Supplementary Information

Synthesis, antimicrobial and molecular docking studies of benzimidazole and benzotriazole based dicationic sulphonophanes

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**Figure S1.** 2D ligplot view of the sulphonophane 1 with DNA gyrase B.

**Figure S2.** 2D ligplot view of the sulphonophane 2 with DNA gyrase B.

**Figure S3.** Pymol view of the sulphonophane 3 with DNA gyrase B.

**Figure S4.** 2D ligplot view of the sulphonophane 5 with DNA gyrase B.
In vitro antimicrobial activity

Antibacterial activity

The antibacterial activity of sulphonophanes 1-8 against human pathogenic bacteria was done by the agar well diffusion assay. The human pathogenic Gram positive bacteria B. subtilis and S. aureus and Gram negative bacteria V. cholera, E.coli, P. vulgaris, P. aeruginosa, K. pneumoniae, S. typhimurium and S. marcescens were obtained from the tissue culture lab, Food Safety and Microbiology Lab, R & D Centre, Anna University. The human pathogens were inoculated into 5mL of sterile Muller-Hinton Broth (MHB), incubated at 37°C for 24 h. The cultures were swabbed on the surface of sterile nutrient agar plates using a sterile cotton swab. Muller-Hinton Agar (MHA) wells were prepared with the help of a sterilized cork borer (9 mm dia). All the sulphonophanes 1-8 were dissolved in 10% DMSO which did not affect the microorganism’s growth, according to our control experiments. Using a micropipette, 50 μL of different concentrations of sulphonophanes (5, 10, 15 to 100 μg)
were added to the wells in the plate. Commercial antibiotics were used as positive reference standard to compare the efficiency of the test compounds.

**Antifungal activity**

The tested human fungal pathogen *C. albicans* was maintained in Sabouraud’s dextrose agar (SDA). The *C. albicans* was inoculated into Sabouraud’s Dextrose Broth (SDA) and incubated at 37 °C for 24 hours. The pathogen was swabbed on the sterile SDA plates using a sterile swab and wells were made using a sterile cork borer (9 mm dia). The sulphonophanes 1-8 were tested for their antifungal activity and their MIC was determined. The sulphonophanes at the concentrations of 5 μg/mL of 10% DMSO was used for this study with Clotrimazole as a positive control. The minimum inhibitory concentration was taken as the lowest concentration of the test compound that showed a prominent inhibition of fungal pathogen growth after 48 h of incubation at 37 °C.

**Molecular docking studies**

The protein in complex with simocyclinone (PDB ID: 2Y3P) was used as the template for the molecular docking studies. GLIDE 9.5 and IFD script from Schrödinger, LLC (New York) was employed as the primary docking engine. The scoring function, called GLIDE score, for computing the binding affinity is an extension of an empirically based Chem-Score function of Eldridge *et al.* OPLS, a molecular mechanics potential energy function was used throughout our calculations. The extra precision mode of GLIDE, which has higher penalties for unfavorable and unphysical interactions, was used for docking. The pictures were generated using LIGPLOT and Pymol. The ADMET parameters were calculated using the QikProp 3.4, Schrödinger, 2011.
$^1\text{H NMR Spectrum (300 MHz, DMSO-d}_6\text{)}$ of precyclophane 10
$^{13}$C NMR Spectrum (75 MHz, DMSO-d$_6$) of precyclophane 10
$^1$H NMR Spectrum (300 MHz, DMSO-d$_6$) of sulphonophane 1
$^{13}$C NMR Spectrum (75 MHz, DMSO-$d_6$) of sulphonophane 1
Mass (ESI) spectrum of sulphonophane 1
$^1$H NMR Spectrum (300 MHz, DMSO-d$_6$) of sulphonophane 3
$^{13}$C NMR Spectrum (75 MHz, DMSO-$d_6$) of sulphonophane 3
Mass (ESI) spectrum of sulphonophane 3
$^1$H NMR Spectrum (300 MHz, DMSO-$d_6$) of sulphonophane 5
$^{13}$C NMR Spectrum (75 MHz, DMSO-d$_6$) of sulphonophane 5
Mass (ESI) spectrum of sulphonophane 5
$^1$H NMR Spectrum (300 MHz, DMSO-$d_6$) of sulphonophane 6
$^{13}$C NMR Spectrum (75 MHz, DMSO-d$_6$) of sulphonophane 6
Mass (ESI) spectrum of sulphonophane 6
$^{1}$H NMR Spectrum (300 MHz, DMSO-$d_6$) of sulphonophane 8
$^{13}$C NMR Spectrum (75 MHz, DMSO-$d_6$) of sulphonophane 8
Mass (ESI) spectrum of sulphonophane 8
Supporting Information References


