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Recent advances in near-infrared fluorescent ligands as a novel frontier in combating antibiotic-resistant bacteria

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ABSTRACT

The emergence and rapid spread of multi-drug-resistant (MDR) bacteria pose a serious and escalating threat to global public health, undermining the effectiveness of conventional antibiotics and demanding urgent development of alternative therapeutic strategies. Among these, phototherapy mediated by organic fluorescent ligands has gained increasing attention as a promising antimicrobial approach due to its spatiotemporal precision, minimal invasiveness, and reduced risk of resistance development. In phototherapeutic antimicrobial applications, near-infrared (NIR) photosensitizers are activated by light to produce reactive oxygen species (ROS) or localized heat, leading to targeted damage of bacterial membranes, proteins, and nucleic acids. This review provides a focused summary of recent advances over the past decade in the design and application of NIR organic fluorescent ligands for antibacterial phototherapy. We discuss key molecular classes which include cyclic tetrapyrroles, phenothiazinium salts, cyanine dyes, BODIPYs and aza-BODIPYs, tetraphenylethene, and triphenylamine analogues, highlighting their structural features, photophysical properties, and mechanisms of action. By consolidating these developments, our aim is to offer a comprehensive and accessible resource that supports future innovation and encourages interdisciplinary collaboration. This review contributes meaningfully to the ongoing scientific and clinical discourse on antimicrobial resistance, highlighting novel phototherapy-based solutions with potential for real-world impact.

1. Introduction

The escalating challenge of antibiotic resistance has prompted an urgent need to revisit and rethink our understanding of antibacterial mechanisms and therapeutic strategies. To provide a comprehensive foundation for this review, we first critically examine the mechanisms underlying traditional antibacterial agents, which have long constituted the cornerstone of infection control. We then explore the drug resistance

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Abbreviations: NIR, near-infrared; ROS, oxygen species; MDR, multidrug-resistant; EPS, extracellular polymeric substances; PTT, photothermal therapy; PDT, photodynamic therapy; PTAs, photothermal agents; PSs, photosensitizers; S_0, the ground state; S_n, short-lived singly excited state; VR, vibrational relaxation; IC, internal conversion; ISC, nonradiative scampering; T_1, longer-lived excited triplet state; PAI, photoacoustic imaging; $^1O_2$, single-linear state oxygen; DNA, deoxyribonucleic acid; RNA, ribonucleic acid; ICG, indocyanine green; ALA, 5-aminolevulinic acid; MB, methylene blue; AMR, antimicrobial resistance; FDA, Food and Drug Administration; NFE, near-field enhancement; PPS, porphyrin polymer vesicle; POPs, porous organic polymers; Ce6, chlorin e6; PDAT, photodynamic antibacterial therapy; PBG, photonic band gap; TB, Toluidine Blue; NB, Nile Blue; LG, lipogel; PACT, photoactivated chemotherapy; APNB, photodynamic antimicrobial; PEG, polyethylene glycol; DMMA, 2,3-dimethylmaleic anhydride; FLI, fluorescence imaging; COF, covalent organic frameworks; BIME, Bacterial Infection Microenvironment; ICT, intramolecular charge transfer; ICy7, iodinated heptamethine cyanine dyes; BODIPY, boron-dipyrromethene; ABDP, asymmetric boron dipyrromethene; PTCE, photothermal conversion efficiency; OHA, oxidized hyaluronic acid; AIE, aggregation-induced emission; UCNPs, upconversion nanocrystals; ET, electron transfer; RENPs, rare-earth-doped nanoparticles; PVP, polyvinylpyrrolidone; ZIF-8, zeolitic imidazolate framework-8; GSH, glutathione; AI, artificial intelligence.

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crisis, delving into the molecular and evolutionary mechanisms that enable bacteria to evade conventional treatments. In response to these limitations, phototherapy has emerged as a promising alternative, offering precise, non-invasive, and resistance-free antibacterial action. We introduce the fundamental principles and advantages of phototherapy, particularly those mediated by near-infrared (NIR) photosensitizers. Finally, we present the core concept of antibacterial phototherapy, detailing how light-activated agents interact with bacterial structures to achieve targeted microbial eradication. Together, these subsections lay the groundwork for understanding the significance and innovation behind NIR fluorescent ligands in combating drug-resistant infections.

1.1. *The mechanism of traditional antibacterial agents*

Traditional antibiotics can be divided into three categories, including antibiotics, semi synthetic antibiotics, and synthetic antibiotics. At present, the main targets of antibacterial drugs include bacterial cell walls (Narendrakumar et al., 2023), cell membranes (Falagas et al., 2010; Hurdle et al., 2011; Poirel et al., 2017), proteins (Rusu and Buta, 2021), and nucleic acids (Campbell et al., 2001; Hooper and Jacoby, 2016).

1.1.1. *Bacterial cell wall inhibitor*

β-Lactam antibiotics are a class of antibacterial drugs that inhibit bacterial cell wall synthesis. They have good bactericidal effects and low toxicity and are widely used in clinical bacterial infection treatment. *β*-Lactam antibiotics can be divided into penicillin, cephalosporin, and atypical antibiotics *β*-lactamides (Narendrakumar et al., 2023), a four-membered 2-azetidinone (β-lactam ring) fused to another five- or six-membered ring, forming a bicyclic system (Chang et al., 2025). The structure of *β*-lactam antibiotics is similar to that of D-Ala-D-Ala at the end of peptidoglycan on the cell wall, and they can competitively covalently bind with penicillin binding proteins, thereby inhibiting the formation of peptidoglycan and damaging the integrity of bacterial cell wall, leading to bacterial lysis and death (Fig. 1).

1.1.2. *Bacterial protein synthesis inhibitor*

Antibiotics that inhibit bacterial protein biosynthesis can be broadly categorized into several classes, including tetracyclines, aminoglycosides, macrolides, and amphenicols. Among them, tetracycline antibiotics exert their antibacterial effect by penetrating bacterial cells through passive diffusion and energy-dependent active transport mechanisms (Blake et al., 2025; Brdova et al., 2024; Ma et al., 2023). Once inside, they reversibly bind to the A site of the 30S ribosomal subunit, specifically interacting with the 16S rRNA. This binding prevents the attachment of aminoacyl-tRNA to the mRNA–ribosome complex, thereby inhibiting the elongation of the nascent peptide chain and ultimately suppressing bacterial protein synthesis and growth. Structurally, tetracyclines are zwitterionic compounds characterized by a hydrogenated tetracyclic benzene backbone (Fig. 2). Their ability to form reversible complexes with ribosomal RNA is central to their mechanism of action, making them effective against a broad spectrum of bacterial pathogens.

Macrolide antibiotics, on the other hand, are defined by their large lactone rings, typically comprising 14–16 members (Fig. 2). These rings are often substituted at the C-3 and C-5 positions with one or more deoxysugar moieties, such as erythromycin and desosamine. Macrolides bind to the "V"-shaped domain of the 50S ribosomal subunit via hydrogen bonding interactions. This binding promotes the premature dissociation of peptidyl-tRNA from the ribosome, thereby interrupting the transpeptidation process and halting peptide chain elongation. As a result, protein synthesis is effectively inhibited, leading to bacteriostatic or bactericidal outcomes depending on the concentration and bacterial species (Svetlov et al., 2021).

1.2. *Drug resistance crisis and mechanism*

With the widespread use of antibiotics, bacteria have developed resistance to various antibacterial drugs, posing a serious challenge to global healthcare systems (Michael et al., 2014). The outbreak of the coronavirus has also led to increased use of antibiotics, further exacerbating the risk of bacterial resistance (Tan et al., 2022). Multidrug-resistant (MDR) bacteria, also known as superbugs with high infectivity and mortality rates, have become a significant threat to human health (Cao et al., 2022). According to conservative estimates by the World Health Organization, the annual death toll due to bacterial resistance is projected to exceed 10 million by 2050 (Zhang et al., 2023d).

The resistance mechanisms of bacteria mainly include forming bacterial biofilms, modifying antibiotics, genetic mutations, reduced cell membrane permeability, and overexpression of efflux pumps (Brdova et al., 2024) (Fig. 3). Bacterial biofilms are extracellular polymeric

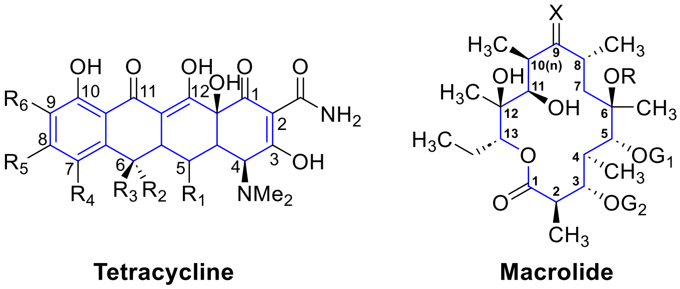

Fig. 2. Chemical structure of tetracycline and macrolide antibiotics.

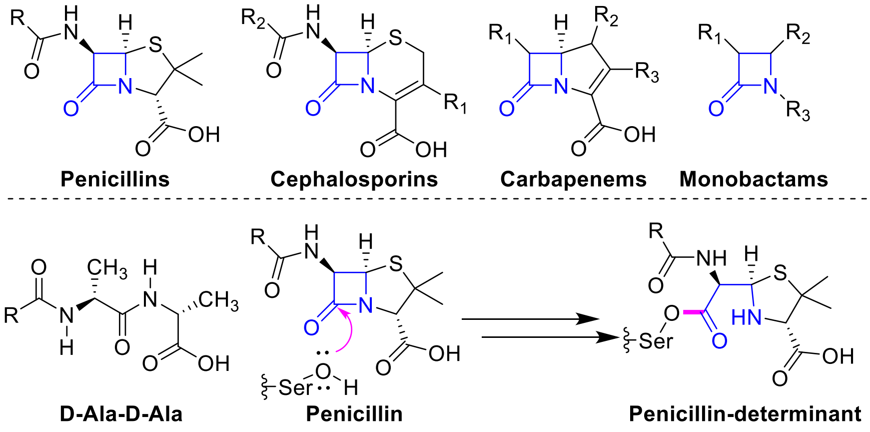

Fig. 1. Common *β*-lactam-based antibiotics and a simplified mechanism of action.

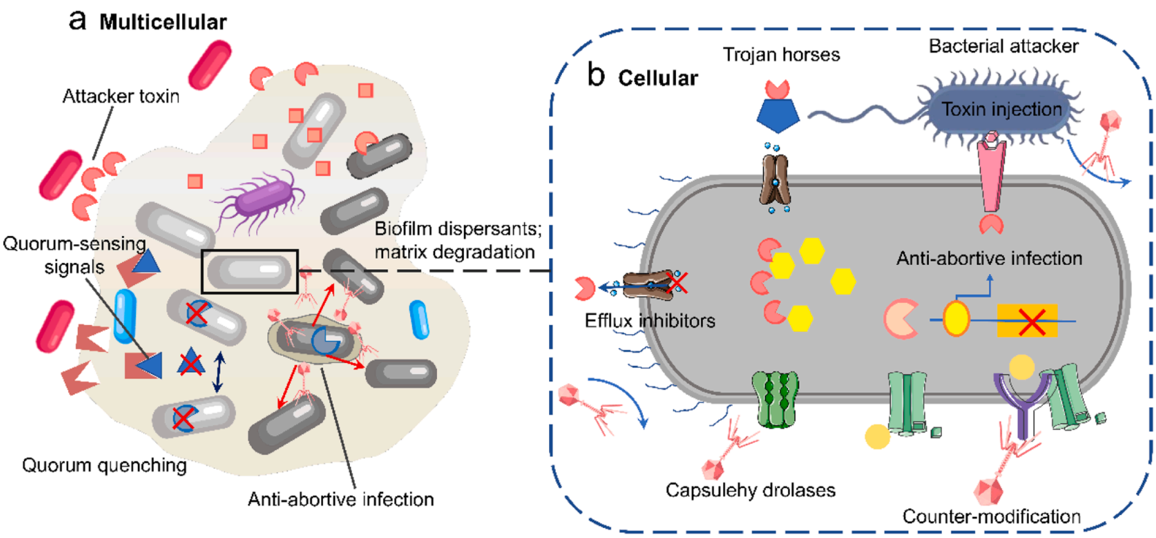

Fig. 3. Bacterial resistance mechanisms to current antibacterial agents. (a) Biofilm formation through bacterial quorum sensing. (b) Mechanisms of bacterial resistance include modifying antibiotics, genetic mutations, reduced cell membrane permeability, and overexpression of efflux pumps.

substances (EPS) secreted by bacteria, mainly composed of polysaccharides, proteins, lipids, and extracellular DNA (Penesyan et al., 2021). They are the main barriers that prevent antimicrobial drugs from entering bacteria (Tshibangu-Kabamba and Yamaoka, 2021) and may increase resistance to antimicrobial agents by about 10–1000 times (Hou et al., 2022). Modification of antibiotics occurs through enzymatic degradation or modification of antibiotic structure, while genetic mutations protect, alter, or overexpress antibiotic targets in bacteria. In addition, bacteria can expel antibiotics from within the bacterial cell through reduced cell membrane permeability or overexpression of efflux pumps. Some bacteria reduce porin expression or express more selective porin variants to decrease cell membrane or cell wall permeability, thus preventing antibiotics from entering the cell. In some instances, bacteria employ multiple antibacterial mechanisms to achieve high levels of antibiotic resistance.

1.3. *Phototherapy mechanism and advantages*

Phototherapy is usually a medical treatment that combines harmless, low-intensity light with exogenous phototherapeutic agents to enhance the therapeutic effect (Ran et al., 2023; Ran et al., 2021a). Phototherapy is a promising alternative therapy against bacterial infections, which mainly consists of photothermal therapy (PTT) and photodynamic therapy (PDT) (Wang et al., 2022a; Wei et al., 2020). PTT is a treatment that directly kills bacteria by converting light energy into heat through photothermal agents (PTAs). At the same time, PDT is an antibacterial treatment through light-induced reactive oxygen species (ROS) production. Compared to conventional antibacterial therapies using preservatives and antibiotics, phototherapy has the advantages of being spatio-temporally selective, non-invasiveness, non-resistant, broad-spectrum antibacterial, and having negligible side effects (Badran et al., 2023; Nguyen et al., 2022; Piksa et al., 2023; Zhou et al., 2023). In particular, NIR phototherapy is a promising alternative to traditional antibacterial methods due to its greater tissue penetration and lower

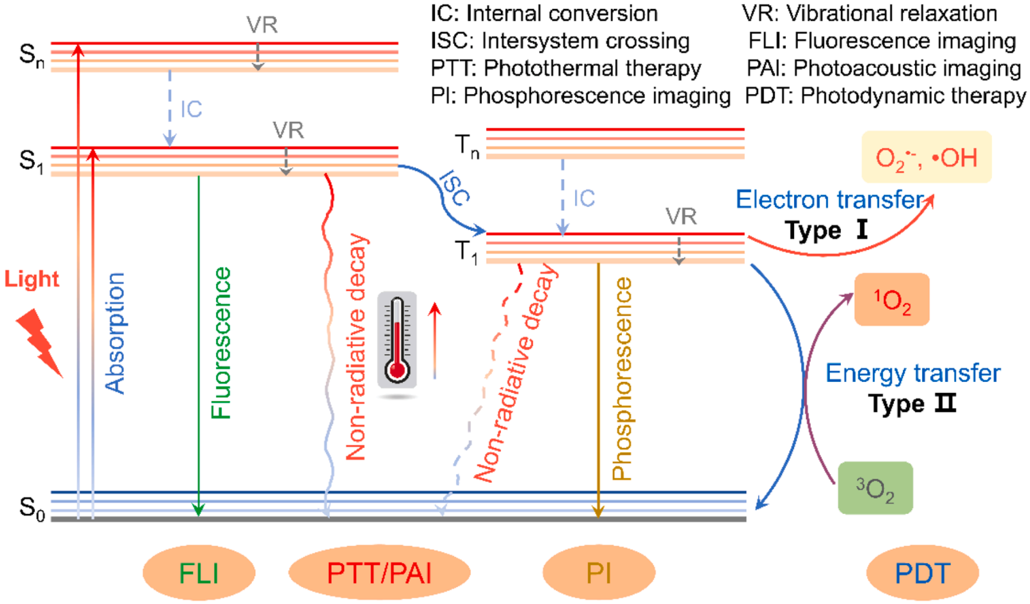

Fig. 4. The mechanisms of phototherapy.

photodamage (Abrahamse et al., 2022; Ebaston et al., 2021; Prakash et al., 2023; Semenova et al., 2023). Using Jablonski diagrams, the photophysical processes of photosensitizers (PSs) under light irradiation can be easily illustrated to elucidate the potential mechanisms of phototherapy (Fig. 4).

Under light excitation at an appropriate wavelength, the photosensitizer can be activated from the ground state (S_0) to a short-lived singly excited state (S_n) of the same spin multiplicity, followed by relaxation through non-radiative vibrational relaxation (VR) and internal conversion (IC) to the lowest vibrational energy level of the excited state (S_1), and subsequently undergo nonradiative scampering (ISC) to form a longer-lived excited triplet state (T_1). Then, the S_1-state electrons relax to the ground state (S_0) by radiative decay, and their energy is converted into fluorescence emission, which is mainly applied to bioimaging. At the same time, the electron from the S_1 state can also return to the ground state by non-radiative decay, and its energy will be converted to heat applied to PTT/photoacoustic imaging (PAI). Electrons in the T_1 state can return to the ground state by transferring energy through phosphorescence emission.

In addition, PSs in the T_1 state may generate ROS for PDT through different photochemical reaction processes (Bucharskaya et al., 2022; Celli et al., 2010; Garapati et al., 2023; Li et al., 2022d). Among them, PS in the excited state for type I PDT reacts directly with biological substrates through electron transfer to form generating radicals and/or radical ions, such as hydroxyl radical (•OH) and superoxide anion ($O_2^{\bullet-}$). For type II PDT, an oxygen-dependent photochemical reaction process, the excited PSs reacts with the surrounding oxygen through energy transfer to form highly reactive single-linear state oxygen ($^1O_2$). Type I and type II PDT can co-occur, and their dominance depends on photosensitizer performance, the reaction environment (substrate type and oxygen concentration), and the interaction between the PSs and substrates (Fan et al., 2016; Li et al., 2022a). Most of the existing PSs is working based on type II PDT mechanism, which is oxygen-dependent, and this property limits their antibacterial efficiency in anoxic environments. In contrast, there are a few types I PSs that can function in anoxic environments (Pham et al., 2021; Xiao et al., 2023; Zhao et al., 2021a).

With the rapid advancement of PSs design and optical technologies, phototherapy-based antibacterial strategies have gained substantial attention in recent years. This approach is increasingly recognized as a green, non-invasive, and highly promising alternative to conventional antibiotics, particularly for treating infections caused by drug-resistant microorganisms (Zhou et al., 2021). The growing body of research highlights phototherapy's potential to overcome limitations associated with traditional antimicrobial agents, offering precise, controllable, and resistance-free mechanisms of action. As such, phototherapy is emerging as a vital component in the development of next-generation antimicrobial therapies, with significant implications for both clinical practice and global public health. Compared to conventional antibiotics, phototherapeutic antibacterial strategies offer several distinct advantages:

(1) Broad-spectrum antibacterial properties. Phototherapy is effective in inactivating a wide range of microorganisms such as bacteria (Kang et al., 2019; Liu et al., 2022b), fungi (Gamelas et al., 2023; Garcia-Fernandez et al., 2012; Zhang et al., 2023c), viruses (Bai et al., 2023; Jurak et al., 2023), and parasites (Mohammed et al., 2023).

(2) Low toxicity and minimal side effects. Phototherapeutic agents are typically designed to achieve high biocompatibility for safe and effective therapeutic applications. Phototherapy is applied directly to the localized site of infection. This targeted treatment approach minimizes exposure to surrounding healthy tissues, thereby reducing potential damage and systemic toxicity.

(3) Non-invasive or minimally invasive. Bacterial infections often occur on the skin surface or in post-operative wounds, making them accessible for phototherapy. For infections located deeper within the body, phototherapeutic agents and excitation light can be delivered precisely to the affected area using endoscopic techniques and optical fibers. This enables targeted treatment with minimal disruption to surrounding tissues (Dai et al., 2009; Jori, 2006).

(4) Low-cost, eco-friendly, efficient, and rapid antimicrobial action. Light is a readily available, low-cost, and renewable resource, making phototherapy a sustainable and environmentally friendly treatment option. Compared to antibiotics, which often require hours or days to take effect, phototherapy can rapidly inactivate pathogens. This is a distinct advantage in managing fast-spreading microbial infections (Ran et al., 2021a).

(5) Low potential for resistance development. Unlike antibiotics, which microorganisms can rapidly develop drug-resistance via different mechanisms such as mutations or efflux pumps, phototherapy exerts antimicrobial effects mainly by inducing localized hyperthermia and generating reactive oxygen species (ROS). These mechanisms enable effective and long-lasting microbial inactivation, including the disruption and removal of biofilms (Hu et al., 2018; Song et al., 2020). More importantly, repeated phototherapeutic treatments are less likely to induce microbial resistance, making it a promising strategy for combating persistent infections.

1.4. General principal of antibacterial phototherapy

For infectious diseases, antibiotics are extremely effective treatments in modern medicine and can significantly reduce their mortality rates (Chung, 2023; Shrivastava et al., 2023). Antibiotics work by inhibiting key aspects of bacterial growth or proliferation, including the synthesis of cell walls and cell membranes and the production of deoxyribonucleic acid (DNA), ribonucleic acid (RNA), and proteins (Kohanski et al., 2010). Unfortunately, the excessive use of antibiotics has led to the emergence of drug-resistant and even multi-drug-resistant bacterial strains (Kim et al., 2021a; Stiborova et al., 2018). Phototherapy has gained attention for its controllability and lack of resistance and is gradually being explored as an alternative strategy for antibacterial (Jana and Chatterjee, 2023; Jose et al., 2023; Liu et al., 2022a). As shown in Fig. 5, the fundamental mechanism of antibacterial phototherapy is illustrated. Unlike antibiotic therapy, the primary targets of phototherapy strategies are the bacteria's various structures and components rather than a single target, thus reducing the potential for resistance to develop. Most importantly, phototherapy produces localized high temperatures or ROS to which the bacteria cannot become resistant (Dalrymple et al., 2010; Ganguly et al., 2018). Therefore, phototherapy circumvents existing resistance mechanisms and is less likely to generate resistance.

During phototherapy, phototherapeutic agents are adsorbed on the bacterial surface or uptake by the bacteria in different ways, such as electrostatic interactions, hydrophobic interactions, and van der Waals forces (Ran et al., 2023). Among them, PTT raises the temperature of the surrounding environment (42–46 °C) by converting light energy into heat via PTAs, which leads to localized thermal damage to the bacteria, which suffer from stresses such as cell shape alteration, imbalance of membrane permeability, cytoplasmic leakage, protein denaturation, and cellular metabolism disruption, resulting in bacterial inactivation (Huo et al., 2021; Qi et al., 2022). In contrast to PTT, on the one hand, type I PDT occurs mainly in the bacterial cell membrane, leading to lipid peroxidation, disrupting bacterial structural integrity, and increasing ionic permeability of the cell membrane (Gehring et al., 2016). On the other hand, type II PDT generates the most threatening ROS ($^1O_2$), which directly causes oxidative damage to unsaturated lipids, DNA, enzymes, and other active molecules, thus effectively killing bacteria (Gnanasekar et al., 2023). Overall, PTT induces bacterial cell death primarily through localized hyperthermia, which leads to thermal damage of microbial cells. This damage can result in protein

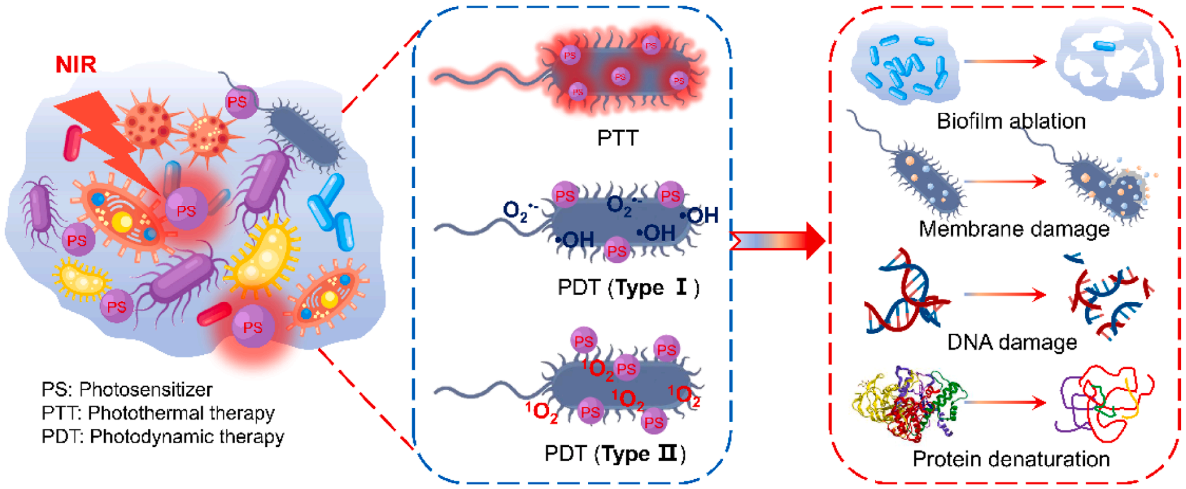

Fig. 5. General principal of antibacterial phototherapy.

denaturation, membrane disruption, enzyme inactivation and cell lysis. In contrast, PDT generates ROS upon light activation, which trigger oxidative stress and lead to bacterial apoptosis. These complementary mechanisms enable effective and targeted antimicrobial action.

In recent years, significant progress has been made in the development of organic fluorescent ligands for light-responsive antibacterial therapies. This review highlights recent advances in the design and application of these ligands for phototherapeutic antibacterial strategies. Key classes of compounds include cyclic tetrapyrroles, phenothiazinium salts, cyanine dyes, BODIPYs and aza-BODIPYs, as well as tetraphenylethene and triphenylamine derivatives. These tailored molecules offer promising avenues for targeted, efficient, and light-activated antimicrobial treatments. In this context, we provide a systematic overview of different types of antibacterial organic fluorescent ligands, as shown in Fig. 6, focusing on their working mechanisms, design strategies, and practical applications. The targets of action of different organic fluorescent ligands are also described in detail. Finally, the challenges and future development directions of antibacterial organic fluorescent ligands in clinical applications are presented.

1.5. Limitations of traditional phototherapy agents and advantages of near-infrared light in phototherapy

1.5.1. Limitations of conventional phototherapy agents

Despite the promising potential of phototherapy in antimicrobial applications, conventional phototherapy agents face several limitations that hinder their clinical translation and widespread use. One of the primary challenges is poor tissue penetration of visible light, which restricts the effectiveness of phototherapy to superficial infections and limits its utility in treating deep-seated bacterial infections (Zhang et al., 2024). Traditional PSs often absorb light in the visible spectrum (400–700 nm), which is strongly scattered and absorbed by biological tissues, resulting in suboptimal activation of the therapeutic agents.

Another significant limitation is phototoxicity and off-target effects, especially when high-intensity light or non-specific PSs are used (Lu et al., 2023; Luo et al., 2024). These can damage surrounding healthy tissues and provoke inflammatory responses. Additionally, many conventional PSs suffer from low photostability, rapid photobleaching, and poor solubility in physiological environments, which compromise their therapeutic efficacy and reproducibility (Wang et al., 2024b).

Moreover, limited selectivity toward bacterial cells over mammalian

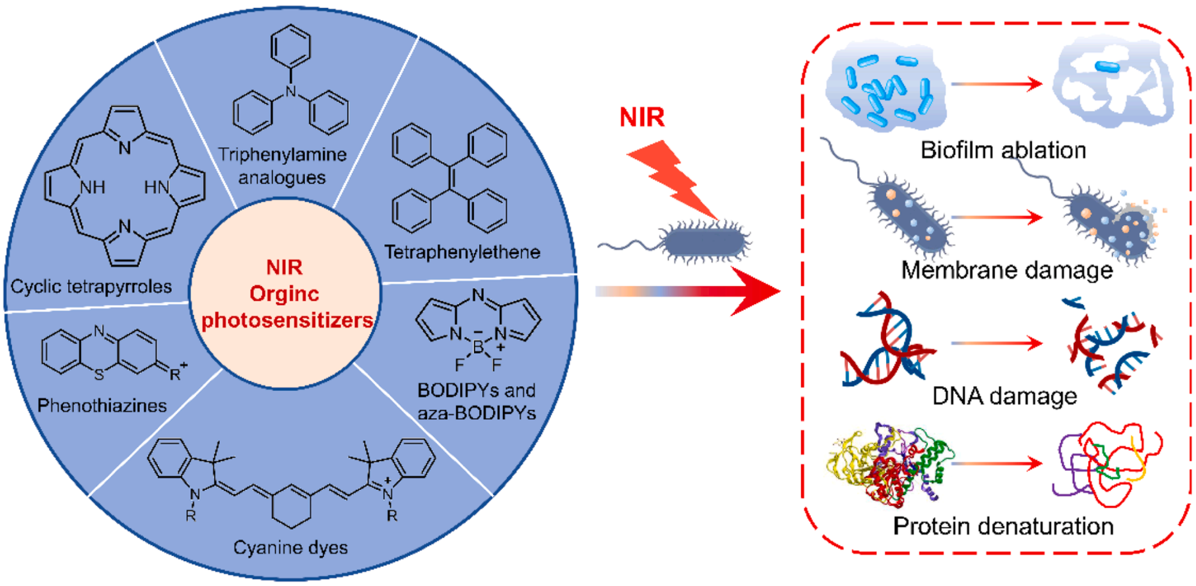

Fig. 6. Schematic illustration of different organic photosensitizers in phototherapeutic antibacterial and antibacterial mechanisms.

cells remains a concern (Ma et al., 2025; Xin et al., 2025). Without targeted delivery mechanisms, PSs may accumulate in non-infected tissues, reducing treatment precision. The inefficient generation of reactive ROS in hypoxic environments, which are common in infected tissues, further reduces the effectiveness of PDT (Abad-Montero et al., 2025; Zhou et al., 2025b).

Recent efforts have focused on overcoming these limitations through the development of nanomaterial-based PSs, which offer improved stability, targeted delivery, and enhanced ROS generation. However, challenges such as cytotoxicity of nanocarriers, complex synthesis, and regulatory hurdles still need to be addressed before these advanced systems can be widely adopted in clinical settings (Gao et al., 2023).

1.5.2. *Advantages of near-infrared light in biomedical and antibacterial phototherapy*

Near-infrared (NIR) light, particularly within the first (700–950 nm) and second biological windows (950–1450 nm), offers distinct advantages for biomedical applications, especially in antibacterial phototherapy (Nguyen et al., 2022). One of the most critical benefits is deep tissue penetration, which allows NIR light to reach infections located beneath the skin or within internal tissues. It is an area where visible light-based therapies fall short. This property significantly expands the therapeutic scope of phototherapy beyond superficial infections.

NIR light also exhibits low scattering and minimal absorption by endogenous chromophores such as haemoglobin and water, enabling more efficient activation of PSs and reducing collateral damage to healthy tissues (Banstola et al., 2025; Xu et al., 2025). Additionally, NIR-triggered phototherapy can be precisely controlled in terms of timing and localization, offering high spatiotemporal selectivity that is crucial for minimizing side effects (Wang et al., 2025c; Zhao et al., 2025).

Photosensitizers activated by NIR light, such as indocyanine green (ICG) and its derivatives (Hu et al., 2025), have demonstrated excellent photothermal conversion efficiency and robust ROS generation, making them suitable for both photodynamic and photothermal therapies. These agents also show low photobleaching rates, enhancing their stability during prolonged irradiation (Mahmut et al., 2023).

Furthermore, NIR-based therapies are compatible with image-guided treatment platforms, allowing real-time monitoring of therapeutic progress (Cheng et al., 2022; Tang et al., 2025). This integration of diagnostics and therapy, which is known as theranostics, is particularly valuable in personalized medicine and infection control.

The development of NIR-II (950–1450 nm) responsive nanomaterials is a rapidly growing field, offering even deeper tissue penetration and reduced background interference. These advancements are paving the way for more effective and minimally invasive treatments for drug-resistant bacterial infections (Thangudu and Su, 2025).

1.6. *The clinical progress of phototherapy in the treatment of antibiotic-resistant bacteria*

Extensive preclinical studies have thoroughly investigated the mechanisms of action of PDT and PTT, optimized therapeutic strategies, and laid the foundation for clinical translation. PDT and PTT exhibit broad-spectrum antimicrobial activity, effectively eliminating multidrug-resistant pathogens such as MRSA and carbapenem-resistant *Enterobacteriaceae* without readily inducing new drug resistance (Cheng et al., 2015; Song et al., 2015; Xue et al., 2017). Studies indicate that single-modality PDT or PTT exhibits limited penetration into mature biofilms (Wang et al., 2022c). Nanocarriers, such as liposomes or polymeric nanoparticles, can enhance penetration through biofilms. By boosting the accumulation of photosensitizers or photothermal agents within biofilms, synergistic PDT/PTT treatment can significantly disrupt biofilm structures (Zhang et al., 2025; Zhou et al., 2025a).

Preclinical studies reveal that PDT can activate local immune responses (Yang et al., 2020). PDT not only directly kills bacteria, but the ROS it generates and the resulting local inflammatory response also recruit and activate neutrophils and macrophages, promoting the clearance of residual bacteria and dead bacterial fragments. This “antibacterial immune” effect provides a new therapeutic dimension (Chen et al., 2025; He et al., 2024; Wang et al., 2023a). The thermal effect of PTT enhances tissue blood flow and drug delivery, significantly improving antimicrobial efficacy (Chen et al., 2020b). In animal models, localized PDT/PTT causes minimal damage to normal tissues, exhibits low systemic toxicity, and demonstrates high biological safety, making it particularly suitable for skin, wound, and mucosal infections (Li et al., 2023a; Liu et al., 2025).

With the advancement of basic research, the pace of clinical translation has accelerated, though it remains primarily focused on treatment trials for localized and superficial infections. Most studies are currently in the preclinical phase, but a small number of early-stage clinical trials have begun exploring treatments for localized infections. PDT primarily conducts localized clinical trials related to chronic wound infections, burn infections, and oral drug-resistant bacterial infections (Bassetti et al., 2020; Cesar et al., 2022). Multiple Phase I/II clinical trials have demonstrated the safety and preliminary efficacy of locally applied 5-aminolevulinic acid (ALA) or methylene blue (MB)-mediated PDT for treating diabetic foot ulcers and chronic venous ulcers complicated by drug-resistant bacterial infections. This approach significantly reduces bacterial bioburden in wounds and promotes healing (Early clinical (Phase I/II)) (Ferreira et al., 2024; Li et al., 2022c). PDT has also been adopted as an adjunctive therapy for treating oral drug-resistant bacterial infections such as peri-implantitis and refractory periodontitis, and has entered clinical practice. Randomized controlled trials support its additional benefits relative to conventional debridement (Clinically adopted adjunct therapy) (Alasqah, 2024; Xue et al., 2017). Small-scale clinical studies have begun exploring the combination of PDT with traditional antibiotics (e.g., for treating post-burn infections caused by drug-resistant bacteria) (Clinically adopted adjunct therapy) (Fang et al., 2025; Feng et al., 2021). Preliminary results indicate that this approach can shorten antibiotic treatment duration and improve patient outcomes.

PTT has been investigated for its clinical potential in treating skin and soft tissue infections, as well as in supporting diagnostic procedures. Based on animal safety and efficacy data from preclinical studies of gold nanoshells or nanorods, the first human Phase I safety study (e.g., NCT04240639) evaluating these gold nanomaterials with PTT for superficial abscesses has been initiated in recent years (He et al., 2018; Song et al., 2015). Some exploratory studies have utilized photothermal agents with photoacoustic imaging capabilities, such as gold nanorods, to achieve integrated visualization and precision treatment at infection sites, with preliminary confirmation of safety (Zarska et al., 2018; Zhao et al., 2017).

Despite ongoing research that has significantly advanced understanding of the antimicrobial mechanisms of PDT/PTT and substantially enhanced its efficacy against drug-resistant bacteria and biofilms through strategies like nanotechnology, early clinical trials have demonstrated clear promise in treating localized infections. However, translating these findings from the laboratory to widespread clinical application still requires breakthroughs in key bottlenecks such as deep tissue penetration techniques, long-term material safety, treatment standardization, and cost control. Future successful translation hinges on close collaboration among materials scientists, clinicians, and regulatory authorities.

1.7. *Clinical and societal impact of phototherapy-based antibacterial technologies*

The rise of antimicrobial resistance (AMR) has become a global health crisis, with projections estimating up to 10 million deaths annually by 2050 if effective countermeasures are not implemented (Cao et al., 2022). In this context, phototherapy-based antibacterial technologies offer a transformative alternative to conventional antibiotics, with the potential to reshape infection control strategies across clinical and public health domains.

Clinically, phototherapy, especially when mediated by NIR-responsive PSs, provides a non-invasive, resistance-free, and highly targeted approach to treating infections. It is particularly effective against biofilm-associated infections, which are notoriously resistant to antibiotics and prevalent in chronic wounds, implants, and surgical sites. The ability to avoid systemic drug administration also reduces the risk of side effects and drug interactions, making phototherapy suitable for vulnerable populations such as immunocompromised patients and the elderly (Wu et al., 2024).

From a societal perspective, the adoption of phototherapy could alleviate the burden on healthcare systems by reducing hospital stays, lowering treatment costs, and minimizing the spread of resistant pathogens. It also supports sustainable antimicrobial stewardship, as it does not contribute to the development of resistance—a major drawback of traditional antibiotics (de la Fuente-Nunez et al. 2023).

Moreover, the integration of phototherapy into portable and wearable devices opens new avenues for point-of-care treatment, especially in resource-limited settings (Wang et al., 2025a). This democratization of advanced antimicrobial technologies could significantly improve access to care in underserved regions.

As research continues to advance, interdisciplinary collaboration among chemists, microbiologists, engineers, and clinicians will be essential to translate laboratory innovations into real-world solutions. Phototherapy-based antibacterial technologies represent not only a scientific breakthrough but also a social imperative in the fight against drug-resistant infections. (Nguyen et al., 2022).

Collectively, this review synthesizes emerging strategies to address multidrug-resistant (MDR) bacterial infections, highlighting organic fluorescent near-infrared (NIR) ligands as a uniquely effective solution. These organic fluorescent NIR ligands address MDR bacteria by enabling photothermal and photodynamic therapies that generate localized hyperthermia and reactive oxygen species, producing a physicochemical, multi-target antibacterial attack that disrupts biofilms, eradicates diverse pathogens, and minimizes the likelihood of resistance development. Compared with inorganic nanomaterials, organic fluorescent ligands may offer superior biocompatibility, lower long-term toxicity, and greater structural tunability. Their chemical structures can be readily modified to optimize photophysical performance, bacterial targeting, and pharmacokinetics, thereby facilitating clinical translation. Coupled with the deep tissue penetration and low phototoxicity of NIR-II light, these advantages position organic fluorescent ligands as a more precise, flexible, and clinically viable platform for non-invasive antimicrobial phototherapy and future public health applications.

2. NIR organic photosensitizers applied in antibacterial phototherapy

To date, a lot of studies have reported the widespread use of natural and synthetic organic PSs in antibacterial phototherapy. Organic PSs have shown excellent antibacterial therapeutic effects in preclinical animal models due to their superior physical and chemical properties, good photostability, good biocompatibility and biodegradability, and ease of modification (Spagnul et al., 2015). In addition, researchers have designed PSs with targeting and response properties based on the microenvironment of the bacterial infection site and the structural properties of the bacteria. For example, due to the strong electronegativity of the bacterial cell wall, cationic groups were introduced into the PS structure to achieve high selectivity against bacteria (Yuan et al., 2014; Zhang et al., 2023a). This design strategy provides a theoretical reference for the development of PS for clinical applications. In this section, we focus on the NIR organic PSs developed for phototherapeutic antibacterial applications.

2.1. *Cyclic tetrapyrroles*

Cyclic tetrapyrroles are abundant in nature and are known as "life pigments" and are characterized by high photoconversion efficiencies and ease of chemical modification, including porphyrin, chlorine, and phthalocyanine (Anas et al., 2021; Nguyen et al., 2022). The ring center is often coordinated with metal atoms (e.g., Zn, Fe, Pd, Si, Co, Sn, and Ga) to improve the photoconversion efficiency. The positive charge on the surface of the cyclic tetrapyrrole is prone to form electrostatic or hydrophobic interactions with negatively charged cell membranes, showing a more effective inhibition of Gram-positive bacteria than Gram-negative bacteria (Nguyen et al., 2022; Zhang et al., 2023a).

The core structure of porphyrins and their derivatives consists of methane-bridged tetrapyrrole substituents, second-generation PSs (Zhang et al., 2018). Porphyrins, the first PS approved by the U.S. Food and Drug Administration (FDA), show excellent anticancer and antibacterial activity. They are water-soluble pigments, including heme proteins such as hemoglobin, cytochromes, and peroxidase (Fig. 7**a**), and can be excited in 600–690 nm. To increase the binding affinity with bacteria, researchers have modified the porphyrin structure by using cationic groups, targeting peptides, and cell-penetrating peptides (cationic antibacterial peptides or apidacin), which show stronger interactions with the bacterial cell wall and significantly enhanced phototoxicity upon light irradiation (Anas et al., 2021). The short excitation wavelengths of the porphyrin-based PS make them poor performers in treating deep bacterial infections. Researchers have also developed innovative strategies to enhance the NIR light responsiveness of porphyrin-based PS, thereby improving their antibacterial efficacy in deep tissue environments (Duan et al., 2023; Wang et al., 2025b).

In response to the differences in O_2 environments in different bacteria, Zhang's team designed a bacterial-responsive cationic porphyrin (TMPyP) that responds to a specific bacterium and then performs adaptive PDT/PTT (Fig. 7**b**) (Hu et al., 2022). In aerobic environments containing aerobic bacteria such as *Bacillus subtilis* and *Pseudomonas aeruginosa*, TMPyP functions as an effective PS. Under PDT, it achieves a bacterial killing efficiency exceeding 99.9%. TMPyP could be reduced in situ to rhizopiridin by reducing-capable parthenogenetic anaerobic bacteria (*E. coli* and *S. typhimuriun*) in anoxic environment, with strong NIR absorption and significant photothermal conversion, and possessed good antibacterial activity (Hu et al., 2022).

The self-assembly of porphyrins into nanoparticles enhances their phototherapeutic performance by increasing surface area for cellular interactions, improving light absorption intensity, and broadening the absorption spectrum. These features collectively contribute to more efficient and effective antibacterial phototherapy. Zhou *et al.* constructed a new Janus Au-porphyrin polymer vesicle (J-AuPPS) heterostructure via a simple one-step photocatalytic synthesis (Fig. 7**c**) (Chen et al. 2023a). A near-field enhancement (NFE) effect is realized between the porphyrin polymer vesicle (PPS) and gold nanoparticles in the J-AuPPS, which enhances its NIR light absorption and the strength of the electric/thermal field at the interface. As a result, J-AuPPS exhibits higher NIR-activated photothermal conversion efficiency (48.4%) and produces more oxygen in the single-line state compared to the non-Janus J-AuPPS (28.4%). As a result, J-AuPPS exhibits excellent dual-mode (PDT/PTT) antibacterial and anti-biofilm properties. Porphyrin-based POPs (PPOPs) are prepared by doping porphyrin into porous organic polymers (POPs). Compared to porphyrin monomers, PPOPs provide enhanced photostability and chemical stability, broadened light absorption region, and improved weak trapping ability due to their extended π-conjugated and hierarchical porous structure (Li et al., 2020a; Li et al., 2020b).

To solve the problems of shallow penetration ability of PSs organization as well as low yield, short lifetime, and short release distance of ROS. Zhang's team prepared a positively charged porous porphyrin-based organic polymer ($\text{FePPOP}_{\text{Hydantoin}}$) for resistance to bacterial infections via a Yamamoto cross-coupling reaction using Fe(III)-

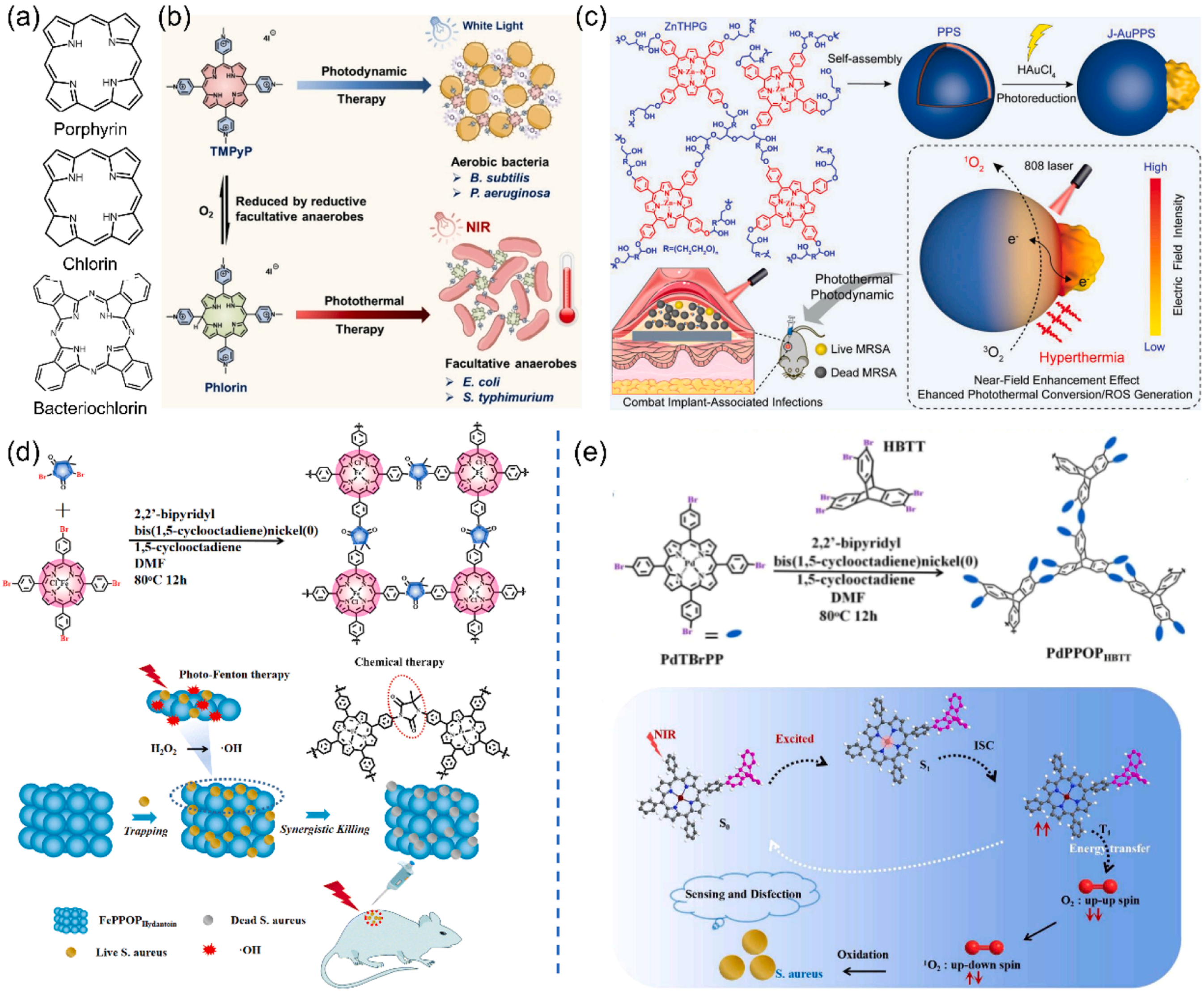

Fig. 7. (a) Chemical structures of antibacterial photosensitizers from the cyclic tetrapyrroles. (b) Schematic representation of bacterial response to TMPyP for adaptive PDT and PTT antibacterial (Hu et al., 2022). Copyright 2022, Wiley. (c) Schematic illustration of the preparation, electromagnetic NFE mechanism of J-AuPPS, and schematic diagram of PTT/PDT bimodal antimicrobial and biofilm ablation (Chen et al. 2023a). Copyright 2022, Wiley. (d) Schematic illustration of the synthesis of $FePPOP_{Hydantoin}$ and its photo-fenton and chemical antibacterial mechanism (Li et al., 2023c). Copyright 2023, Royal Society of Chemistry. (e) Schematic illustration of the $PdPPOP_{HBTT}$ synthesis process and the mechanism of $^1O_2$ production by PDT (Li et al., 2023b). Copyright 2023, Royal Society of Chemistry.

5,10,15,20-tetra-(4'-bromophenyl) porphyrinic acid (FeTBrPP) and hydantoin as monomers (Fig. 7**d**) (Li et al., 2023c). The extended π-conjugated framework in $FePPOP_{Hydantoin}$ gives it excellent peroxidase catalytic activity and NIR light-enhanced photo-Fenton activity. The introduction of hydantoin units also significantly enhanced the chemical antibacterial activity of $FePPOP_{Hydantoin}$. Such $FePPOP_{Hydantoin}$ can achieve synergistic antibacterial activity with photo-Fenton therapy and chemical therapy. The research team also designed a bifunctional POPs material based on porphyrin and trichothecenes ($PdPPOP_{HBTT}$) for the sensitive detection and eradication of bacteria (Fig. 7**e**) (Li et al., 2023b). $PdPPOP_{HBTT}$ has a hierarchical 3D porous structure and excellent NIR absorption, which produces a large amount of $^1O_2$ when irradiated by NIR light. $PdPPOP_{HBTT}$ has successfully achieved sensitive detection of *S. aureus* and efficient removal of *S. aureus* and *E. coli*.

Similar to porphyrins, chlorin is a dihydroporphyrin macrocycle consisting of three fully aromatic pyrrole rings and one partially reduced pyrrole ring (pyrroline). Compared to porphyrins, both chlorins and phthalocyanines exhibit stronger absorption in the red and NIR regions, enabling deeper tissue penetration and enhancing their suitability for phototherapeutic applications. Among them, chlorin e6 (Ce6) is a highly efficient photosensitizer widely used in PDT due to their low toxicity and ease of synthesis. However, its poor water solubility is the main reason hindering its application. To improve the water solubility of Ce6 as well as to enhance the PDT effect. Hu et al. designed a synergistic anti-biofilm system for the biofilm microenvironment (Fig. 8**a**) (Hu et al., 2020). Supramolecular nanocarriers (α-CD-Ce6-NO-DA) were prepared by the host-guest interaction between α-CD-based prodrugs (α-CD-NO and α-CD-Ce6) and the pH-sensitive copolymer PEG-(KLAKLAK)2-DA. The nanocarriers showed charge inversion and positively charged α-CD-Ce6-NO-DA in the acidic environment of the biofilm (pH=5.5), which effectively penetrated the biofilm and adhered to the negatively charged bacterial surface. After penetrating the biofilm, the nanocarrier can release NO triggered by glutathione (GSH) and continuously consume GSH. In addition, the NO can react with light-triggered $^1O_2$ to generate RNS ($ONOO^-$) with more vital bactericidal ability, further improving the PDT efficiency (Hu et al., 2020). Thus, the

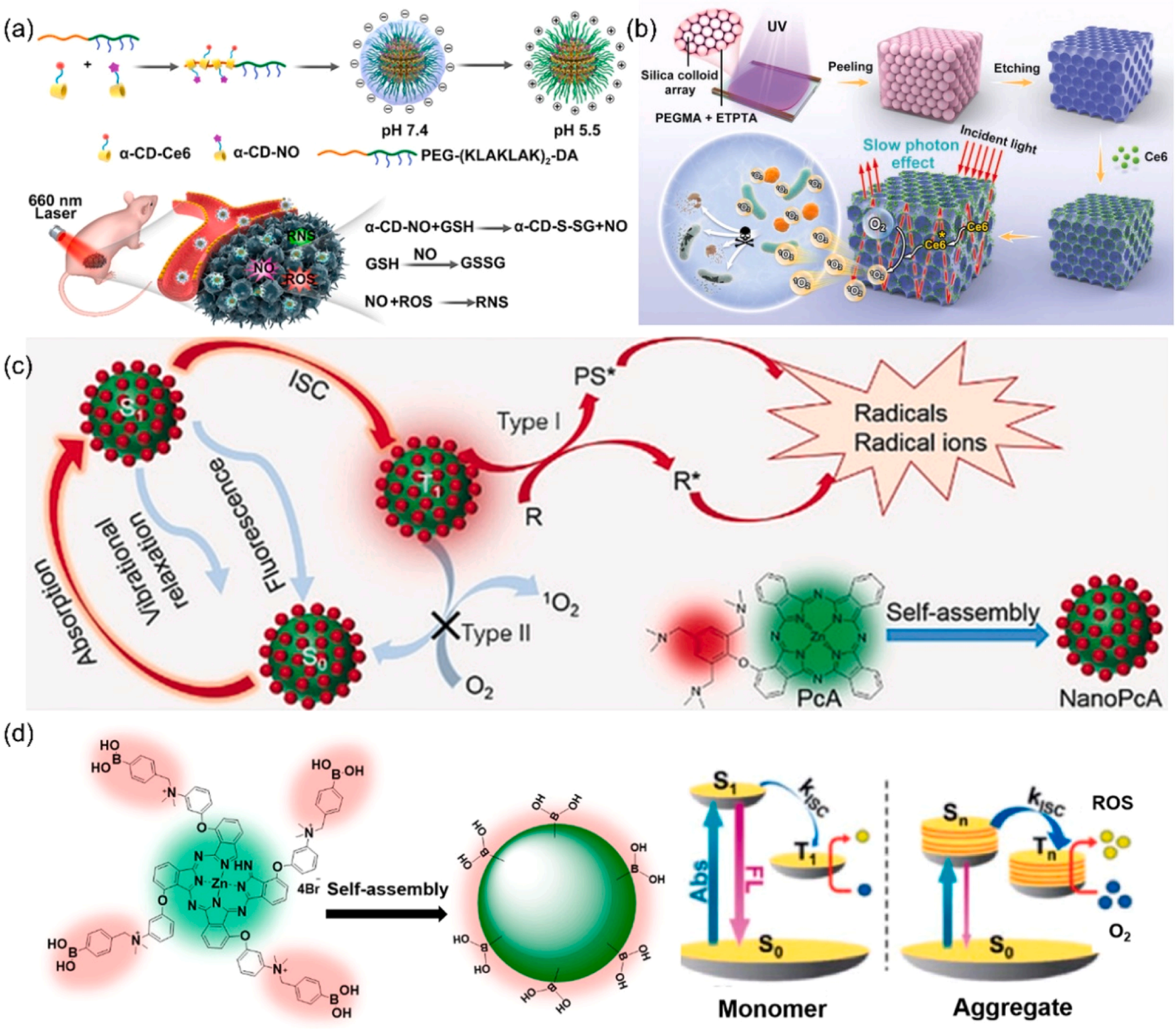

Fig. 8. (a) Schematic diagram of the preparation process of α-CD-Ce6-NO-DA nanocarriers and the related mechanism of synergistic eradication of MRSA biofilm by $^1O_2$ and NO. Copyright 2020, American Chemical Society (Hu et al., 2020). (b) Schematic illustration of decorating IOPG with Ce6 and its improvement of PDT antibacterial (Wang et al., 2023b). Copyright 2023, Wiley. (c) Preparation process of self-assembled phthalocyanine nanoparticles (NanoPcA) and photodynamic therapy mechanism (Li et al., 2018). Copyright 2018, Wiley. (d) Boronic acid modified phthalocyanine aggregation for enhanced photodynamic therapy (Lee et al., 2020). Copyright 2020, Royal Society of Chemistry.

supramolecular nanocarriers with switchable surface charges exhibited excellent NO synergistic photodynamic scavenging of MRSA biofilms.

To improve photodynamic antibacterial therapy (PDAT) limited by limited photon absorption and low quantum yield of PSs. Zhou's team prepared a blue-edge slow photon-enhanced PDAT platform based on IOPG decorated with Ce6 that can effectively utilizes light to inactivate bacteria (Fig. 8**b**) (Wang et al., 2023b). The generation efficiency of $^1O_2$ can be modulated by the relative positions of the photonic band gap (PBG) of the IOPG and the absorption band of Ce6. The slow-photon effect of Ce6/IOPG$_{694}$, combined with the effective dispersion of Ce6, results in an enhancement factor of up to a maximum of 69.5-fold under low-light irradiation when the blue edges of the PBG are matched to the absorption band of Ce6. The enhancement factor of Ce6/IOPG$_{694}$ showed improved antibacterial efficiency against *S. aureus* and *E. coli*. Ce6/IOPG$_{694}$ serves as the first proof-of-concept demonstrating that the blue-edge slow photon effect in IOPG can be utilized to design a promising platform for the promotion of $^1O_2$ production and enhancement of PDAT activity.

In addition, phthalocyanines are macrocyclic molecules similar to porphyrins with a main chain of isoindole substituents linked by a secondary amine bridge. Phthalocyanines have excitation wavelengths between 660 and 700 nm (Zheng et al., 2021). Like porphyrins, the self-assembly of phthalocyanines into phthalocyanine nanoparticles (NanoPcA) also promotes ROS generation, enhancing PDT(Zhao et al., 2021c). Yoon's team prepared self-assembled NanoPcA using 2,4,6-tris-(N, N-dimethylaminomethyl)phenoxy-substituted Zn(II) phthalocyanine as a monomer (Fig. 8**c**) (Li et al., 2018). Unlike conventional phthalocyanine-based PSs that are highly dependent on O_2, NanoPcA exhibited efficient type I photoreaction due to the presence of amino groups, generating abundant $O_2^{\bullet -}$ and exhibiting excellent photodynamic antibacterial activity against both *P. aeruginosa* and *E. coli*. Next, the research group used boric acid-modified phthalocyanine to synthesize boric acid-functionalized phthalocyanine (PcN4-BA) (Fig. 8**d**) (Lee et al., 2020). PcN4-BA exhibits an uncommon phenomenon, the aggregation-enhanced PDT effect. The intermolecular interactions in the aggregated state significantly reduce the energy gap between the singlet and triplet states (ΔE_{ST}). PcN4-BA efficiently generates ROS through both type I and type II photochemical reaction mechanisms. Therefore, PcN4-BA exhibits excellent performance in PDT antibacterial.

2.2. Phenothiazinium salts

Phenothiazines are a class of cationic dyes consisting of a tricyclic skeleton with strong absorption between 600 and 800 nm, mainly consisting of Methylene Blue (MB), Toluidine Blue (TB), and Nile Blue (NB) (Fig. 9**a**). Due to good photochemical and photophysical properties and their typical cationic nature, phenothiazines have been widely studied as antimicrobial PSs. Unlike Cyclic tetrapyrrole, phenothiazines have high bactericidal efficacy against both Gram-positive and Gram-negative pathogenic bacteria.

MB is a mono-cationic phenothiazine dye consisting of a tricyclic π-system with a chromatic side group and is a clinical treatment for chronic periodontitis and oral mucositis (Boccalini et al., 2017). Due to the complex environmental characteristics of the oral cavity (e.g., continuous salivation, mastication, tongue movement, etc.), it is difficult for existing MB delivery systems to be maintained at the lesion site to achieve long-term therapeutic effects, which leads to unsatisfactory antibacterial results and insignificant periodontal regeneration. Chen

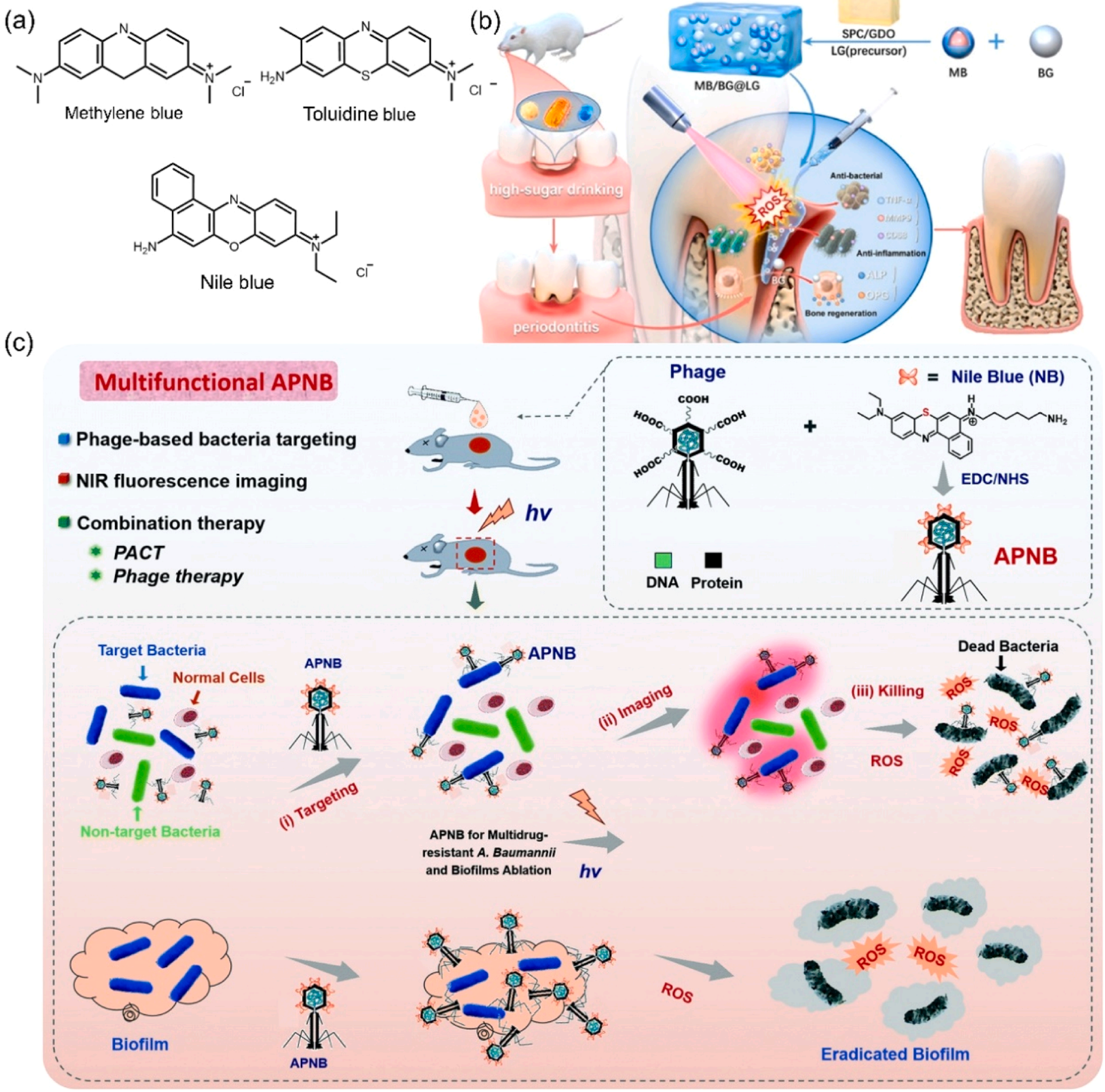

Fig. 9. (a) Chemical structures of antibacterial photosensitizers from the phenothiazinium salts. (b) Schematic illustration of the MB/BG@LG synthesis process and treatment of chronic periodontitis (Chen et al., 2023c). Copyright 2023, Elsevier. (c) Schematic diagram of a multifunctional antimicrobial system (APNB) based on ABP phage and NB for treating multidrug-resistant Acinetobacter *baumannii* infections and their biofilms (Ran et al., 2021b). Copyright 2021, Royal Society of Chemistry.

et al. developed a multifunctional slow-release drug delivery system (MB/BG@LG) by encapsulating MB and bioactive glass (BG) into a lipogel (LG) precursor via the Macrosol technology (Fig. 9**b**) (Chen et al., 2023c). MB/BG@LG sustains the release for 16 days and rapidly fills irregular bone defects caused by periodontitis via in situ hydration. Under 660 nm light irradiation, the ROS produced by MB can reduce the local inflammatory response by inhibiting bacterial growth and effectively promoting periodontal tissue regeneration. MB has been tried to treat other types of bacterial infections, such as drug-resistant urinary tract infections, in addition to dental applications (Huang et al., 2018).

TB and NB are organic PSs with excellent antibacterial properties widely used in dentistry (Ran et al., 2021a; Wainwright and McLean, 2017; Wainwright et al., 2016). photoactivated chemotherapy (PACT) often suffers from inefficient ROS generation and a lack of bacterial targeting ability, limiting its clinical application (Bonnet, 2023; Bretin et al., 2024). Peng's research team developed a unique NB and phage (ABP)-based photodynamic antimicrobial (APNB) for precise bacterial eradication and efficient ablation of biofilms (Fig. 9**c**) (Ran et al., 2021b). This NB photosensitizer was structurally modified with sulfur atoms, and it exhibited excellent ROS generation capability. In addition, phage can provide specific binding of APNB to pathogenic microorganisms, and the fluorescence of NB allows for easy assessment of the treatment process and real-time monitoring of the therapeutic efficacy. APNB has demonstrated remarkable results in combating multidrug-resistant *Acinetobacter baumannii* (MDR-AB) infections and biofilm ablation.

2.3. Cyanine dyes

Cyanine dyes are a class of excellent fluorescent dyes characterized by a conjugated organic small molecular system consisting of an odd number of carbon atoms forming a resonating methine conjugated chain and being terminated by two nitrogen-containing heterocycles (Fig. 10**a**). By leveraging the altered photophysical and chemical properties resulting from group protonation, researchers can facilitate electrostatic interactions between the photosensitizers and the negatively charged bacterial membrane surfaces, enhancing binding efficiency. Zhao *et al.* developed a pH-reversible asymmetric Cyanine-based near-infrared photosensitizer nano-encapsulated system for specific fluorescence imaging and photodynamic antibacterial at the site of bacterial infection (Zhao et al., 2020). The study used pH-reversible activated asymmetric cyanine (Acy) photosensitizer as the fluorescence imaging unit. It introduced a pyridinyldithio group (–S–S–Py), the mimic of allicin, as an auxiliary antibacterial group to further enhance its antibacterial effect (Acy–S–S–Py) (Fig. 10**b**). Based on this, the nanocapsule was self-assembled using distearyl phosphatidyl ethanolamine (DSPE) and functionalized polyethylene glycol (PEG) modified with 2,3-dimethylmaleic anhydride (DMMA), possessing switchable charges and intelligent targeting ability, encapsulating DSPE-PEG-DMMA@Acy–S–S–Py (Fig. 10**c**).

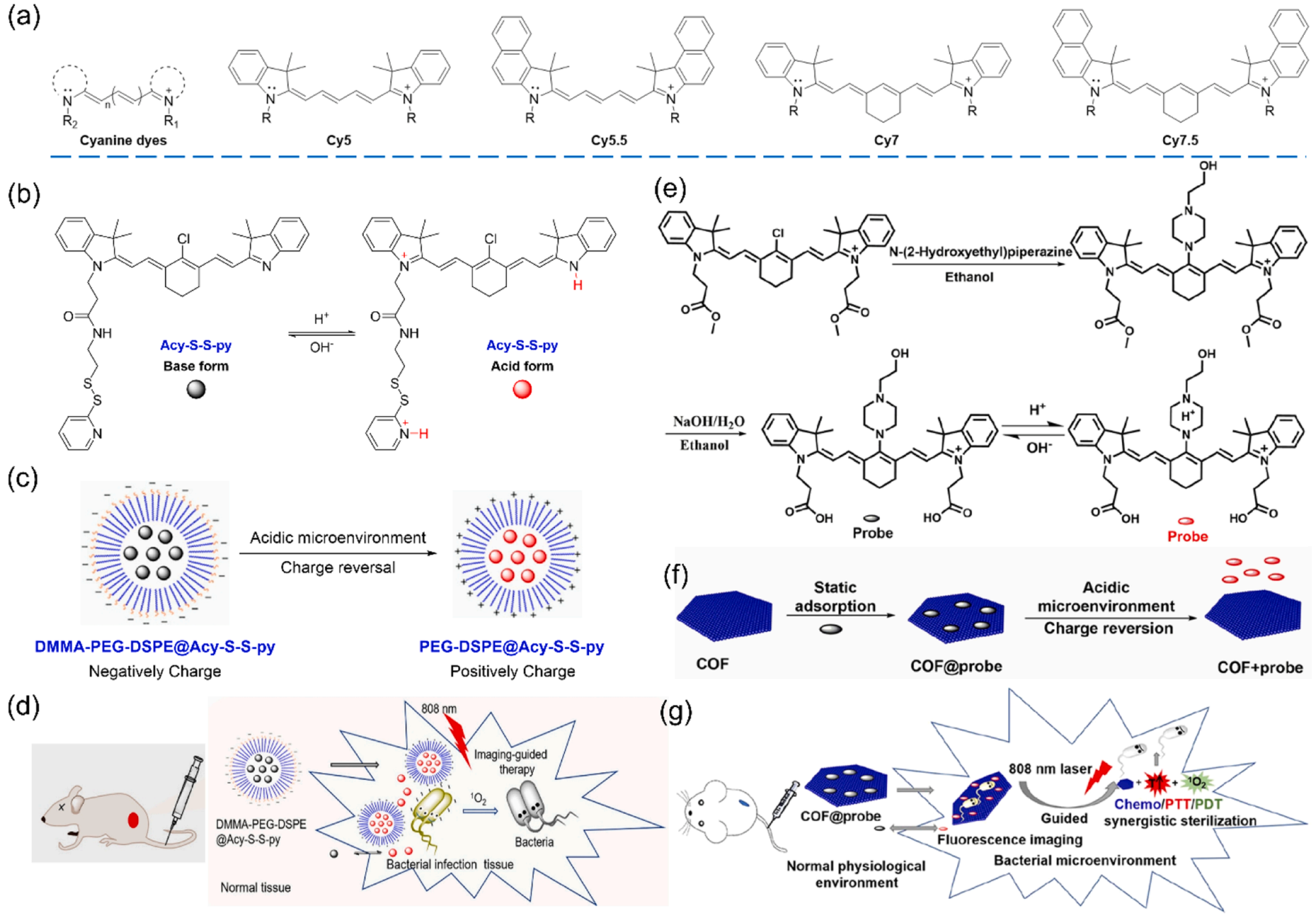

Fig. 10. (a) Chemical structures of cyanine dyes. (b) Schematic for the design and synthesis of the Acy-S-S-Py photosensitizer. (c) Schematic for the design and preparation of the DSPE-PEG-DMMA@Acy-S-S-Py nanocapsule. (d) Illustration of DSPE-PEG-DMMA@Acy-S-S-Py as a pH reversibly switchable theranostic platform for precision bacteria-targeting NIR fluorescence imaging-guided smart photodynamic sterilization (Zhao et al., 2020). Copyright 2020, American Chemical Society. (e) Synthetic route of the PTT/PDT-in-one agent. (f) Schematic diagram for preparing the COF@probe platform. (g) Illustration of the COF@probe theranostic platform for precision imaging-guided chemo/PTT/PDT synergistic sterilization. (Liu et al., 2021) Copyright 2021, American Chemical Society.

In a mouse model experiment, DSPE-PEG-DMMA@Acy–S–S–Py underwent charge conversion due to the acidic microenvironment (pH=5.5) at the site of bacterial infection, allowing for its "smart" targeting toward the site and achieving NIR fluorescence imaging of the bacterial infection site. Simultaneously, under acidic conditions (pH=6.0) and irradiation with 808 nm near-infrared laser (0.6 W cm^{-2}), significant $^{1}O_2$ production was observed, thereby achieving effective photodynamic antibacterial action against *S. aureus* (Fig. 10**d**). Moreover, the nanocapsule exhibited enhanced blood circulation to accelerate wound healing. The findings indicate that the nanocapsule effectively addresses the limitations of continuously activated photodynamic therapeutic agents, particularly in treating deep tissue infections and minimizing non-specific damage. This approach may offer a promising strategy for managing both skin infections and deep tissue inflammation.

Yan and co-workers developed a hydroxyethylpiperazine-modified NIR cyanine dye that enables targeted fluorescence imaging (FLI) at sites of bacterial infection. In addition to its imaging capabilities, the dye exhibits both photodynamic and photothermal antibacterial effects (Liu et al., 2021). Symmetric cyanine dyes with pH-reversible activation characteristics were synthesized (Fig. 10**e**), wherein the piperazine group undergoes protonation in the acidic microenvironment of the infection site, enabling targeted binding to carboxylic acid and phosphate groups on the bacterial cell membrane surface. This disrupts the charge balance of the bacterial membrane, leading to the rupture of the bacterial cell membrane. Therefore, these dyes serve as bacteria-specific imaging units and photosensitive and thermosensitive agents.

In addition, guanidine-based polymers possess cationic antimicrobial properties and interact with the bacterial cell membrane. A smart nanoplatform was constructed using guanidine-based covalent organic frameworks (COF) as the nanocarrier and chemotherapeutic drugs via electrostatic self-assembly (Fig. 10**f**). The piperazine-modified cyanine dye was loaded into an antibacterial active arginine-based COF lamella to create an intelligent therapeutic diagnostic platform (COF@probe) for detecting and treating bacterial infections. When COF@probe circulates to the infection site, the protonated cyanine dye probe is dissociated from the COF, leading to fluorescence restoration of the cyanine dye probe and activation of the photodynamic and photothermal properties of the piperazine-modified cyanine dye (Fig. 10**g**). This platform efficiently eradicates *S. aureus* and *E. coli* in infected wounds through combined chemotherapy, photodynamic, and photothermal antibacterial therapy, promotes blood circulation to accelerate wound healing, and exhibits minimal side effects, thus demonstrating great potential for practical applications.

Metabolic labeling strategy is a labeling technique that involves chemical molecules participating in cellular metabolic processes without damaging the cells (Zheng et al., 2024). Introducing D-amino acid groups as the basic component of bacterial cell walls can participate in peptidoglycan metabolism, explicitly labeling the peptidoglycan of bacterial cell walls. Li *et al.* developed a multimodal synergistic antibacterial therapy that combines metabolic labeling with photothermal and photodynamic effects (Li et al., 2022b). They coupled a commercially available NIR cyanine dye (IR820) with D-propargylglycine (a type of D-amino acid, DAA) to synthesize a PS (IR820-DAA) with metabolic labeling properties (Fig. 11**a**). IR820-DAA can be enzymatically embedded into the bacterial cell wall to achieve NIR metabolic labeling. Additionally, under 808 nm laser excitation, IR820-DAA exhibits a synergistic photothermal and photodynamic antibacterial effect.

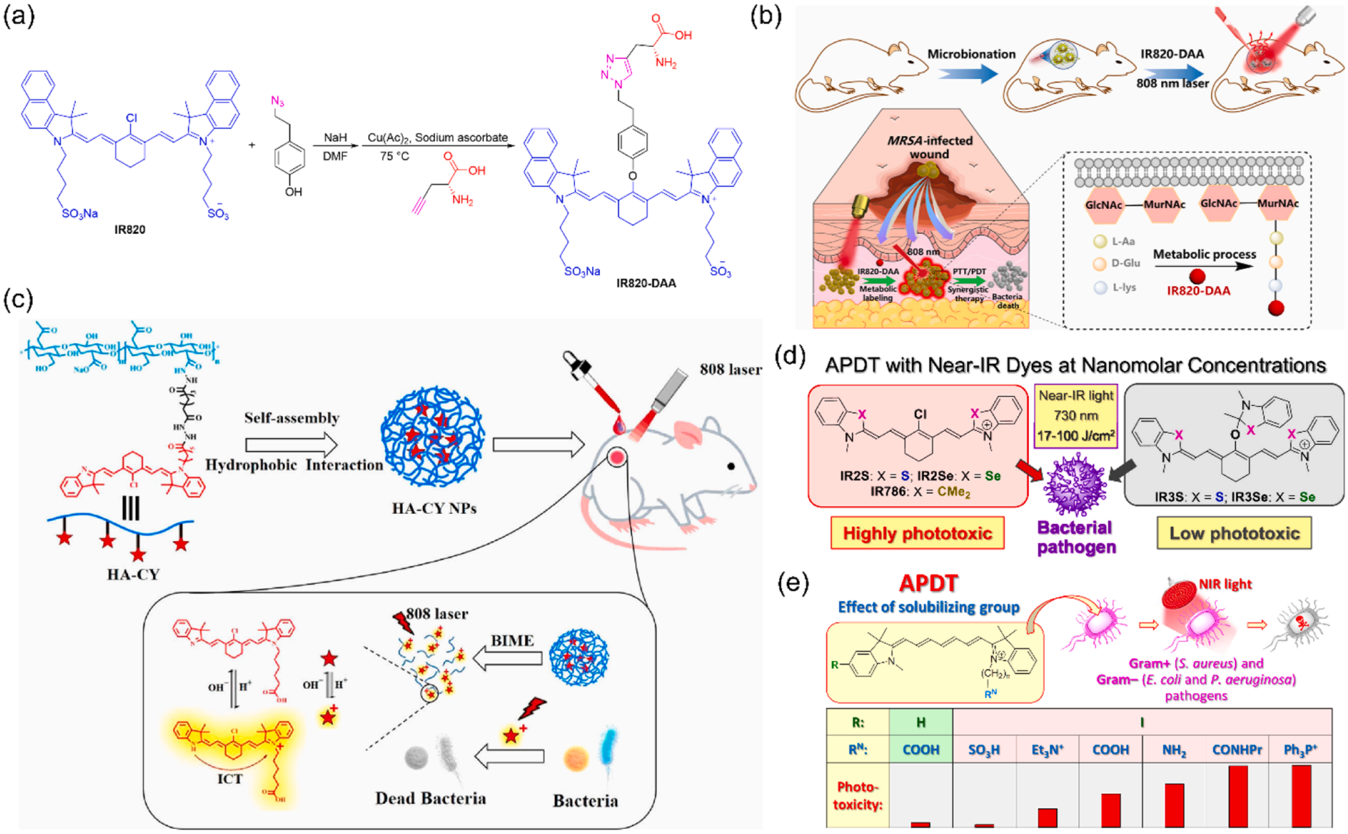

Fig. 11. (a) Synthetic route of IR820-DAA. (b) Schematic illustration of a metabolic labeling strategy for *in vivo* antibacterial therapy based on IR820-DAA (Li et al., 2022b). Copyright 2022, American Chemical Society. (c) Schematic concept of preparing HA-CY nanoparticles and their application for the PDT of bacterial infections (Huang et al., 2023a). Copyright 2023, American Chemical Society. (d) Schematic illustration of the structures and antimicrobial mechanisms of di- and tri-substituted cyanine compounds (Prakash et al., 2023). Copyright 2023, Elsevier. (e) Schematic illustration of the structures and antimicrobial mechanisms of solubilizing group cyanine derivatives (Semenova et al., 2023). Copyright 2023, MDPI.

After irradiation with an 808 nm laser, IR820-DAA is activated. It generates significant heat and ROS, resulting in approximately 70% clearance of methicillin-resistant *Staphylococcus aureus* (MRSA) biofilm, effectively eliminating *Staphylococcus aureus* and MRSA both *in vitro* and *in vivo*. The *in vivo* mouse model experiments demonstrate that IR820-DAA promotes wound healing without significant side effects (Fig. 11**b**). This study reveals a metabolic labeling-based synergistic antibacterial strategy, providing a new approach to the clinical treatment of bacterial infections.

Bacterial Infection Microenvironment (BIME) is a specific microenvironment in which bacteria reside. It includes characteristics such as the overexpression of hyaluronidase, hypoxia, and varying surface temperatures in certain bacteria (Huang et al., 2023b; Zhang et al., 2023d), in addition to the low pH and negatively charged bacterial cell membrane surface described in the studies. Huang *et al.* developed an acid-responsive near-infrared cyanine (HA-CY) nanoplatform by covalently coupling hyaluronic acid (HA) with acid-responsive cyanine units, aiming to enhance the antibacterial effect of photodynamic therapy (Fig. 11**c**) (Huang et al., 2023a). Under BIME conditions, due to the overexpression of hyaluronidase, the HA-CY nanoparticles dissociate, releasing cyanine PSs. Simultaneously, in the acidic BIME, cyanine dye undergoes protonation, allowing protonated cyanine dye to effectively attach to the negatively charged bacterial membrane surface and promote the generation of $^1O_2$ through intramolecular charge transfer (ICT). Under pH= 5.5 conditions, the bacterial biofilm treated with HA-CY+L achieved a clearance rate of approximately 90%, and inhibition rates of $> 99\%$ were observed against Gram-positive bacteria (*S. aureus*) and Gram-negative bacteria (*E. coli*). Animal experimental results showed that the wound healing rate in the HA-CY+L treatment group was significantly higher than in the other groups. Therefore, the nanoplatform with cascade BIME-responsive characteristics provides a new strategy for targeting bacterial infection sites and has tremendous potential for highly efficient photodynamic antibacterial therapy.

To develop NIR organic PSs with enhanced bactericidal activity, introducing heavy atoms such as bromine (Ciubini et al., 2019), iodine (Semenova et al., 2023; Zou et al., 2017), sulfur, silicon, and selenium (Magalhães et al., 2019) to improve bacterial phototoxicity. Prakash *et al.* introduced sulfur and selenium heavy atoms to construct a series of cyclohexene-based NIR cyanine dyes (Prakash et al., 2023), IR786 with indolenine di-substituted, IR2S with benzothiazole di-substituted, IR2Se with benzoselenazole di-substituted, IR3S with benzothiazole tri-substituted and IR3Se with benzoselenazole tri-substituted (Fig. 11**d**). Among them, the dyes with two substituted groups (IR2S and IR2Se) exhibited greater phototoxicity against bacteria than those with three substituted groups (IR3S and IR3Se). The cyanine dye IR2Se with two benzoselenazole groups could eradicate *S. aureus* at 5–10 nM concentrations and a NIR light dose of 33 $J{\cdot}cm^{-1}$. Furthermore, it could completely kill *E. coli* at a concentration of 10–25 μM and a NIR light dose of 200 $J{\cdot}cm^{-2}$, even at low doses of NIR light, maintaining good antibacterial activity.

The cyanine dyes also displayed good phototoxicity against *Staphylococcus aureus* at a concentration of 1 nM and a near-infrared light dose of 33 $J{\cdot}cm^{-2}$. Additionally, it exhibited significant dark toxicity against *E. coli* at a concentration of 10 μM. Therefore, the benzisoselenazole and benzothiazole cyanine dyes with two substituted groups, IR2Se and IR2S, can be further utilized to develop highly efficient photodynamic antimicrobial agents.

Furthermore, Semenova *et al.* synthesized a series of iodinated heptamethine cyanine dyes (ICy7) by introducing iodine atoms and different polar substituents (Semenova et al., 2023), including negatively charged carboxylic (ICy7COOH) and sulfonic ($ICy7SO_3H$) group, positively charged triphenylphosphonium ($ICy7PPh_3$) and triethylammonium ($ICy7NEt_3$), and neutral amide group (ICy7CONHPr) (Fig. 11**e**). Among them, the dyes with neutral and positively charged groups exhibited high phototoxicity against Gram-positive and Gram-negative bacteria at nanomolar and micromolar concentrations. The iodinated heptamethine dyes ICy7CONHPr and $ICy7PPh_3$ with positive charges could completely kill *Staphylococcus aureus* at a concentration of 0.05 μM and a lower near-infrared light dose of 33 $J{\cdot}cm^{-2}$. These photosensitizers effectively kill *E. coli* at a concentration of 50 μM with a light dose of 200 $J{\cdot}cm^{-2}$, and *Pseudomonas aeruginosa* at just 5 μM with a light dose of 100 $J{\cdot}cm^{-2}$. Therefore, the heavy atom effect increased the production of singlet oxygen, and the cationic group effect facilitated cellular uptake, contributing to a significant improvement in the photodynamic therapeutic efficacy of these PSs.

2.4. BODIPYs and aza-BODIPYs

Boron-dipyrromethene (BODIPY) is a crucial fluorescent organic dye with unique chemical and optical properties, such as a high molar extinction coefficient and fluorescence quantum yield. It has narrow absorption and fluorescence emission peaks, enabling high detection sensitivity in analytical applications. Due to its good structural stability, it has been widely applied as a fluorescent dye for biological labeling. The BODIPY structure contains multiple modifiable sites, and its wavelength can be red-shifted into the NIR region through conjugation. After being irradiated with NIR light, it releases absorbed photon energy mainly through fluorescence and non-radiative thermal relaxation, exhibiting good photoacoustic imaging and photothermal effects. However, its poor water solubility often requires the formation of nanostructures through encapsulation with hydrophilic chains for antibacterial phototherapy. Like BODIPY in structure, aza-BODIPY reduces the HOMO-LUMO energy levels by introducing a central nitrogen atom in its core ring. This compound exhibits a high absorption coefficient, near-infrared absorption (650–1060 nm), and easy structural modulation, making it widely used in near-infrared phototherapy (Fig. 12**a**) (Bai et al., 2019; Chen et al., 2018a; Chen et al., 2018b; Shi et al., 2020).

Song *et al.* prepared a asymmetric boron dipyrromethene (ABDP) probe encapsulated within cholesterol-modified polyethylene glycol polymer ($Chol\text{-}PEG_{2000}\text{-}NH_2$) to construct a dual-mode photothermal/photodynamic antimicrobial agent (ABDP NPs) (Song et al., 2022a), providing a new material for the treatment of MRSA infections (Fig. 12**b**). Under 808 nm NIR laser irradiation, ABDP NPs exhibited outstanding bactericidal efficacy against *S. aureus*, *E. coli*, and MRSA. Animal experimental results revealed that ABDP NPs exhibited excellent *in vivo* antibacterial capability against MRSA infections in mice while also preventing the formation of an inflammatory environment in MRSA-infected wounds and effectively promoting wound healing.

Yu *et al.* incorporated diphenylamine and benzo[*b*]thiophene as electron donors into the electron acceptor aza-boron-dipyrromethene (aza-BODIPY) and synthesized two NIR dyes, BDP-4PTZ and BDP-4DPA (Yu et al., 2021). The only difference between the two dyes is the connectivity of a sulfur (S) atom between the two benzene rings in BDP-4PTZ. Two nanocomposites with good water solubility and biocompatibility, BDP-4PTZ NPs and BDP-4DPA NPs, were prepared through co-precipitation with the hydrophilic polymer Pluronic® F-127 (Fig. 12**c**). Under 660 nm irradiation, BDP-4PTZ NPs and BDP-4DPA NPs exhibited good photothermal conversion efficiencies (43% and 50%, respectively) and reactive ROS generation performance (approximately 3.6 times and 6 times that of cyanine dyes). *In vitro* antibacterial experiments showed that both BDP-4PTZ NPs and BDP-4DPA NPs effectively disrupted bacterial membranes to eradicate drug-resistant bacteria. Furthermore, treatment with BDP-4DPA NPs after 660 nm irradiation effectively eliminated bacterial abscesses without adverse effects. Therefore, through precise molecular engineering, sulfur-free BDP-4DPA exhibited synergistic photothermal and photodynamic antimicrobial activity, offering promising potential for the development of effective antimicrobial phototherapies.

NO is the first discovered gaseous signaling molecule widely used to treat bacterial infections (Garren et al., 2021; Hibbard and Reynolds, 2020) and other areas. Researchers have extensively utilized photo-responsive N-nitrosoamine groups to develop NO donors for

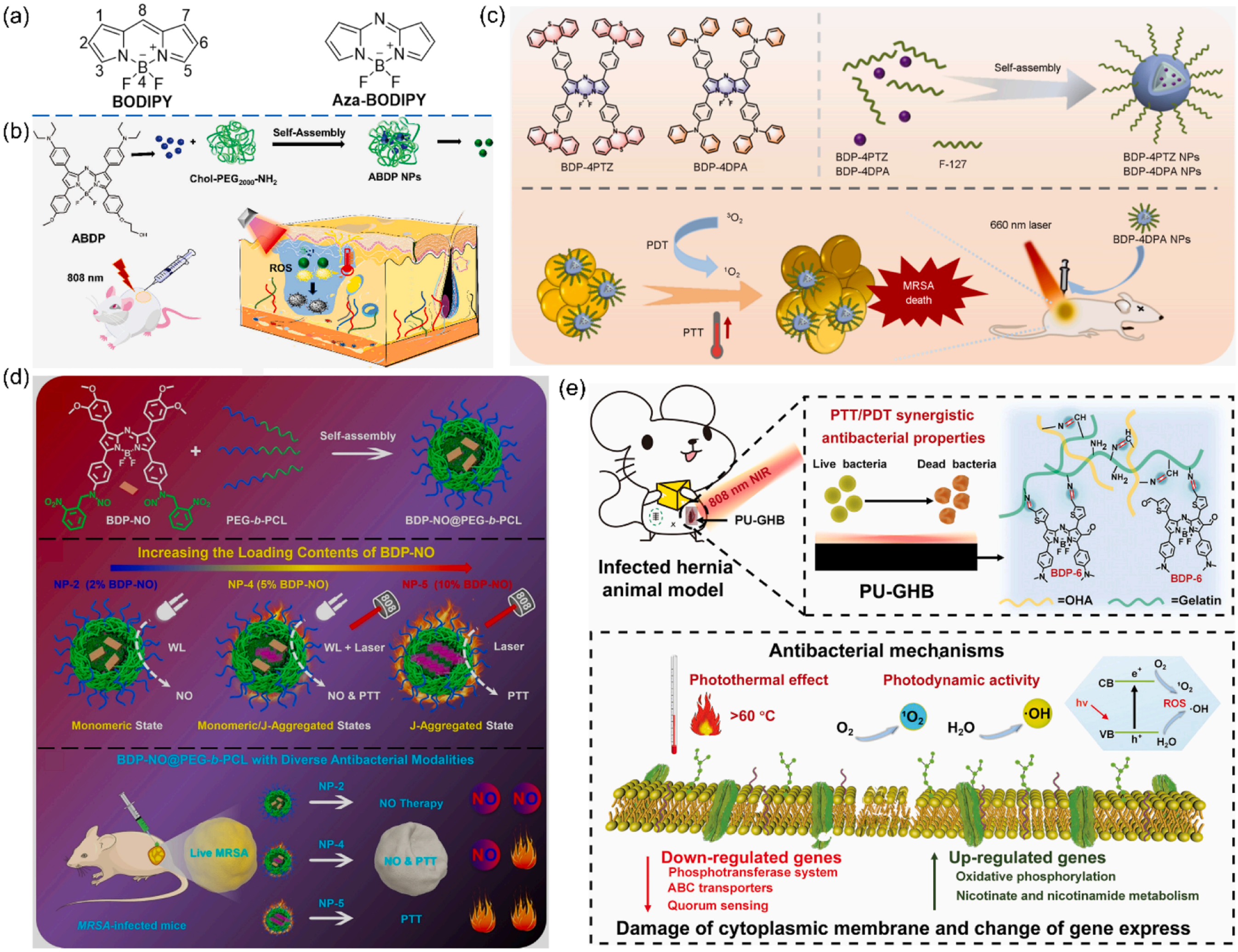

Fig. 12. (a) Chemical structure of BODIPY and aza-BODIPY. (b) Schematic representation of the preparation and application of the ABDP NPs for PTT/PDT synergic therapy of MRSA-infected mice (Song et al., 2022a). Copyright 2022, Springer Link. (c) Schematic illustration of the self-assembly of BDP-4DTZ and BDP-4DPA NPs and the synergistic photothermal and photodynamic antibacterial therapy (Yu et al., 2021). Copyright 2022, Springer Link. (d) Schematic illustration of BDP-NO@PEGb-PCL micelle nanoparticle assembly, regulation of BDP-NO aggregation state mediated by the content of BDP-NO within micelles, and its application in MRSA infection treatment (Bao et al., 2022). Copyright 2022, Wiley. (e) Schematic diagram of the synergistic antibacterial action of PU-GHB via PDT/PTT and its underlying mechanisms (Zhang et al., 2023b). Copyright 2023, Wiley.

achieving the localized NO release spatially and temporally controlled (Zhou et al., 2018) (Li et al., 2025). Additionally, J-aggregates are highly ordered assemblies of organic dyes that exhibit a red shift in peak fluorescence compared to monomeric dyes, making them widely applicable in fluorescence imaging. Bao *et al.* reported the synthesis of a near-infrared J-aggregate nanogel (BDP-NO@PEG-b-PCL) that releases NO (Bao et al., 2022) (Fig. 12**d**). By incorporating a photo-responsive aza-BODIPY structure unit onto the N-nitrosoamine moieties, a near-infrared J-aggregate was constructed, forming aza-BODIPY derivatives capable of releasing NO. The introduction of the *o*-nitrobenzaldehyde group effectively suppressed the intermolecular interactions of the BDP-NO aromatic groups. BDP-NO, capable of releasing NO, was encapsulated into PEG-b-PCL micellar nanoparticles, allowing for precise control over the aggregation state of BDP-NO, thus promoting the formation of J-aggregates within the microgel nanospheres.

BDP-NO@PEG-b-PCL was synthesized as a combination of NO release, PTT, or both, resulting in a multifaceted antibacterial approach. By modulating the loading capacity of BDP-NO within the microgel nanoparticles, both NO release and photothermal conversion efficiency (PTCE) could be finely tuned, thereby achieving multiple antimicrobial mechanisms, including individual utilization of NO release, PTT, or their combined effect. The combination of NO and PTT significantly enhanced the antimicrobial activity in the MRSA-infected mouse model. Integrating NO signaling molecules with near-infrared J-aggregates opens new avenues for biomedical applications.

Conventional organic molecules and compounds containing heavy metal atoms are typically limited by poor bleaching and low quantum yield, thus incapable of generating singlet oxygen (Sun et al., 2019; Turksoy et al., 2019). Inorganic carbon and silicon-based nanomaterials' limited long-wavelength absorption and poor biodegradability hinder their extensive study in PDT (Wu et al., 2019). To overcome these limitations, Zhang *et al.* developed a multifunctional antibacterial coating for medical devices using a heavy-atom-free BODIPY-based photosensitizer BDP-6 (Fig. 12**e**) (Zhang et al., 2023b). The aldehyde group of BDP-6 was covalently attached to the surface coating of the medical device. This antibacterial coating, known as PU-GHB, was prepared by combining BDP-6, oxidized hyaluronic acid (OHA), and gelatin into a film-forming solution, followed by crosslinking the amino groups of gelatins, BDP-6, and OHA on the surface of PU through a *Schiff* base. PU-GHB exhibited excellent *in vitro* PTT/PDT synergistic antibacterial performance against both sensitive and MDR bacteria. The antibacterial mechanism involved temperature elevation to decrease bacterial activity, disruption of bacterial cell membranes, and enhanced permeability of reactive oxygen species through the bacterial cell membrane. Furthermore, PU-GHB demonstrated significant anti-infective performance, good biocompatibility, and photoacoustic imaging properties in an infected abdominal wall hernia model.

2.5. Tetraphenylethene

Most hydrophobic PSs tend to aggregate in aqueous solutions, resulting in quenching and reduced production of $^1O_2$, consequently weakening the effectiveness of photodynamic antibacterial treatment (Du et al., 2022). Moreover, nanoparticles with enhanced penetration and retention properties do not fully accumulate at the infection site, leading to potential side effects on normal tissues using PSs. As a result, the combination of aggregation-induced emission PS and bacteria-targeting nanoparticles has gained significant attention (Gao et al., 2024; Zhu et al., 2022).

Tetraphenylethylene (TPE) is a well-known organic molecule with practical applications in various fields. It belongs to the class of

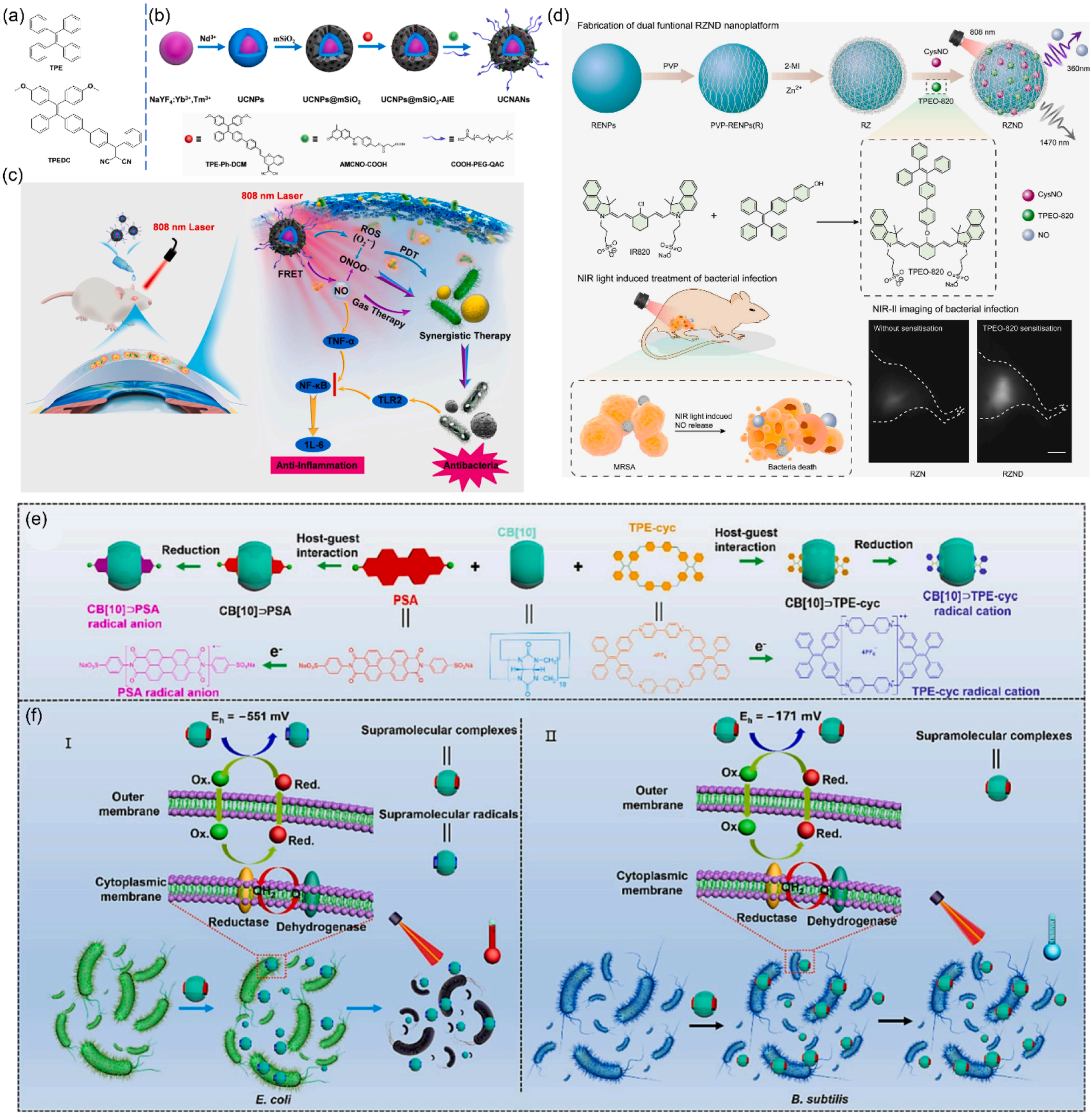

Fig. 13. (a) Chemical structure of TPE and TPEDC. (b) Schematic illustration of the synthetic route to UCNANs. (c)Schematic of UCNANs-mediated photodynamic therapy (PDT) and nitric oxide (NO) therapy for refractory keratitis (Zhang et al., 2022a). Copyright 2022, Elsevier. (d) Schematic illustration of the preparation of the dual-functional RZND nanoplatform and its application in NIR-II imaging and antibacterial treatment of MRSA infection sites, scale bar: 500 µm (Zhu et al., 2023). Copyright 2023, Elsevier. (e) Chemical structures of supramolecular complexes (CB [10]⊃PSA and CB [10]⊃TPE-cyc) and supramolecular radicals. (f) Schematic diagram of supramolecular radicals-mediated PTT to selectively fight against *E. coli* (I) over *B. subtilis* (II) (Wu et al., 2023). Copyright 2023, Elsevier.

π-conjugated molecules, characterized by a central core of four phenyl rings connected by ethylene linkers (Fig. 13**a**). TPE exhibits interesting optical properties, including aggregation-induced emission (AIE), which refers to the phenomenon of enhanced fluorescence upon aggregation. This unique property has gained significant attention in the field of materials chemistry. It has led to the development of various AIE-active compounds for applications such as bioimaging, optoelectronic devices, and sensing (Ren et al., 2025; Xu et al., 2023; Zhu et al., 2025).

PDT generates $O_2^{\bullet -}$, which not only kill bacteria directly but also react with NO to produce a more potent oxidizing and nitrosating agent, peroxynitrite ($ONOO^-$), with better antibacterial effects than NO, $O_2^{\bullet -}$, or even •OH (Deng et al., 2021; Wang et al., 2021). Zhang *et al.* developed a nanoplatform that combines NIR light response, NO therapy, and photodynamic therapy to treat refractory keratitis synergistically (Zhang et al., 2022a). This nanoplatform consists of upconversion nanocrystals (UCNPs) as the light-responsive core and mesoporous silica as the shell for loading aggregation-induced emission AIEgens photosensitizer TPE-Ph-DCM.

In addition, bacterial targeting molecule COOH-PEG-quaternary ammonium compound (COOH-PEG-QAC) and AMC-type NO donor (AMCNO-COOH) are connected to UCNP@mSiO_2-AIE through an amide reaction to form UCNANs. COOH-PEG-QAC can bind to the negatively charged portion of the bacterial cell wall through electrostatic interactions, leading to nanoparticle accumulation at the infection site (Fig. 13**b**) (Zhang et al., 2022a). Under 808 nm light irradiation, UCNANs convert NIR photons to UV and visible photons, which can be used to excite AMCNO to release NO and activate TPE-Ph-DCM to produce $O_2^{\bullet -}$. NO and $O_2^{\bullet -}$ can further react with each other to generate highly active $ONOO^-$ molecules, significantly enhancing the antibacterial ability. Moreover, UCNANs inhibit the expression of TLR2 and TNF-α, thereby suppressing the expression of NF-κB and further inhibiting the expression of pro-inflammatory cytokine IL-6, significantly suppressing the inflammatory response of the cornea (Fig. 13**c**) (Zhang et al., 2022a).

Electron transfer (ET) in prokaryotes is a crucial metabolic activity. At the end of the electron transport chain, electrons in the respiratory cells combine with oxygen through a series of redox reactions, generating transmembrane redox potential (Eh) (Benarroch and Asally, 2020), which is used to identify bacterial species and assess microbial growth stages. Based on this redox potential, the PS targeting specific bacterial redox environments was developed, providing new possibilities for selective antibacterial treatments.

Wu *et al.* constructed two water-soluble supramolecular complexes as NIR PS based on the redox potentials of bacteria and specifically killed facultative anaerobic bacteria (Wu et al., 2023). These supramolecular complexes (CB [10]⊃PSA and CB [10]⊃TPE-cyc) were constructed through host-guest interactions between CB [10] and a perylene diimide derivative (PSA) or a tetracationic cyclophane (TPE-cyc) (Fig. 13**e**). Under reducing conditions such as those present in facultative anaerobic bacteria like *E. coli*, their redox potentials were reduced to −551 mV, and CB [10]⊃PSA and CB [10]⊃TPE-cyc were *in situ* reduced to CB [10]⊃ PSA radical anion and CB [10]⊃TPE-cyc radical cation, respectively. The π-π stacking interactions between PSA of TPE-cyc and CB [10] were weakened, significantly enhancing the stability of the two supramolecular radicals. Under NIR light irradiation, both supramolecular radicals were activated and effectively killed *E. coli* through PTT. In contrast, the redox potential of aerobic bacteria *B. subtilis* could reach −171 mV, which is not able to reduce CB [10]⊃PSA and CB [10]⊃TPE-cyc to radicals, resulting in no significant phototherapeutic antibacterial effects (Fig. 13**f**). After killing bacteria, the supramolecular radicals are re-oxidized to supramolecular complexes by the surrounding air, with no toxic side effects on normal human cells.

Nitric oxide is regulated in various biological pathways and has been widely studied in antibacterial activity and wound healing (Xu et al. 2022a).

In addition, rare-earth-doped nanoparticles (RENPs) can serve as carriers for NO and convert NIR light to ultraviolet light. RENPs also exhibit down-conversion emission in the NIR-II, making them widely applicable for tissue imaging and drug release (Yan et al., 2022). Dye-sensitized RENPs possess excellent upconversion and down-conversion emission properties, making them widely used in deep tissue imaging and in situ generation of NO. Zhu *et al.* developed a hybrid nanoplatform utilizing dye-sensitized RENPs for enhanced NIR-II bioimaging and NIR light-triggered NO release in photodynamic therapy against MRSA (Fig. 13**d**) (Zhu et al., 2023). Initially, RENPs were modified with polyvinylpyrrolidone (PVP) and *in situ* introduced with zeolitic imidazolate framework-8 (ZIF-8) on the surface (RENPs@ZIF-8, referred to as RZ NPs). Subsequently, NO donors (CysNO) and near-infrared dyes (TPEO-820) were immobilized in ZIF-8 to sensitize RENPs and enhance their luminescent performance (Fig. 13**d**). Thanks to the large absorption cross-section and high extinction coefficient of the synthesized NIR dyes, the RENPs achieved a 102-fold enhancement in upconversion emission and an 8.5-fold increase in down-conversion emission within the NIR-II region (Zhu et al., 2023). The resulting RENPs@ZIF-8@CysNO@TPEO-820 nanoplatform (referred to as RZND) showed a 3.6-fold increase in NIR-II luminescence intensity compared to the non-sensitized nanoparticles (RZN) *in vivo*. When tested in a mouse leg abscess model, RZND demonstrated excellent antibacterial effects against MRSA under 808 nm light excitation (0.5 W cm^{-2}) (Fig. 13**d**).

Guanidinium-rich compounds can be applied as the universal biomimetic receptors targeting bacteria (Kim et al., 2021b). T780T, an efficient synergistic agent for PTT and PDT in NIR region, was developed (Zhao et al., 2021b). To enhance hydrophilicity and functionality, Qiao *et al.* incorporated positively charged guanidine (Gu) into the design of a NIR photosensitizer, resulting in the development of positively charged T780T-Gu (Fig. 14**a**) (Qiao et al., 2023). T780T-Gu can penetrate the biological membrane and bind to the polar surfaces of bacterial cell membranes through electrostatic interactions (Fig. 14**b**). Under 808 nm laser irradiation, T780T-Gu converts light energy into heat and ROS, leading to protein denaturation and cell membrane rupture. The results demonstrate that T780T-Gu exhibits synergistic antibacterial effects through PTT and PDT against *H. pylori* biofilm and multidrug-resistant clinical strains. Moreover, RNA-seq–based transcriptomic analysis was performed to investigate the antibacterial mechanism of T780T-Gu. The results indicate that phototherapy-induced antibacterial effects are primarily attributed to disruptions in cell integrity, metabolic processes, and cellular defense mechanisms.

The current PDT platforms primarily concentrate on visible light (400–700 nm) and NIR-I (700–1000 nm) (Chen et al. 2020a; Chen et al., 2023b; Luo et al., 2023; Wu et al., 2018; Xiao et al., 2022; Xiong et al., 2020). Nevertheless, limitations arise, including significant scattering, tissue absorption, low phototherapy efficiency, and restricted imaging and treatment depth. Thus, the development of NIR-II PS holds importance for deep tissue imaging. Due to aggregation-induced quenching and the poor stability of most NIR-II organic fluorophores, the advancement of NIR-II fluorescent dyes for phototherapy applications remains significantly constrained. Furthermore, only a limited number of AIEgens exhibit emission in the NIR-II region. This scarcity highlights the considerable potential for developing NIR-II AIEgens with strong fluorescence and high phototoxicity for advanced phototherapeutic applications.

In 2022, Xu *et al.* reported an AIE-based NIR-II photothermal diagnostic and therapeutic fluorophore called ZSY-TPE (Xu et al., 2020), which could be utilized for imaging and phototherapy. ZSY-TPE comprises a skeleton ZSY that emits NIR-II fluorescence or photoacoustic signals and a classic aggregation-induced emission fluorophore, TPE (Fig. 14**c**). It can be effectively applied for combined therapy against malignant tumors and bacterial infections by integrating PTT and PDT, both triggered by ROS and heat generated under 808 nm laser irradiation. This dual mechanism promotes cell apoptosis and pathogen elimination. (Fig. 14**c**).

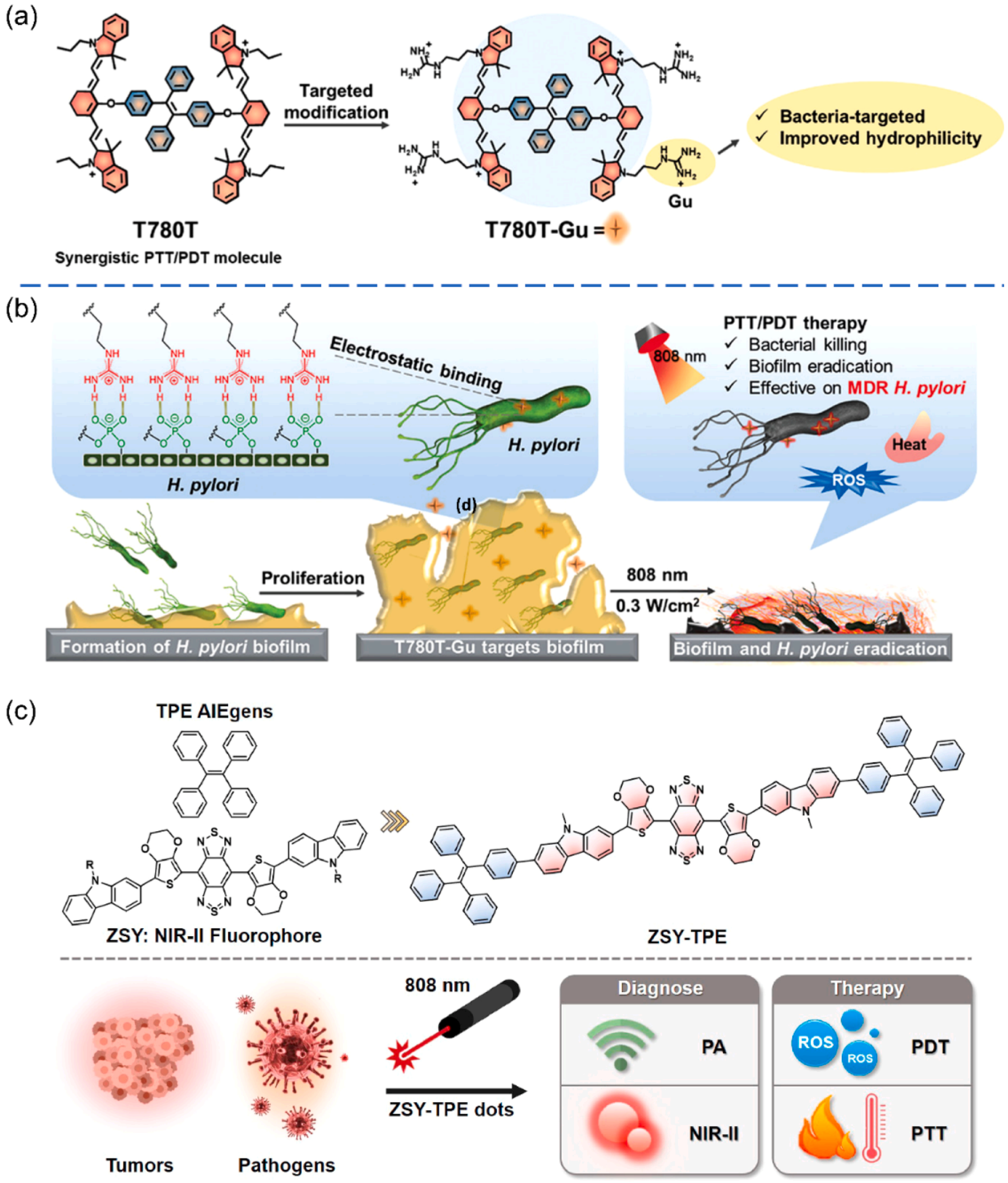

Fig. 14. (a) Schematic diagram of the T780T-Gu molecular design that combines the targeting ability of bacteria and hydrophilicity. (b) Eradication of *H. pylori* biofilms and MDR strains by synergistic PTT/PDT effect-mediated treatment with T780T-Gu (Qiao et al., 2023). Copyright 2023, Wiley. (c) Schematic illustration showing the design and biomedical application of single laser-activated ZSY-TPE (Xu et al., 2020). Copyright 2020, Elsevier.

2.6. *Triphenylamine analogues (TPA)*

Triphenylamine derivatives are commonly used as aggregation-induced emission PS for biomedical imaging and phototherapy. (Fig. 15a). Combining NIR PS and photothermal agents through nano-precipitation enables the integration of advantages from both photodynamic and photothermal antibacterial therapies, allowing for effective treatment of deep-tissue bacterial infections without significant

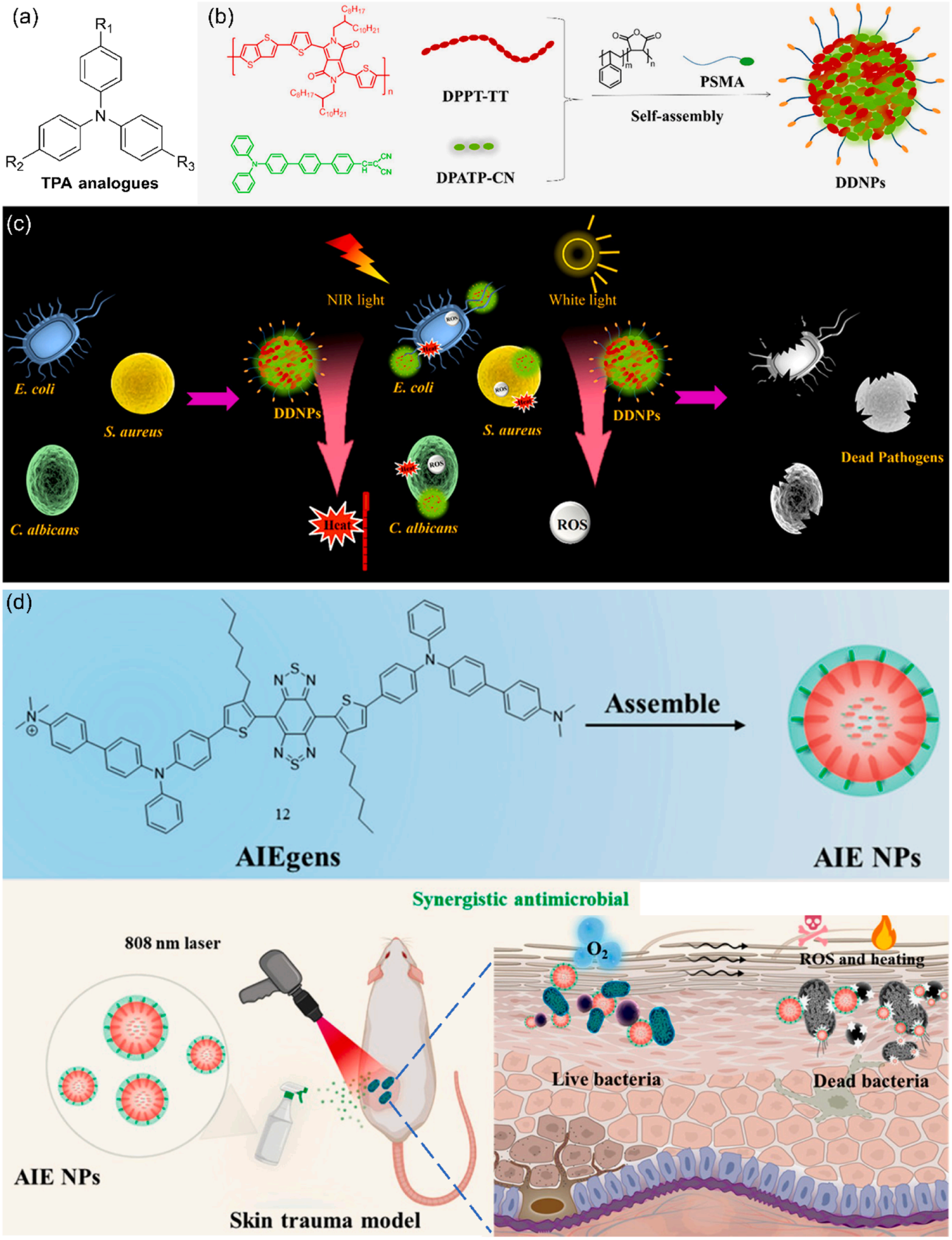

Fig. 15. (a) Chemical structure of TPA analogues. (b) Schematic diagram of preparation of DDNPs and chemical structures of DPPT-TT and DPATP-CN. (c) Schematic illustration of dual-modal activated DDNPs for synergistic photothermal and photodynamic killing of pathogens (Liang et al., 2020). Copyright 2020, American Chemical Society. (d) Synthesis of positively charged AIE NPs. (e) PTT and PDT mediated adhesive hydrogel show applications in wound healing (Wang et al., 2022b). Copyright 2022, American Chemical Society.

cytotoxicity to normal tissues. Liang *et al.* developed dual-doped nanoparticles (DDNPs) containing a photothermal-conjugated polymer (DPPT-TT) and a triphenylamine derivative (DPATP-CN) (Fig. 15**b**) (Liang et al., 2020). DDNPs convert light energy into high heat under 808 nm light irradiation. It also generates ROS in the presence of ambient oxygen under white light irradiation. Under combined irradiation of NIR and white light, DDNPs effectively eradicated *E. coli*, *S. aureus*, and *C. albicans* (Fig. 15**c**).

Incorporating near-infrared AIE PS into nanomaterials can address the poor solubility issues of traditional photosensitizers while enabling targeted antibacterial therapy. Using PTT and PDT dual modes enhances the light-triggered antibacterial strategy, effectively reducing the heat and activator or oxidizer required for light therapy. Wang et al. developed targeted bacteria-specific AIE nanoparticles (AIE-NPs) with high water solubility, good biocompatibility, and excellent photostability, enabling bacterial PTT and PDT combined therapy under 808 nm light irradiation (Fig. 15**d**) (Wang et al., 2022b). The introduction of a positively charged functional group ($–N^+Me_3$) into the PS with AIE results in a highly distorted structure. The compound was found able to target bacteria and generates 1O2 and heat, achieving antibacterial rates of 99.9% and 99.8% against S. aureus and E. coli, respectively. Also, in vivo experiments have shown that PTT and PDT dual-mode treatment triggered by such AIE NPs could eliminate Staphylococcus aureus and accelerate the healing of bacterial-infected skin wounds (Fig. 15**e**).

3. Summary and outlook

In this review, we have highlighted recent advances in photosensitizers for phototherapeutic antibacterial applications, encompassing a diverse range of molecular classes such as cyclic tetrapyrroles, phenothiazinium salts, cyanine dyes, BODIPYs and aza-BODIPYs, tetraphenylethene, and triphenylamine analogues. These PSs have been engineered to address the unique challenges posed by bacterial infections, including hypoxic microenvironments, acidic pH, elevated levels of GSH and hydrogen peroxide (H_2O_2), and the structural complexity of bacterial cell walls and biofilms.

Innovative strategies have emerged to enhance the therapeutic efficacy and safety of PSs, including molecular modifications, nanomaterial integration, and microenvironment-responsive designs. Mechanistic insights into PS activation, target specificity, and antibacterial pathways have been thoroughly discussed. In addition, Table 1 provides a comprehensive overview of key components in antibacterial phototherapy, including advanced PSs, therapeutic agents, light sources, target sites, clinical applications, and treatment modalities.

Despite notable progress, even some PSs having entered clinical trials currently, several critical challenges remain before widespread clinical adoption can be realized:

(1) Limited tissue penetration: The shallow penetration depth of UV and visible light restricts phototherapy to surface-level infections. This limitation hinders treatment of deep-seated infections such as pneumonia or enteritis. To overcome this, NIR light–excited PSs, particularly those operating in the second NIR window (NIR-II, 1000–1700 nm), offer deeper tissue penetration and reduced phototoxicity. In addition, UCNPs, which absorb NIR light and emit shorter wavelengths, can serve as energy transducers to activate PSs in deeper tissues, expanding the therapeutic reach of phototherapy. Notably, advances in flexible optical fibers and medical endoscopy technology have made it possible to precisely deliver therapeutic light to deep-seated lesions within the body (Sun et al., 2025). This "intracavitary photodynamic antimicrobial therapy" offers a highly promising new strategy for treating deep infections caused by drug-resistant bacteria. Its feasibility has been thoroughly validated in preclinical mouse models of pneumonia and enteritis. Taken together, the development of NIR photosensitizer platforms and innovations leveraging fiber optics and endoscopy are enabling near-infrared photodynamic antimicrobial therapy to overcome tissue penetration limitations. This approach is emerging as a highly promising, precise, minimally invasive treatment strategy against deep-seated drug-resistant bacterial infections, with its clinical translation progress accelerating.

(2) Hypoxia in infection sites: Most PSs rely on oxygen-dependent Type II mechanisms, which are less effective in hypoxic environments typical of bacterial infections. To address this, Type I PSs that generate reactive radicals independent of oxygen are being developed. Moreover, nanocarriers that deliver exogenous oxygen or nanoenzymes that catalyze endogenous H_2O_2 into oxygen can significantly enhance phototherapeutic efficacy under hypoxic conditions (Alamer and Nasiruzzaman, 2024; Ali et al., 2025).

(3) Target specificity and safety: Many PSs target bacterial membranes based on membrane potential, which risks collateral damage to host cells. Recently, researchers invented a smart responsive photosensitizer by combining a photosensitizer "prodrug" with specific responsive groups. This innovation utilizes bacterial-specific biochemical signals (such as specific enzymes: nitroreductase (Ran et al., 2024), β-lactamase (Luo et al., 2025), lipase (Song et al., 2022b), and hyaluronidase (Ran et al., 2017) or microenvironmental factors like weak acidity (Liu et al., 2024), high H_2S concentration (Wang et al., 2024a), and reducing conditions (Oldroyd et al., 2024)) as "triggers". This induces irreversible chemical changes in the prodrug molecules (e.g., bond cleavage, reduction, protonation), thereby restoring or enhancing their photophysical properties (absorption, fluorescence, inter-system crossing), ultimately achieving efficient, in situ ROS generation for targeted antibacterial action. Taken together, the targeted and enzyme-responsive/bacteria-triggered smart photosensitizers represent a powerful strategy to overcome drug resistance and enhance antibacterial selectivity. Future designs should focus on enhancing bacterial specificity through ligand-receptor targeting, enzyme-responsive activation, or exploiting unique bacterial metabolic pathways.

(4) Limitations of monotherapy: Phototherapy alone may be insufficient to eradicate bacteria and disrupt resilient biofilms. Synergistic approaches, such as combining phototherapy with chemotherapy, immunotherapy, or emerging gas therapies (e.g., nitric oxide, carbon monoxide, hydrogen), can amplify antibacterial effects. Gas-light synergistic therapy, for instance, leverages the diffusibility and bioactivity of therapeutic gases with the precision of light activation, offering a promising avenue for treating complex infections.

(5) Adaptability to complex *in vivo* microenvironments: Preclinical models cannot fully replicate the intricate microenvironments encountered during human infections (such as light absorption and scattering by necrotic tissue, pus, and blood), which may significantly diminish actual therapeutic efficacy *in vivo*.

(6) Lack of standardized and individualized treatment protocols: Parameters such as light power, drug dosage, and timing of exposure are highly dependent on infection type, location, and bacterial species, yet no widely accepted standardized treatment protocols have been established. In addition, there is a lack of clinical data to guide the impact of individual variations—such as tissue optical properties—on treatment efficacy.

(7) Cost-effectiveness and accessibility: Many novel nano-photodynamic/photothermal agents involve complex synthesis processes and high production costs, and their application requires specialized light-emitting equipment. These factors limit their adoption in primary healthcare facilities or resource-constrained regions.

Looking forward, the field of phototherapeutic antibacterial research is poised for transformative breakthroughs. Continued innovation in photosensitizer design, coupled with advanced delivery strategies, holds the key to overcoming current limitations and unlocking new clinical possibilities. In an era marked by escalating antibiotic resistance, phototherapeutic antimicrobials offer a powerful, non-invasive alternative for combating bacterial infections.

Interdisciplinary collaboration, including but not limited to chemistry, nanotechnology, microbiology, and clinical medicine, is essential for the development of next-generation photosensitizers that are highly selective, minimally toxic, and therapeutically robust. The integration of smart nanocarriers, real-time imaging technologies, and stimuli-responsive activation mechanisms will further enhance the precision

Table 1
Summary and potential applications of NIR organic photosensitizers for phototherapeutic antibacterial.

Photosensitizers	Phototherapy agent	Light source	Target site	Application		Antibacterial mechanism	Ref.
				Organism (Antimicrobial efficiency)	Model		
Cyclic tetrapyrroles	TMPyP	730 nm (1.0 W cm^{-2})	Cell membrane	*E. coli* and *S. typhimuriun* (All >99.9%)	Subcutaneous abscesses	PDT (II) / PTT	(Hu et al., 2022)
	J-AuPPS	808 nm (1.0 W cm^{-2})	/	MRSA (97.76%)	Implant-associated infection	PDT (II) + PTT	(Chen et al. 2023a)
	FePPOP$_{\text{Hydantoin}}$	808 nm (0.7 W cm^{-2})	Cell membrane	*S. aureus* (> 99.9%)	Skin wound infection	Photo-Fenton therapy	(Li et al., 2023c)
	PdPPOP$_{\text{HBTT}}$	808 nm (0.7 W cm^{-2})	Cell membrane	*S. aureus* and *E. coli* (All nearly 100%)	Skin wound infection	PDT (II)	(Li et al., 2023b)
	α-CD-Ce6-NO-DA	660 nm (0.2 W cm^{-2})	Cell membrane	MRSA (>90%)	Subcutaneous infection	PDT (II) + NO	(Hu et al., 2020)
	Tph-BDP-COF	808 nm (2.0 W cm^{-2})	/	*E. coli* (97%)	/	PDT + PTT	(Zhao et al., 2023)
	Pc-pDMAEMA-C4	680 nm (0.64 W cm^{-2})	Cell membrane	*S. aureus* and *E. coli* (>95% and >78%)	Skin wound infection	PDT (II)	(Xu et al., 2022b)
	TFPP-QA/CP5	660 nm (0.4 W cm^{-2})	Cell membrane	MRSA and *E. coli* (>95% and >78%)	Skin wound infection and biofilm catheter	PDT	(Xia et al., 2022)
	Ce6/IOPG	665 nm (20 mW cm^{-2})	/	*S. aureus* and *E. coli* (94.5% and 91.5%)	/	PDT (II)	(Wang et al., 2023b)
	NanoPcA	655 nm (0.4 W cm^{-2})	Cell membrane	MR S. *Aureus* and ESBL *E. coli* (All 100%)	/	PDT (I)	(Li et al., 2018)
	PcN4-BA	655 nm (0.4 W cm^{-2})	Cell membrane	MR S. *Aureus* and ESBL *E. col* (All nearly 100%)	/	PDT	(Lee et al., 2020)
Phenothiazinium salts	MB/BG@LG	660 nm (0.1 W cm^{-2})	/	*S. aureus* and *E. coli*	Chronic periodontitis	PDT	(Chen et al., 2023c)
	C$_{12}$-MB	660 nm (30 mW cm^{-2})	Cell membrane	*P. aeruginosa and S. aureus* (73% and 70%)	/	PDT (II)	(Zhang et al. 2022b)
	NBS-N, NBSe-N	665 nm (50 mW cm^{-2})	/	*S. aureus* and *E. coli* (>67% and >50%)	Skin wound infection	PDT	(Wu et al., 2022)
	APNB	660 nm (20 mW cm^{-2}	/	MRAB (97%)	Skin wound infection	PDT	(Ran et al., 2021b)
Cyanine Dye	PEG-DSPE@Acy-S-S-py	808 nm (0.6 W cm^{-2})	Cell membrane	*S. aureus* and *E. coli* (All >99.9%)	Subcutaneous infection	PDT	(Zhao et al., 2020)
	COF@probe	808 nm (0.6 W cm^{-2})	Cell membrane	*S. aureus* and *E. coli* (All >95%)	Subcutaneous infection	Chemo, PTT, and PDT(II)	(Liu et al., 2021)
	IR820-DAA	808 nm (1.0 W cm^{-2})	biofilm and cell wall	MRSA (98%)	Skin wound infection	PTT + PDT (II)	(Li et al., 2022b)
	HA-Cy	808 nm	biofilm and Cell membrane	*S. aureus* and *E. coli* (All >99%)	Skin wound infection	PDT (II)	(Huang et al., 2023a)
	IR2S, IR2Se and IR786	730 nm (33 J cm^{-2} for *S. aureus* and 200 J cm^{-2} for *E. coli*)	Cell membrane	*S. aureus* and *E. coli* (All >99%)	/	PDT	(Prakash et al., 2023)
	ICy7CONHPr and ICy7PPh$_3$	730 nm (56 W cm^{-2})	Cell membrane	*S. aureus*, *E. coli* and *P. aeruginosa* (All >99%)	/	PDT	(Semenova et al., 2023)
aza-BODIPY	ABDP NPs	808 nm (2.0 W cm^{-2})	Cell membrane	*S. aureus*, *E. coli*, and MRSA (All >99%)	Skin wound infection	PTT + PDT	(Song et al., 2022a)
	BDP-4PTZ NPs and BDP-4DPA NPs	660 nm (0.7 W cm^{-2})	Cell membrane	*S. aureus*and MRSA (All >99%)	Bacterial abscess	PTT + PDT (II)	(Yu et al., 2021)
	BDP-NO@PEG-*b*-PCL	808 nm (375 mW cm^{-2})	Cell membrane	*S. aureus*, *E. coli*, and MRSA (All >99%)	Bacterial abscess	PTT + PDT	(Bao et al., 2022)
	PU-GHB	808 nm (1.5 W cm^{-2})	Cell membrane	*S. aureus*, *E. coli*, MRSA, and VRE (All >99%)	Infected abdominal wall hernia	PTT + PDT	(Zhang et al., 2023b)
Triphenylamine	UCNANs	808 nm (0.4 W cm^{-2})	biofilms and Cell membrane	*S. aureus* and *P. aeruginosa* (All >99%)	Bacterial keratitis	PDT (I) + NO	(Zhang et al., 2022a)
	CB [10]⊃TPE-cyc	808 nm (1.5 W cm^{-2})	Cell membrane	*E. coli* and *B. subtilis* (All nearly 100%)	Subcutaneous abscess	PTT	(Wu et al., 2023)
	RZND	808 nm (0.5 W cm^{-2})	Cell membrane	MRSA (99)	Leg abscess	NO	(Zhu et al., 2023)

(*continued on next page*)

Table 1 (*continued*)

Photosensitizers	Phototherapy agent	Light source	Target site	Application		Antibacterial mechanism	Ref.
				Organism (Antimicrobial efficiency)	Model		
Triphenylamine	T780T-Gu	808 nm (0.3 W cm^{-2})	biofilm and Cell membrane	MDR *H. pylori* (97%)	/	PDT+ NO	(Qiao et al., 2023)
	ZSY-TPE	808 nm (10 mW cm^{-2})	Cell membrane	*S. aureus*	Subcutaneous abscess	PTT + PDT (II)	(Xu et al., 2020)
	DDNPs	808 nm (600 mW cm^{-2})	Cell membrane	*E. coli*, *S. aureus*, and *C. albicans* (>70%, >90%, and >99%	/	PTT + PDT	(Liang et al., 2020)
	AIE NPs	808 nm (0.1–0.2 mW cm^{-2})	Cell membrane	*S. aureus* and *E. coli* (99.9% and 99.8%)	Skin wound infection	PTT + PDT (II)	(Wang et al., 2022b)

and efficacy of phototherapy. Moreover, the incorporation of artificial intelligence (AI) into the design and optimization of multifunctional PTT/PDT platforms presents a promising frontier. AI-driven approaches may accelerate the discovery of novel photosensitizers, predict optimal treatment parameters, and enable personalized therapeutic regimens tailored to specific bacterial strains and infection microenvironments, particularly in the context of drug-resistant pathogens.

To fully realize the clinical potential of this modality, future research must address key challenges such as limited tissue penetration, hypoxic infection environments, and off-target effects. Promising strategies include the use of NIR-II light for deeper tissue access, oxygen-independent photosensitizer mechanisms, and targeted delivery systems that discriminate between bacterial and host cells. Moreover, combining phototherapy with complementary approaches, such as chemotherapy, immunotherapy, or emerging gas therapies (e.g., NO, CO, H_2), can yield synergistic effects, particularly in eradicating biofilms and multidrug-resistant pathogens.

In conclusion, phototherapeutic antibacterial agents represent a frontier of precision medicine. With sustained research and technological refinement, they have the potential to revolutionize infection treatment, offering safer, more effective, and personalized solutions for global health challenges.

CRediT authorship contribution statement

Wing-Leung Wong: Writing – review & editing, Funding acquisition, Formal analysis, Conceptualization. **Ying-Ying Zheng:** Visualization, Formal analysis, Data curation. **Jia-Peng Dong:** Visualization, Software, Formal analysis, Data curation. **Ze-Xin Chen:** Visualization, Software, Formal analysis, Data curation. **Yao-Xun Zeng:** Writing – original draft, Visualization, Software, Formal analysis, Data curation. **Wen-De Zheng:** Writing – original draft, Visualization, Formal analysis, Data curation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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