\rightarrow$ L |
| S$_0$ $\rightarrow$ S$_2$       | 422/2.94          | 0.0214            | H $\rightarrow$ L |
|                                |                   | 50%               |                   |
| S$_0$ $\rightarrow$ S$_3$       | 411/3.01          | 0.1623            | H $\rightarrow$ L |
|                                |                   | 92%               |                   |
| AHM-Al-S$_1$                     |                   |                  |                   |
| S$_1$ $\rightarrow$ S$_0$       | 530/2.34          | 0.9313            | L $\rightarrow$ H |
|                                |                   | 97%               |                   |

Fig. 8 Frontier molecular orbitals involved in the UV–vis absorption of AHM and AHM-Al complex and the emission of AHM-Al.
AHM-Al complex (Fig. 8). This indicates that AHM-Al complex is more stabilized than that of AHM-a. For AHM-Al, the electron is confined to the A part, and the distribution region of the electron does not change significantly before and after the excitation. Meanwhile, the emission process of AHM-Al is studied. As shown in Table 5, the $S_1 \rightarrow S_0$ emission with large oscillator strength of 0.9313 generates $\pi \rightarrow \pi^*$ transition character, which means the AHM-Al is emissive. Moreover, $Al^{3+}$ is not involved in the emission process, which eliminates the original TICT state.

Conclusions

In conclusion, the sensor AHM has been researched and analyzed by DFT and TD-DFT theoretical methods. The imine nitrogen of the sensor is adjacent to the $-OH$ group, and the sensor has a large spectral shift for $Al^{3+}$ ions due to the presence of polar groups such as hydroxyl and amine. Furthermore, the trivalent form of these groups has a high affinity for the $Al^{3+}$ ion. In acetonitrile solvent, the AHM exhibits weak fluorescence emission because of ESIPT and C–N isomerization. Upon adding of $Al^{3+}$, the AHM coordinates with the metal ions and eliminates the TICT state. The coordination $Al^{3+}$ with AHM deprotonates the phenolic hydroxyl groups preventing the intrahydrogen bonding with imine nitrogen ($O$–$H$'–$N$) and also inhibits the ESIPT. Based on the characteristics of sensor AHM, it is widely used in real life, such as cell imaging and dipstrip test.

Supplementary information

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Author contribution

Xiumin Liu performed data collection, analysis, and writing. Hengwei Zhang performed data collection and analysis. Sen Liu performed data analysis. Yi Wang performed the study’s conception, design, data collection, analysis, writing, editing, review, and supervision. Peng Zhang performed the study’s conception, editing, review, and supervision.

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Declarations

Conflict of interest

The authors declare no competing interests.

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