

Supporting Information

Highly Effective Inactivation of SARS-CoV-2 by Conjugated Polymers and Oligomers

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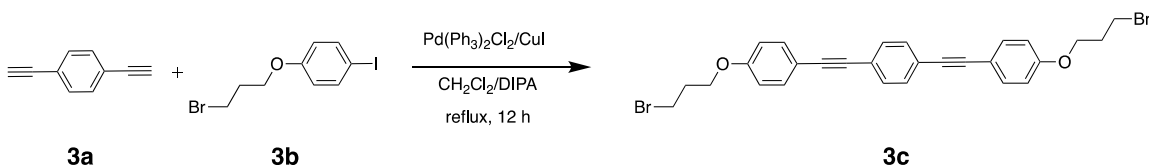
Materials

All starting materials and reagents were obtained from commercial sources (Sigma-Aldrich, Fisher Scientific) and used without further purification. All reactions were performed under a nitrogen atmosphere, unless stated otherwise. Compounds **1**, **2**, **3b**, **poly-4** and **poly-5** were synthesized by following the literature procedure.¹⁻⁵

Characterization Methods

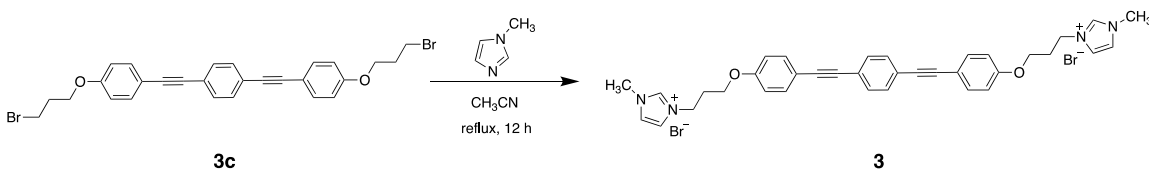
UV-Visible spectra for all the samples were recorded at a concentration of 10 $\mu\text{g/mL}$ in water using the PerkinElmer Lambda 35 UV-Vis spectrophotometer.

1,4-bis((4-(3-bromopropoxy)phenyl)ethynyl)benzene (**3c**).



To a degassed solution of **3a** (300 mg, 2.378 mmol) and **3b** (1.62 g, 4.756 mmol) in 60 mL CH_2Cl_2 and 20 mL diisopropyl amine, $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (167 mg, 0.238 mmol), CuI (90 mg, 0.476 mmol) were added. The mixture was refluxed for 12 h. The product was separated between saturated aq. NH_4Cl and CH_2Cl_2 , and washed with D.I. water. The CH_2Cl_2 layer was dried over anhydrous Na_2SO_4 and distilled off the solvent under reduced pressure. The crude product was passed through a silica gel column using hexane/DCM as the mobile phase to isolate **3c** as a pale white solid. Yield: 710 mg (76 %).

3,3'-((((1,4-phenylenebis(ethyne-2,1-diyl))bis(4,1-phenylene))bis(oxy))bis(propane-3,1-diyl))bis(1-methyl-1H-imidazol-3-ium) bromide (**3**).



To a solution of **3c** (500 mg, 0.905 mmol) in 30 mL CH₃CN, 1-methylimidazole (164 mg, 2 mmol, 2.2 eq.) was added and refluxed for 12 h. The precipitated solid product was filtered and was washed with cold CH₃CN. The product was dried under high vacuum to remove any trace amount of solvent. Yield: 600 mg (93 %). HRMS (**3**²⁺ ion calculated 278.1413, found 278.1427).

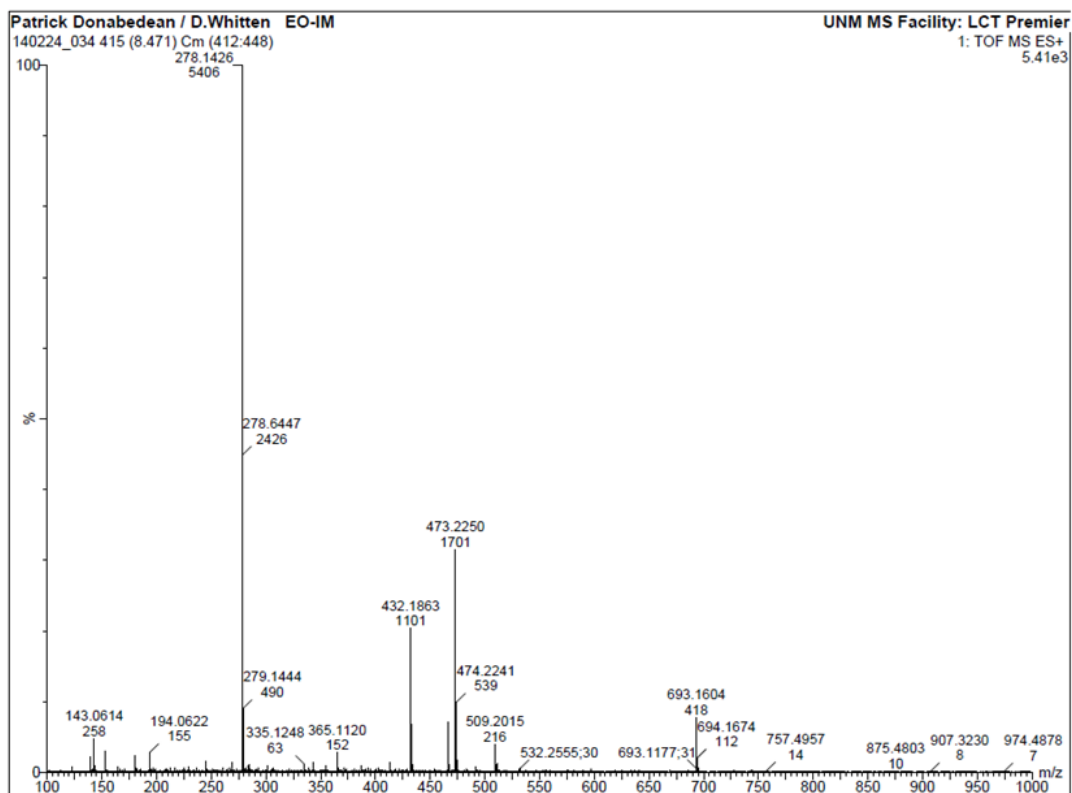


Figure S-1. High resolution mass spectrum of oligomer **3**.

Photolysis Light Sources

Samples were exposed to light for the indicated periods using using a Luzchem photoreactor (Luzchem.com) equipped with either near-UV or visible light sources. The spectral distribution of the light from the two sources is shown below.

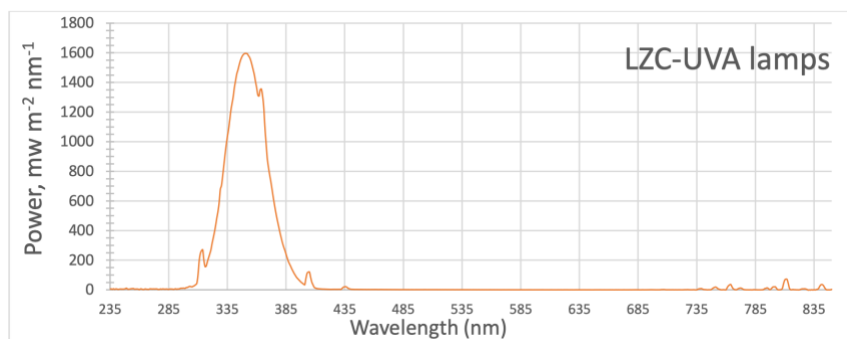


Figure S-2. Spectral distribution for LZC-UVA lamps used for near-UV irradiation of samples. The irradiance at the sample with this light source is $6.7 \text{ mW}\cdot\text{cm}^{-2}$.

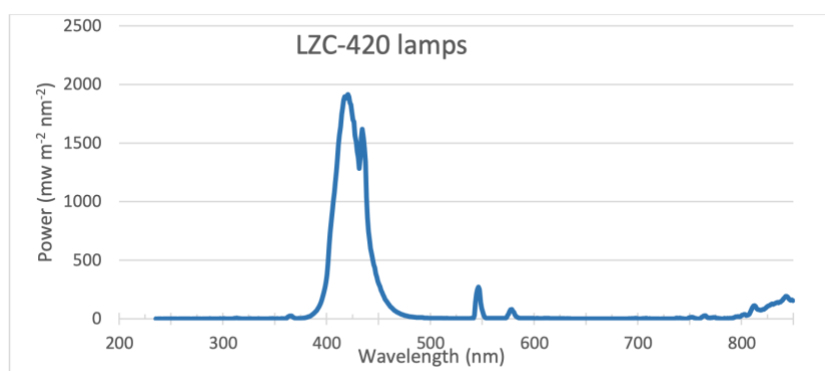


Figure S-3. Spectral distribution for LZC-420 lamps used for visible irradiation of samples. Visible region irradiance at the sample with this light source is $6.7 \text{ mW}\cdot\text{cm}^{-2}$.

References

1. Tan, C.; Pinto, M. R.; Schanze, K. S. Photophysics, aggregation and amplified quenching of a water-soluble poly(phenylene ethynylene), *Chem. Commun.* **2002**, 446–447.
2. Zhang, L.; Lou, X.; Yu, Y.; Qin, J.; Li, Z. A New Disubstituted Polyacetylene Bearing Pyridine Moieties: Convenient Synthesis and Sensitive Chemosensor toward Sulfide Anion with High Selectivity, *Macromolecules* **2011**, 44, 5186–5193.
3. Donabedian, P. L.; Pham, T. K.; Whitten, D. G.; Chi, E. Y. Oligo(p-phenyleneethynylene) Electrolytes: A Novel Molecular Scaffold for Optical Tracking of Amyloids, *ACS Chem. Neurosci.* **2015**, 6, 1526-1535.
4. Zhao, X. Y.; Pinto, M. R.; Hardison, L. M.; Mwaura, J.; Muller, J.; Jiang, H.; Witker, D.; Kleiman, V. D.; Reynolds, J. R.; Schanze, K. S. Variable Band Gap Poly(arylene ethynylene) Conjugated Polyelectrolytes, *Macromolecules* **2006**, 39, 6355-6366.
5. Huang, Y.; Pappas, H. C.; Zhang, L.; Wang, S.; Cai, R.; Tan, W.; Wang, S.; Whitten, D. G.; Schanze, K. S. Selective Imaging and Inactivation of Bacteria over Mammalian Cells by Imidazolium-Substituted Polythiophene, *Chem. Mater.* **2017**, 29, 6389-6395.