

Supporting Information

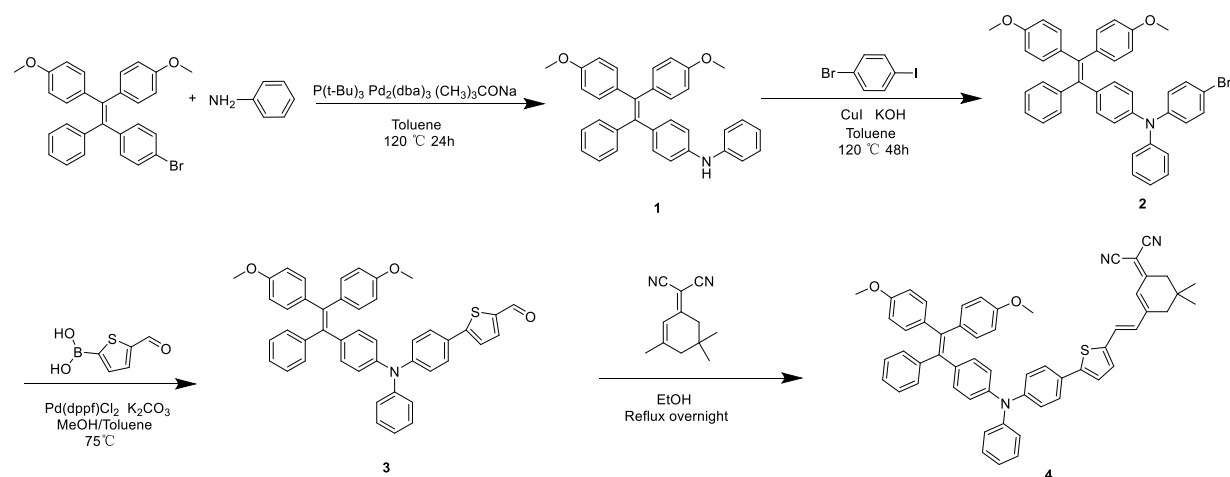
Precise Molecular Engineering of Type I Photosensitizer with Aggregation-Induced Emission for Image-Guided Photodynamic Eradication of Biofilm

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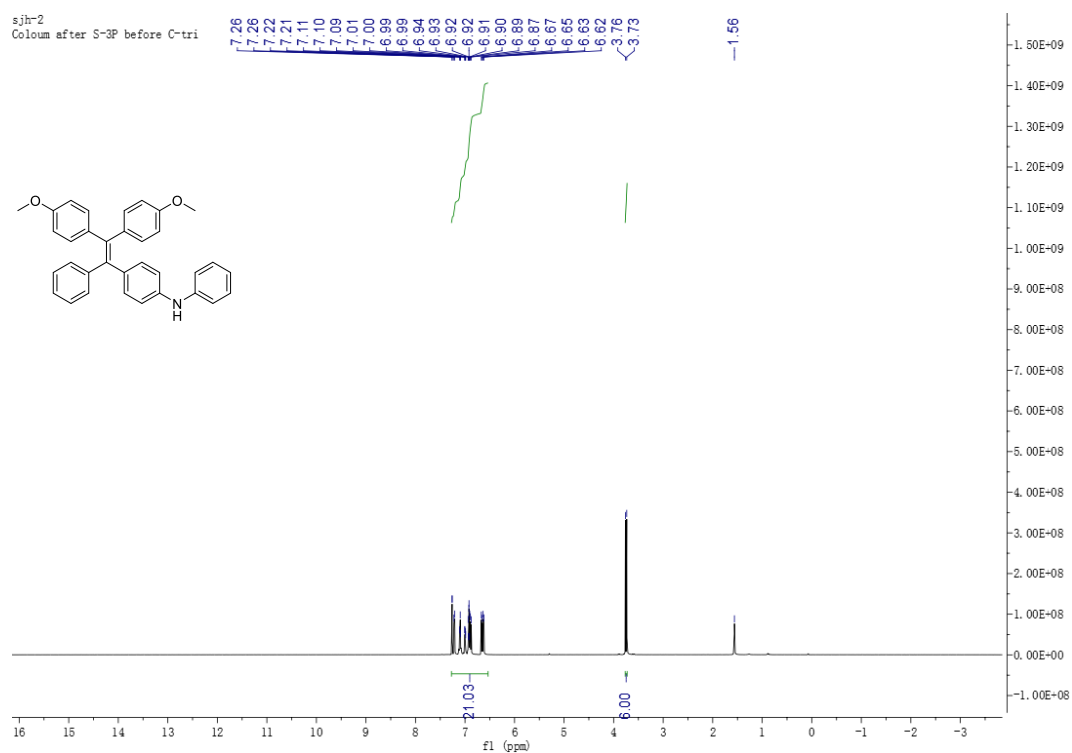
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Synthesis of TTTDM

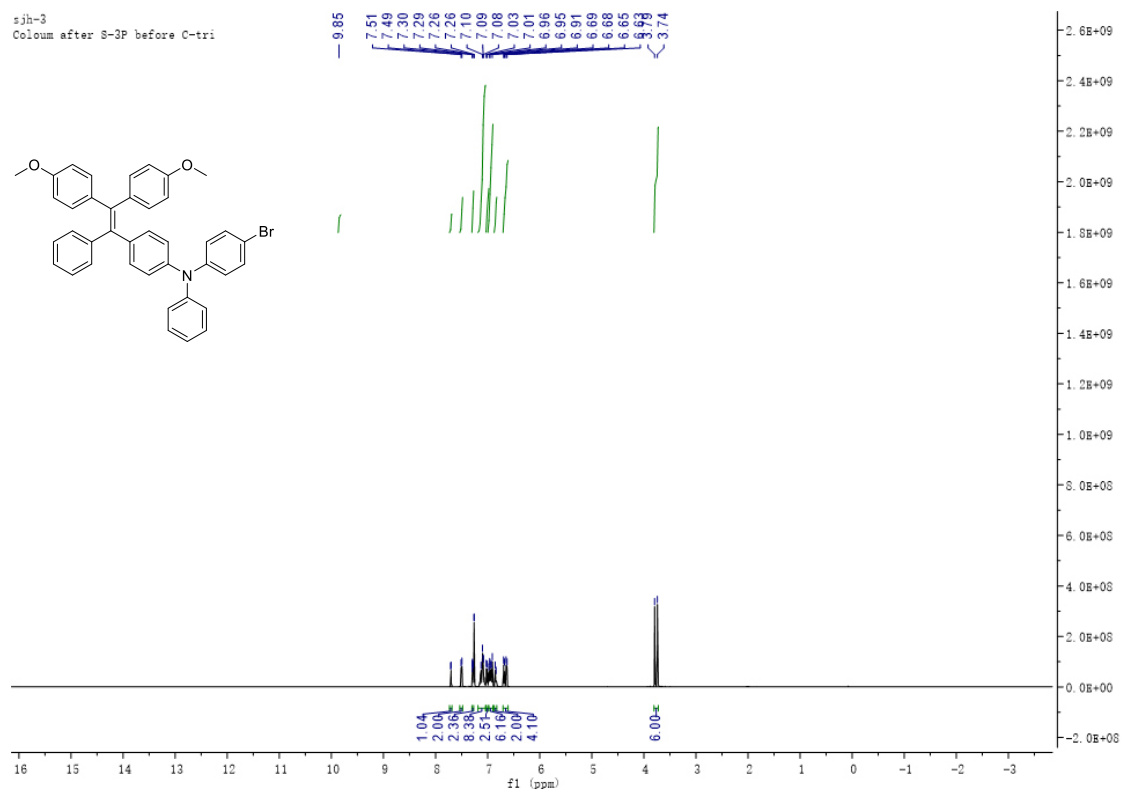


Scheme S1. Synthesis of Type-I photosensitizer TTTDM.

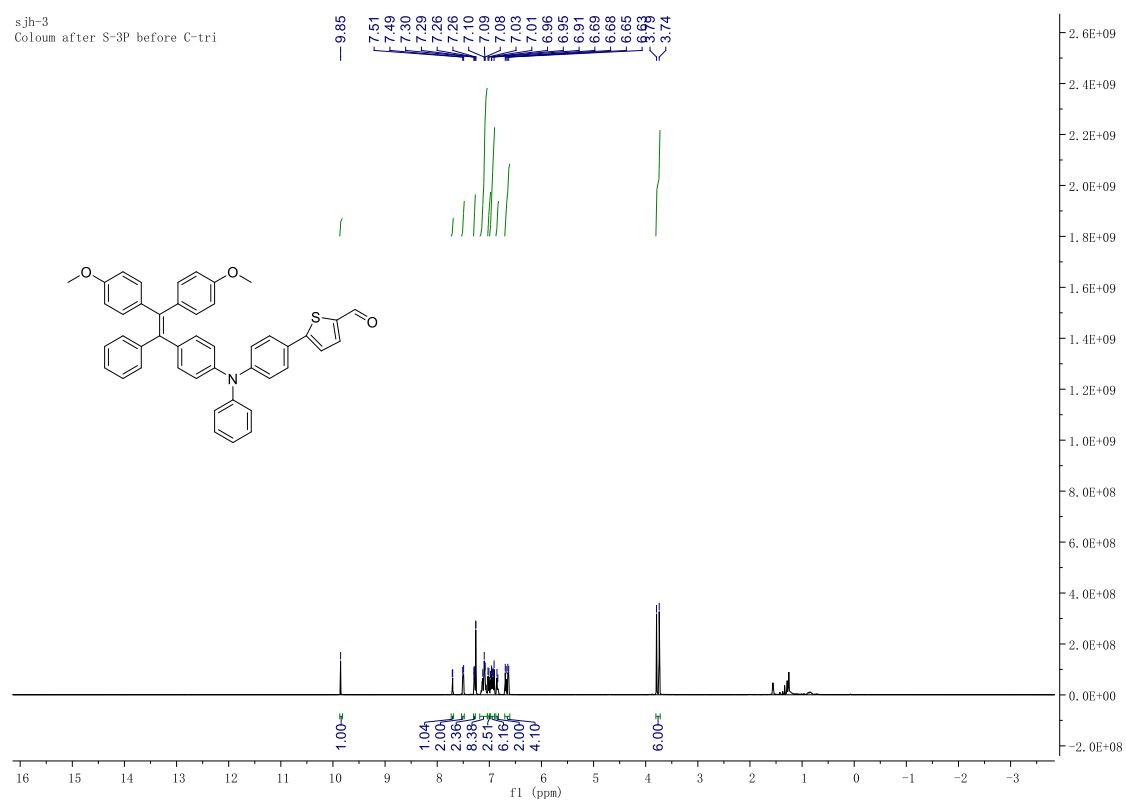
^1H NMR Spectra of intermediate and TTTDM



^1H NMR Spectra of intermediate **1** (CDCl₃, 298 K) Purity= 99%

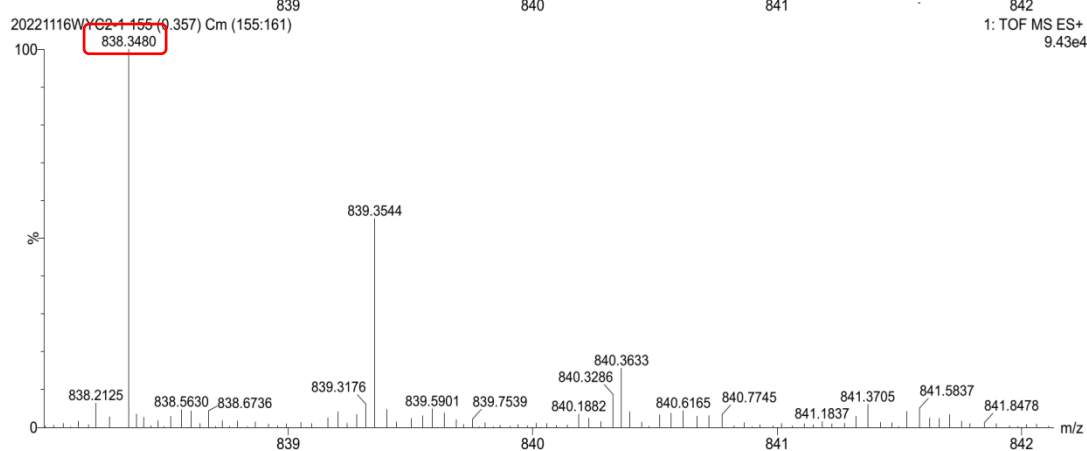
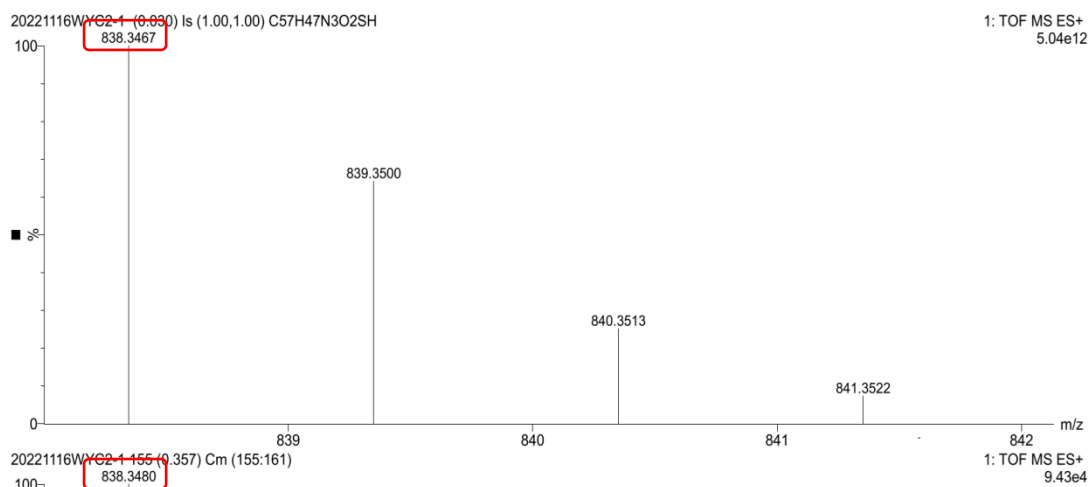


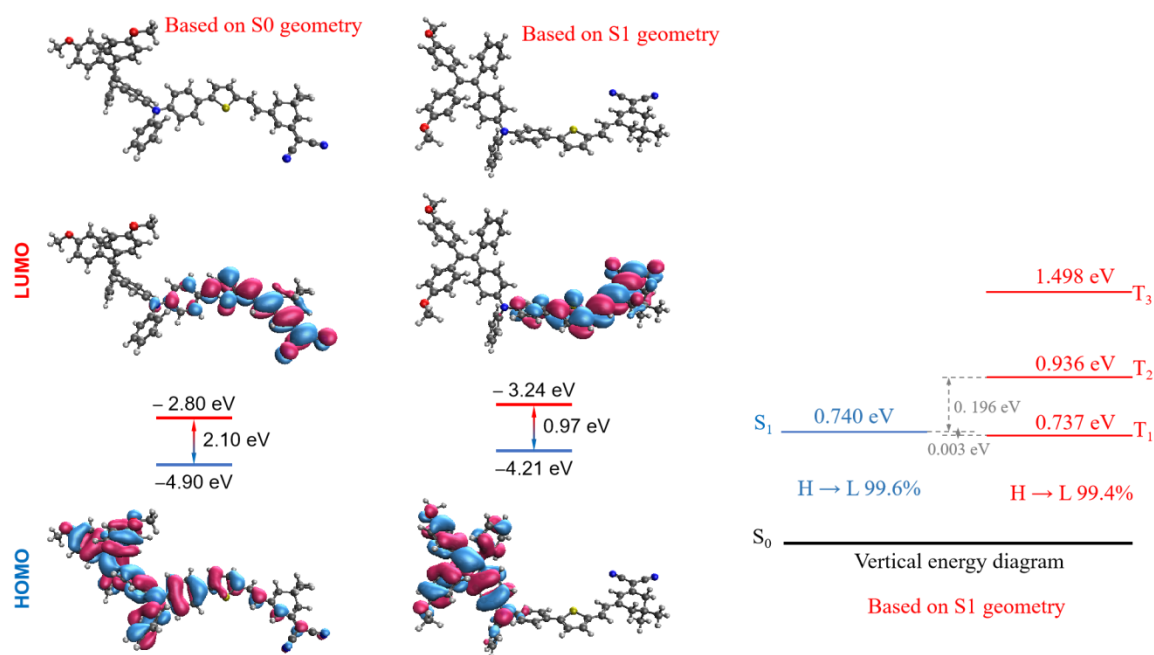
¹H NMR Spectra of intermediate 2(CDCl₃, 298 K) Purity= 100%



¹H NMR spectrum of intermediate 3 (CDCl₃, 298 K) Purity= 93 %

Mass spectrum of TTTDM





**Figure S1 Theoretical calculation
Computational details**

The ground-state geometries of the molecule was optimized using density functional theory (DFT) method at the theoretical level of B3LYP-D3/6-31g(d,p). Time-dependent DFT (TD-DFT) method was utilized at the same level of theory to calculate energy levels of singlet, triplet states and their gap (eV) based on the optimized singlet-state geometries.[1] Above quantum chemical calculations were carried out by using Gaussian 16 program (Revision A.03).[2] The HOMO and LUMO were displayed using IQmol molecular viewer package (Vision 3.0.1).

[1] C. Adamo and D. Jacquemin. The calculations of excited-state properties with Time-Dependent Density Functional Theory. *Chem. Soc. Rev.* 42 (2013), 845.

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16*, Gaussian, Inc., Wallingford CT, 2016.

Digital photos of biofilm samples



Figure S2. Digital photos of biofilm samples

SEM

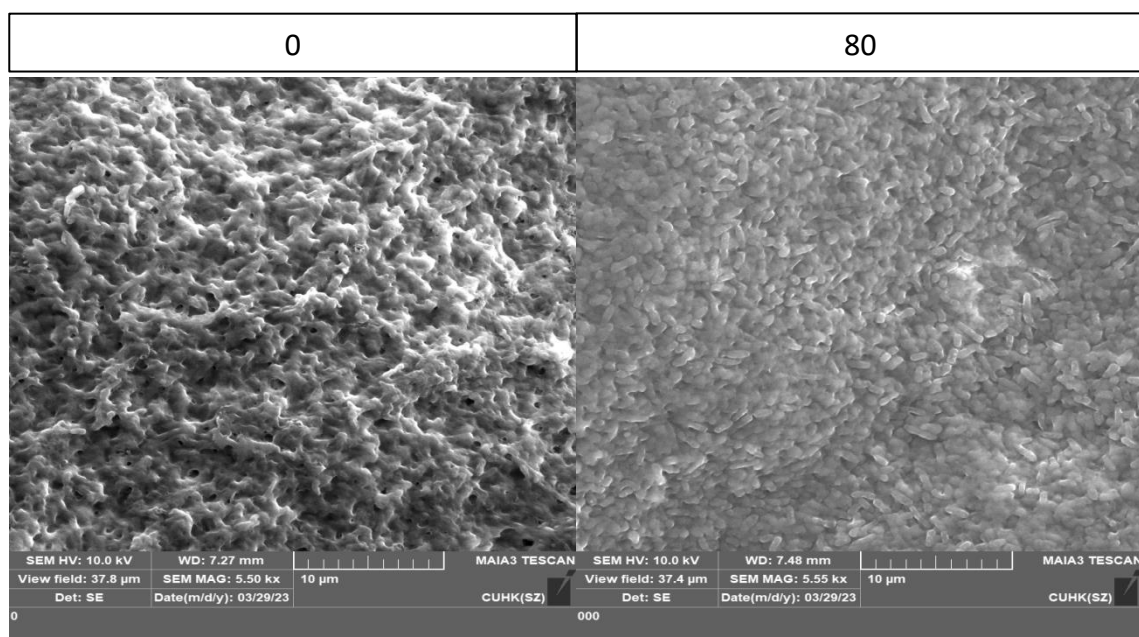


Figure S3. SEM images of *P.aeruginosa* biofilms after treatment with different concentrations under light conditions (white light 30 mW cm⁻² for 1 h).