Supporting material for

Unlocking the Antibiofilm Potential of Natural Compounds by Targeting the NADH:quinone Oxidoreductase WrbA

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Table S1. MM-GBSA terms resulted in the output of the Prime calculations and then used for PCA. The abbreviation used in the mnuascript (Figure 5) are highligted in bold.

Term	Description
r_psp_MMGBSA_dG_Bind(NS)_**Coulomb**	Coulomb energy
r_psp_MMGBSA_dG_Bind(NS)_**Covalent**	Covalent binding energy
r_psp_MMGBSA_dG_Bind(NS)_**Hbond**	Hydrogen-bonding energy
r_psp_MMGBSA_dG_Bind(NS)_**Lipo**	Lipophilic energy
r_psp_MMGBSA_dG_Bind(NS)_**Packing**	Pi-pi packing energy
r_psp_MMGBSA_dG_Bind(NS)_**Solv_GB**	Generalized-Born electrostatic solvation energy
r_psp_MMGBSA_dG_Bind(NS)_**vdW**	Van der Waals energy
TOTAL (**ΔG**)	Binding free energy value
r_psp_Prime_MMGBSA_ligand_efficiency (**LE**)	ΔG / (number of heavy atoms)
r_psp_Prime_MMGBSA_ligand_efficiency_sa (**LE_sa**)	ΔG / (number of heavy atoms)$^{2/3}$ *This efficiency metric approximates the effect of surface area*
r_psp_Prime_MMGBSA_ligand_efficiency_ln (**LE_ln**)	ΔG / (1 + ln(number of heavy atoms))