Supplementary data to:

Original article:

SYNTHESIS, STRUCTURAL STUDIES, AND INHIBITORY POTENTIAL OF SELECTED SULFONAMIDE ANALOGUES: INSIGHTS FROM IN SILICO AND IN VITRO ANALYSES

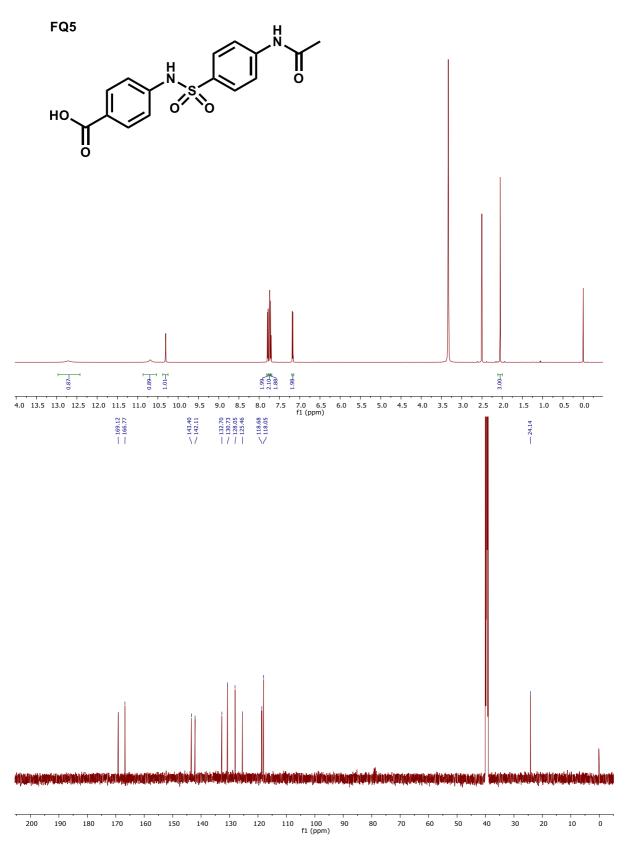
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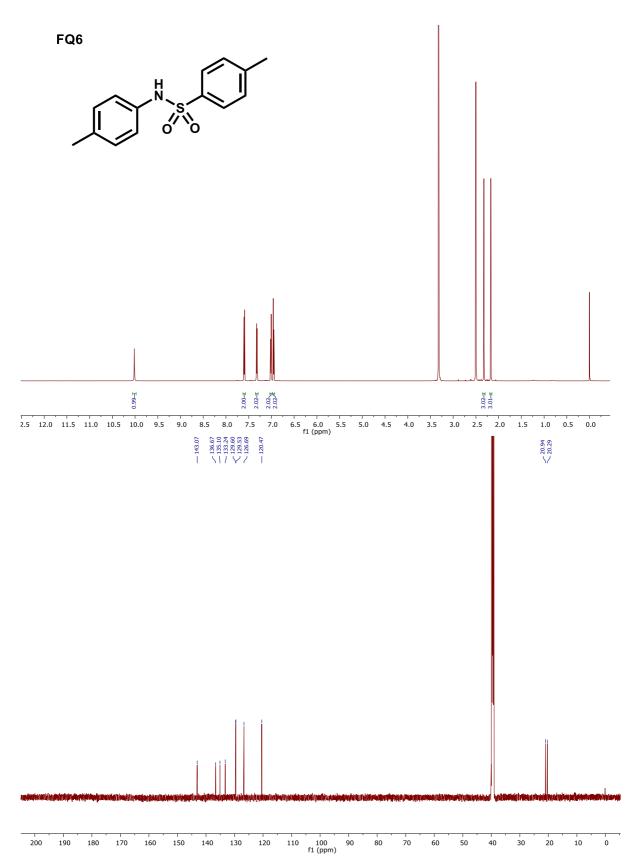
https://dx.doi.org/10.17179/excli2024-8118

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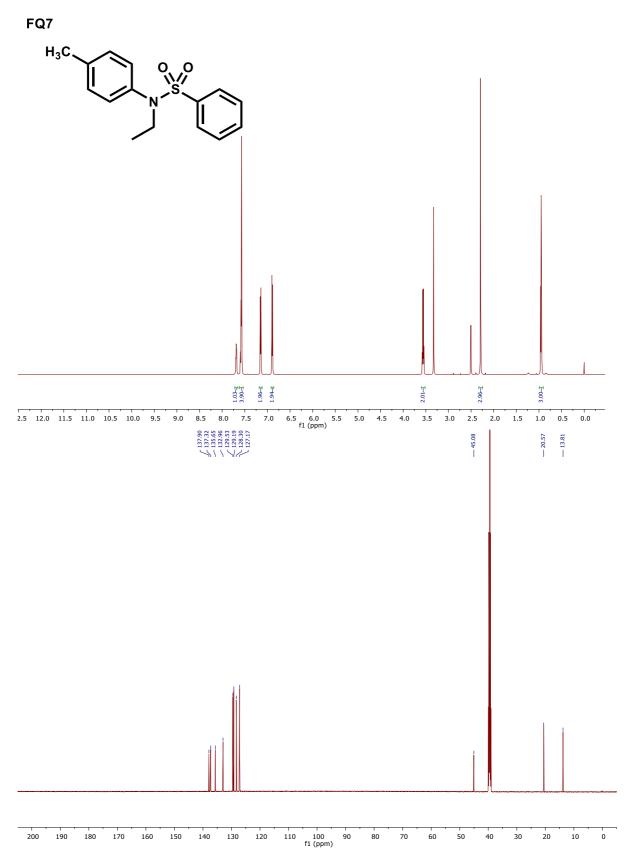
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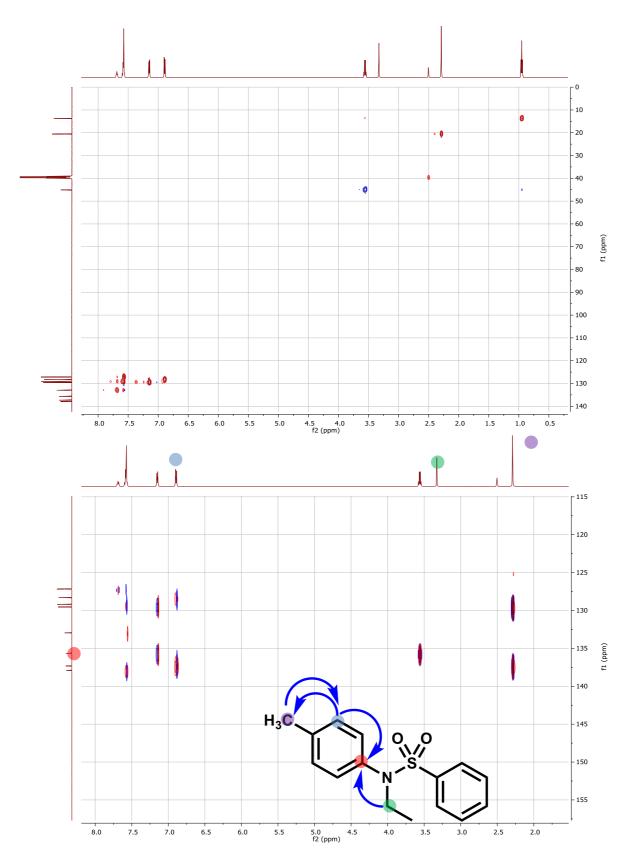
Supplementary Figure 1: ¹H and ¹³C NMR (DMSO-d6) spectra for compound FQ5



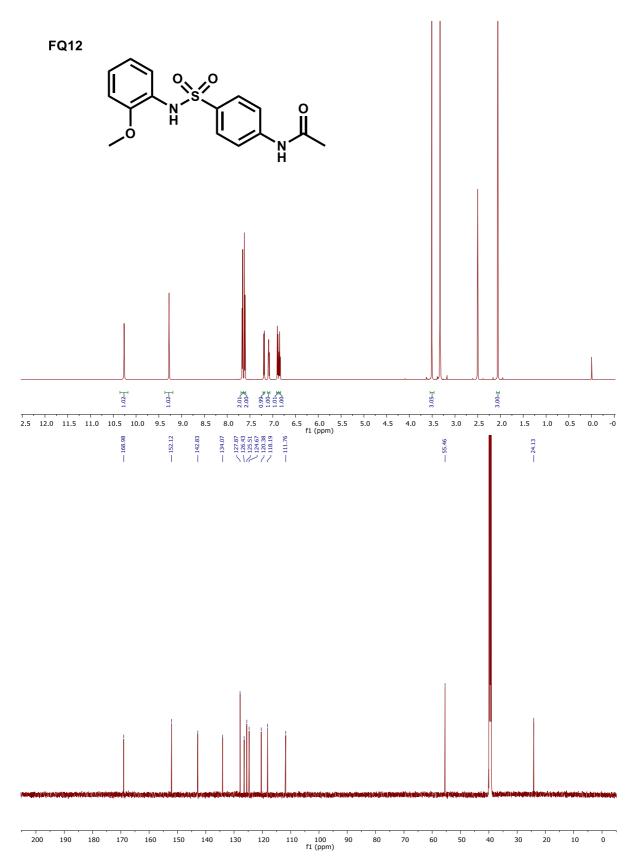
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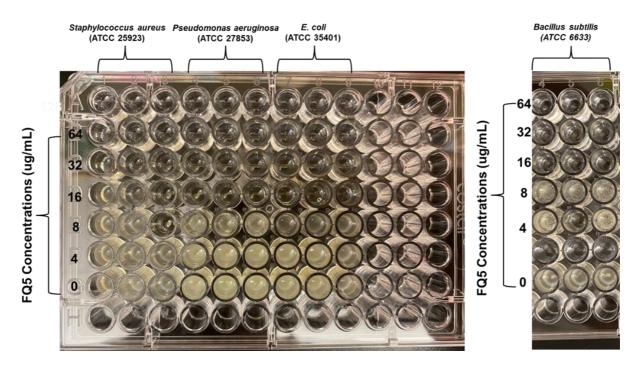
Supplementary Figure 3: ¹H and ¹³C NMR (DMSO-d6) spectra for compound FQ7



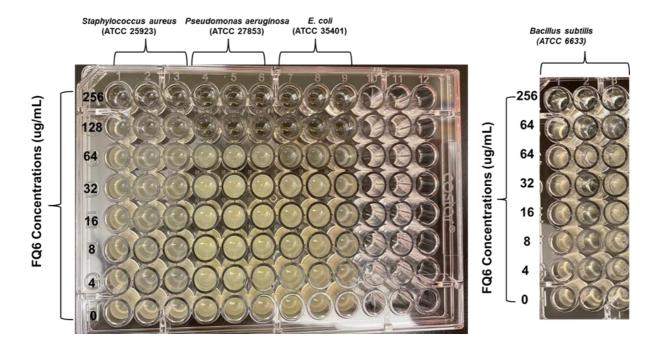
Supplementary Figure 4: HSQC and HMBC spectra (DMSO-*d6*) for compound FQ7, with zoomed- in region and key correlations highlighted



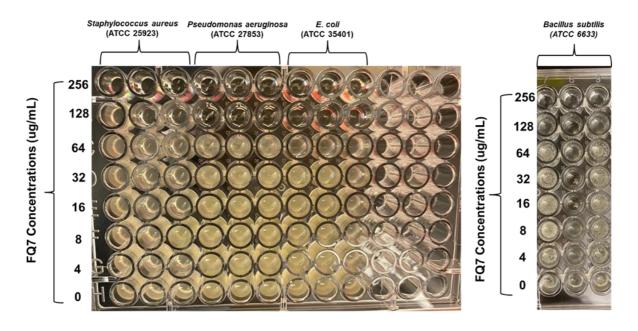
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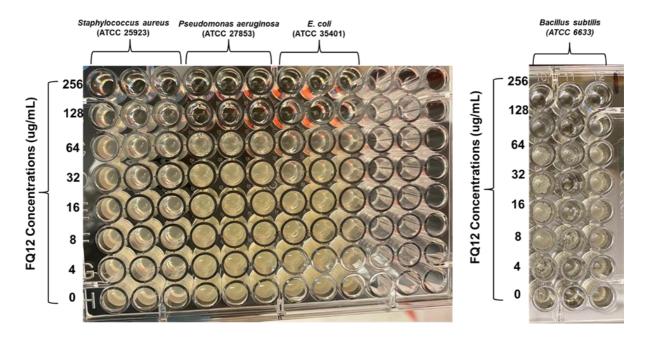
Supplementary Figure 6: Minimum Inhibitory Concentration (MIC), in $\mu g/mL$, of FQ5 against selected bacterial strains



Supplementary Figure 7: Minimum Inhibitory Concentration (MIC), in μ g/mL, of FQ6 against selected bacterial strains



Supplementary Figure 8: Minimum Inhibitory Concentration (MIC), in μ g/mL, of FQ7 against selected bacterial strains



Supplementary Figure 9: Minimum Inhibitory Concentration (MIC), in µg/mL, of FQ12 against selected bacterial strains

Supplementary Table 1: Additional Predicted ADMET properties

Compound	Caco2 permeability (> 0.90)	No. Rotatable Bonds (> 10)	SASA (300.0- 1000.0)	S+MDCK (5-1130)
Sulfadiazine	0.36	4	475.42	167.49
FQ5	0.18	6	598.54	7.78
FQ6	1.31	3	519.07	249.23
FQ7	1.04	4	513.25	791.88
FQ12	0.18	6	595.53	109.41

Abbreviations: Caco2 permeability = permeability of compound across a human colon carcinoma cell line monolayer; SASA = solvent accessible surface area; S+MDCK = solubility plus Madin-Darby canine kidney (MDCK) cell permeability