coatings

Supplementary Materials: Antimicrobial Ceramic Filters for Water Bio-Decontamination

Olga Ferreira [1,2], Patrícia Rijo [3,4], João Gomes [2,5], Ricardo Santos [6], Sílvia Monteiro [6], Rita Guedes [1], Maria Luísa Serralheiro [1], Marisa Gomes [7], Luciana C. Gomes [7], Filipe J. Mergulhão [7] and Elisabete R. Silva [1,2,*]

1 BioISI—Biosystems & Integrative Sciences Institute, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal; orferreira@fc.ul.pt (O.F.); cpn.ritaguedes@gmail.com (R.G.); mlserralheiro@fc.ul.pt (M.L.S.)
2 CERENA—Centro de Recursos Naturais e Ambientais, Departamento de Civil, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal; jgomes@deq.isel.ipl.pt
3 CBIOS —Research Center for Biosciences & Health Technologies, Universidade Lusófona, Campo Grande 376, 1749-024 Lisboa, Portugal; p1609@ulusofona.pt
4 Instituto de Investigação do Medicamento (iMed.ULisboa), Faculdade de Farmácia da Universidade de Lisboa, Avenida Professor Gama Pinto, 1649-003 Lisboa, Portugal
5 Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa (ISEL-IPL), Rua Conselheiro Emídio Navarro 1, 1959-007 Lisboa, Portugal
6 Laboratório de Análises, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal; ricardosantos@tecnico.ulisboa.pt (R.S.); silvia.monteiro@tecnico.ulisboa.pt (S.M.)
7 LEPABE—Laboratory for Process Engineering Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-645 Porto, Portugal; marisagomes@fe.up.pt (M.G.); luciana.gomes@fe.up.pt (L.C.G.); filipem@fe.up.pt (F.J.M.)
* Correspondence: ersilva@fc.ul.pt; Tel.: +351-217500991

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SI.1 Functionalization of Econea Biocide

The functionalization of Econea (E) biocide (Figure S1) was carried out in accordance with Silva et al. (2019) [1,2]. Briefly, it can be devised in three main steps:

(i) dissolution of the Econea biocide in dried ethyl acetate (p.a. Sigma-Aldrich), at a content ranging from 15 to 30 wt.%). The biocide, the 4-bromo-2-(4-chloropheny)-5-(trifluoromethyl)-1H-pyrrole-3-carbonitrile, 97% purity, was obtained from Janssen PMP, Beerse—Belgium;

(ii) reaction of functionalization between the diisocyanate 4,4 diphenyl diisocyanate-monomeric (MDI), with an isocyanate (NCO) content of 33.4% ± 0.1%, and an average functionality of 2, and the biocide in solution. Briefly, the reaction was performed in a three-necked round bottom flask, under inert atmosphere conditions and continuous stirring (300–400 rpm) at 40 ± 5 °C for about 1 h per gram of biocide. The biocide solution was added dropwise into de MDI kept in the round bottom flask at 40 ± 5 °C;

(iii) after the functionalization, the obtained biocidal precipitated (EM) was collected by filtration, purification and after a drying step. The drying was performed by solvent evaporation under reduced pressure in a Buchi R-210/215 rotary evaporator.

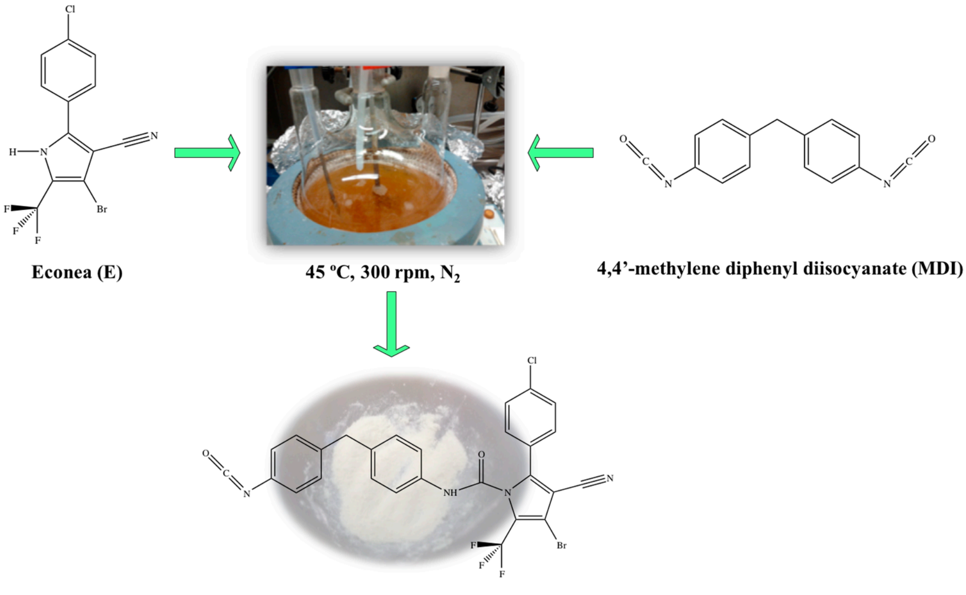

Figure S1. Eco-friendly strategy to generate the isocyanate derivative of Econea biocide and promote its grafting in polymeric matrices [3].

SI.2 Antimicrobial Effects of Biocides against methicillin-Resistant *Staphylococcus Aureus*

The antimicrobial effects of biocides Econea (E) and its isocyanate-functional derivative (EM) against methicillin-resistant *Staphylococcus aureus* (MRSA) bacteria were evaluated upon direct contact of the biocidal agents with the bacterium. Figure S2 shows the assay results after an incubation period of 48 h at 37 °C.

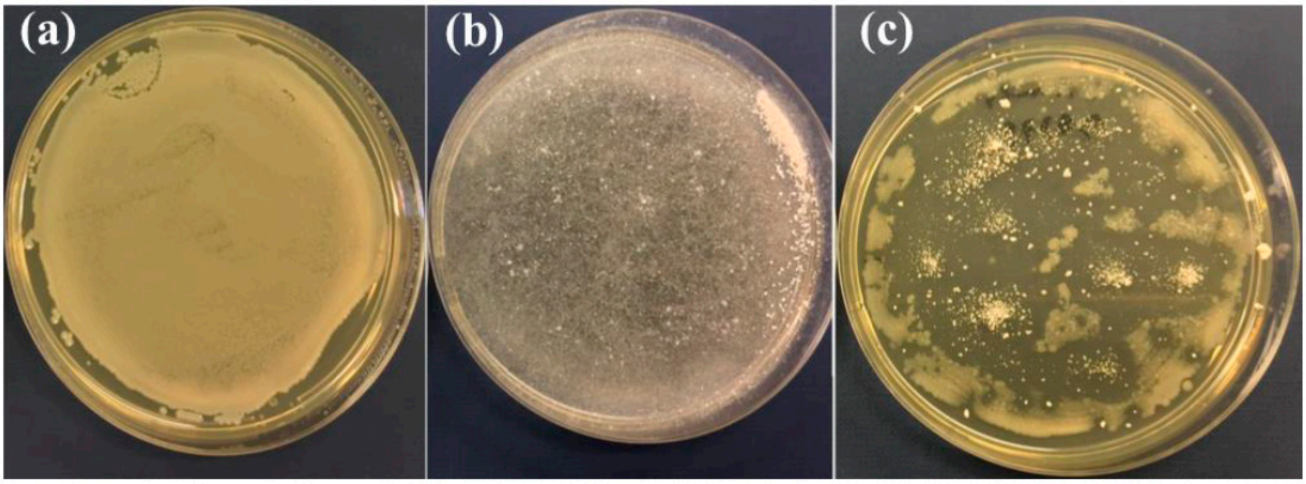

Figure S2. Antimicrobial activity of Econea biocide (**b**) and its isocyanate functionalized derivative (EM) (**c**) against MRSA (ATCC 33591) (**a**).

SI.3 Minimum Bactericidal Concentration (MBC) of Biocides against methicillin-Resistant *Staphylococcus Aureus*

The MBC values against methicillin-resistant *Staphylococcus aureus* (MRSA) bacteria were evaluated to confirm the bactericidal and bacteriostatic properties of the studied biocides, Econea (E) and its isocyanate-functional derivative (EM). After MIC determinations and for each set of wells that did not show any growth of MRSA bacteria, a loopful of broth was collected and inoculated on sterile Mueller-Hinton (MH) agar.

Figure S3 shows the MBC assay results for the biocides after an incubation period of 24 h at 37 °C

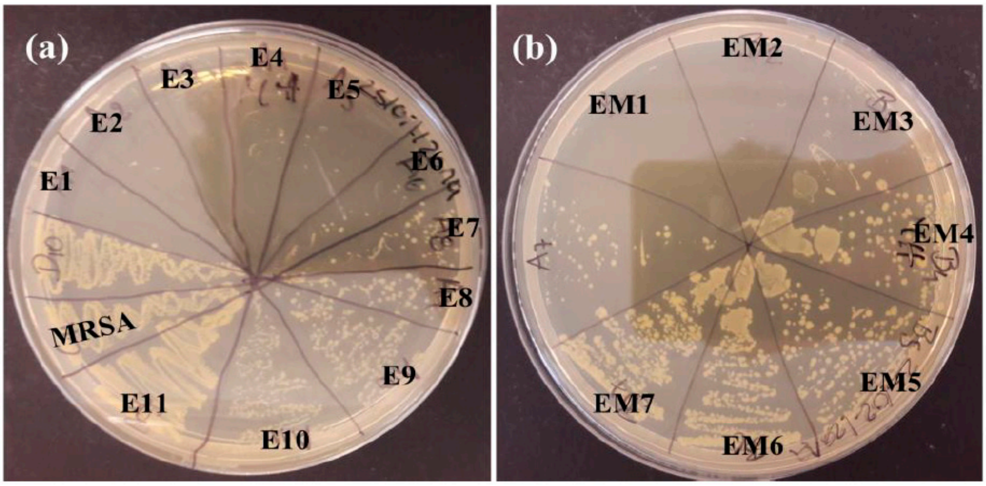

Figure S3. Minimum bactericidal concentration (MBC) assay against methicillin-resistant *Staphylococcus aureus* (MRSA) for Econea biocide (E) (**a**), ranging from 500 µg/mL (E1) and 0.49 µg/mL (E11), and for the isocyanate functional Econea derivative (EM) (**b**), ranging from 500 µg/mL (EM1) and 7.81 µg/mL (EM7). MRSA is a free bacteria culture assay, without any established contact with the biocides.

SI.4 Antimicrobial Effects of Biocidal PU Coatings against methicillin-Resistant *Staphylococcus Aureus* and *Enterococcus Faecalis*

The antimicrobial effects of biocides Econea (E) and its isocyanate-functional derivative (EM) against methicillin-resistant *Staphylococcus aureus* (MRSA) and *Enterococcus faecalis* (Ef) were evaluated upon direct contact of the biocidal agents with the different bacteria. Figure S4 shows the bioassay results after an incubation period of 48 h at 37 °C.

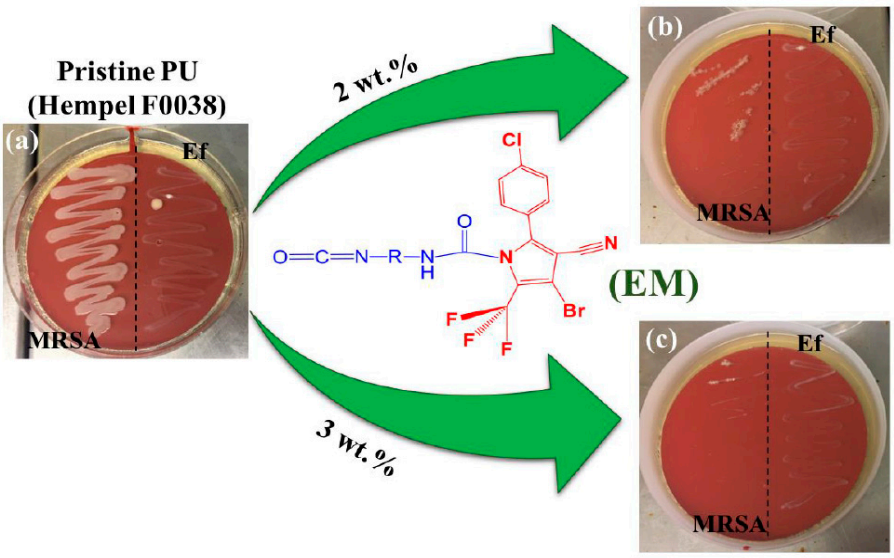

Figure S4. Antimicrobial susceptibility against MRSA and *E. faecalis* (Ef) bacteria of (**a**) pristine polyurethane (PU) based coating (control) and PU-based coating containing grafted Econea biocide at different contents, 2 wt.% (**b**) and 3 wt.% (**c**).

SI.5 UHPLC-MS/MS Chromatograms of Leaching Waters

To identify the compounds in the leaching waters obtained from the submersion tests of coated monolithic filters, UHPLC/MS-MS analyses were carried out. Figure S5 (a) and (b) presents the chromatograms in the negative (ESI −) and positive (ESI +) ionization modes, respectively, for the monolithic filters coated with the pristine polydimethylsiloxane (X3-PDMS) and polyurethane (PU) coatings (CM/X3-PDMS and CM/PU), and those containing incorporated Econea (CM/X3-PDMS-E and CM/PU-E) or grafted Econea (CM/X3-PDMS-EM and CM/PU-EM).

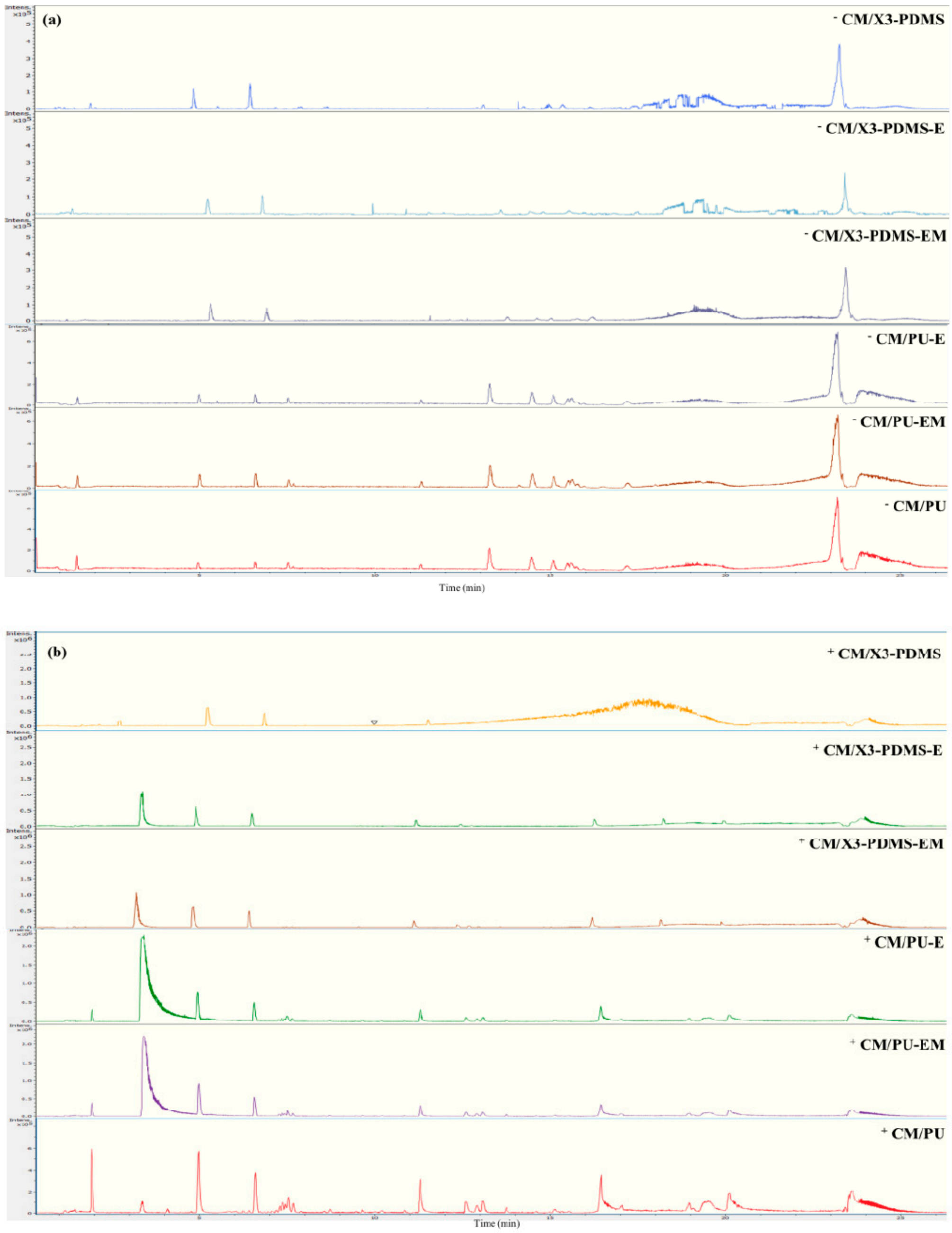

Figure S5. Base peak chromatograms from the analyses of leaching waters from monoliths (CM) coated with polyurethane (PU) and polydimethylsiloxane (PDMS) based coatings with incorporated Econea (CM/X3-PDMS-E and CM/PU-E), grafted Econea (CM/X3-PDMS-EM and CM/PU-EM), and biocide free (CM/X3-PDMS and CM/PU): ESI (−) (**a**) and ESI (+) (**b**).

SI.6 Chemical Structures of Econea and BCCPCA Compounds

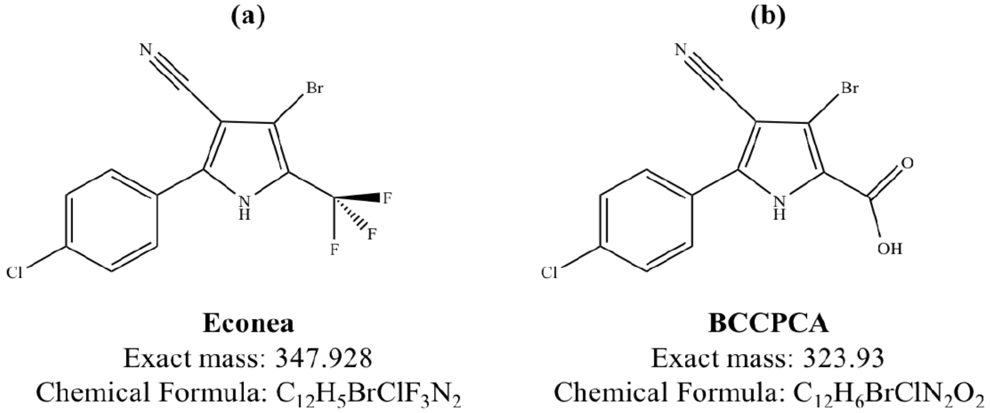

Figure S6. Chemical structure of 4-bromo-2-(4-chlorophenyl)-5-(trifluoromethyl)-1H pyrrole-3-carbonitrile (Econea) (**a**) and 3-bromo-5-(4-chlorophenyl)-4-cyano-1H-pyrrole-3-carboxylic acid (BCCPCA) (**b**).

SI.7 Contact Angle Measurements of Coatings (Wettability)

The hydrophobicity of the polydimethylsiloxane (PDMS) based coatings (pristine X3-PDMS and PDMS-EM containing grafted Econea) and polyurethane (PU) based coatings (pristine PU and PU-EM containing grafted Econea) were assessed on coated polyvinyl chloride (PVC) substrates (2 cm × 2 cm), through contact angles measurements *vs* time, in accordance with the ASTM standard D5725-99 (2003), and applying the sessile drop method using a gastight syringe to generate distilled water drops inside a closed chamber (25 °C). The images were recorded and analyzed in a range of 0 to 600 s using an optical equipment described elsewhere [4], and the Axisymmetric Drop Shape Analysis—profile (ADSA-P) Program. The values of the contact angle correspond to the average of at least 10 experiments. Tests were also performed in triplicate on independent coated substrates for each tested formulation. Some of the data provided were adapted from a previous work [2].

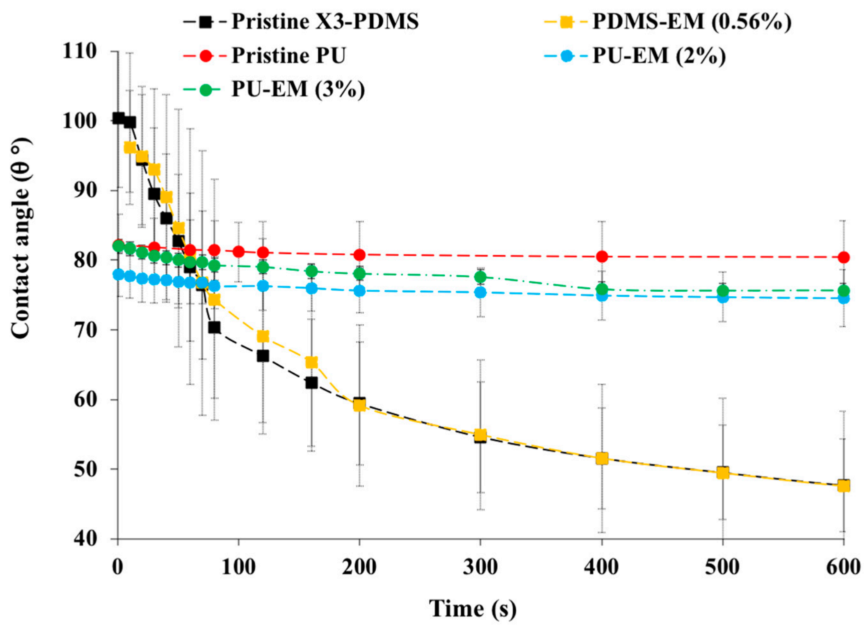

Figure S7. Contact angle measurements of water on polydimethylsiloxane (PDMS) and polyurethane (PU)-based marine coatings.

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