

Antimicrobial properties of new polyamines conjugated with oxygen containing aromatic functional groups

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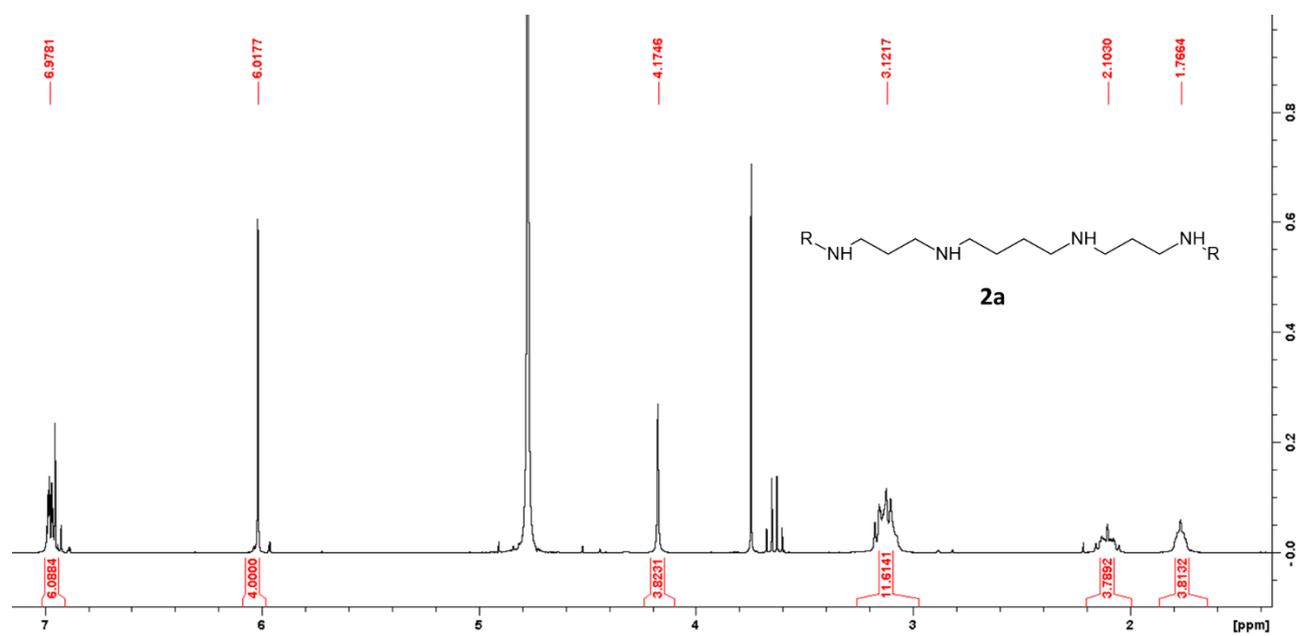
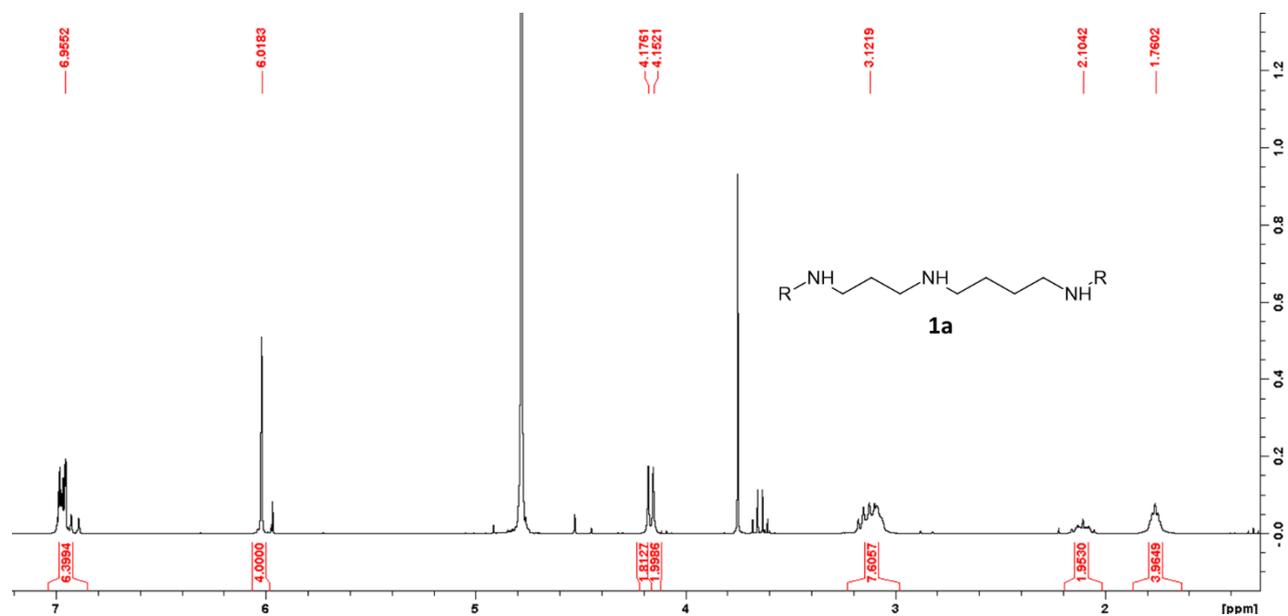
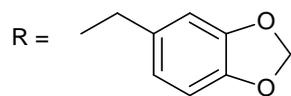
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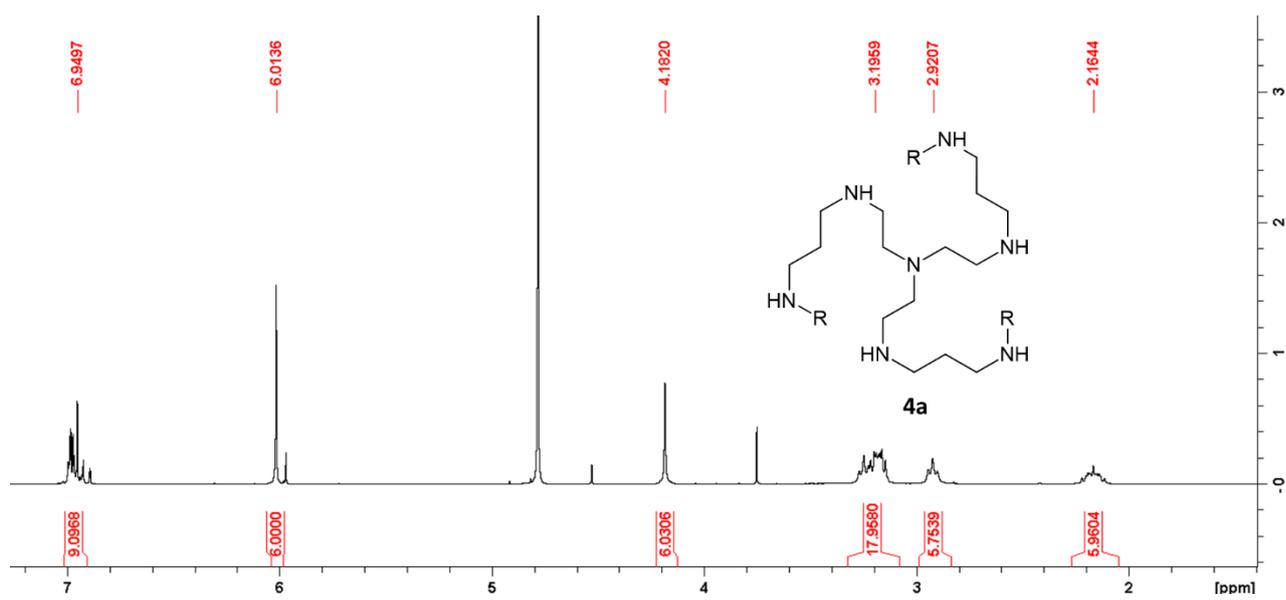
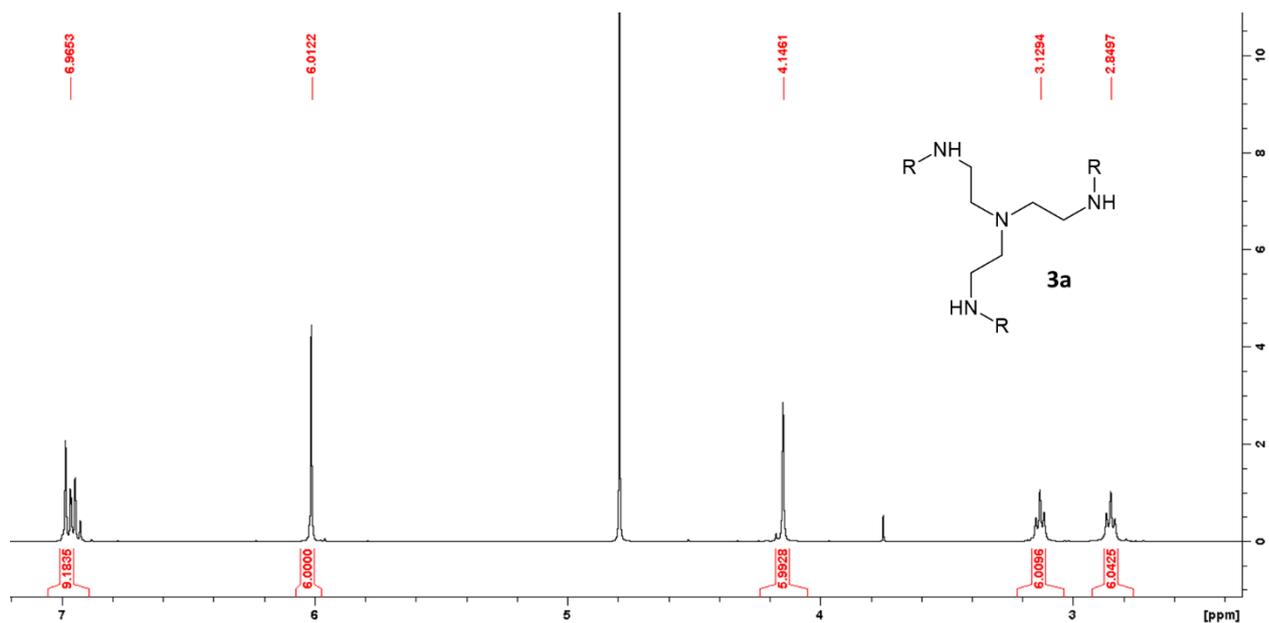
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Figure S1. ¹H NMR spectra of the new compounds





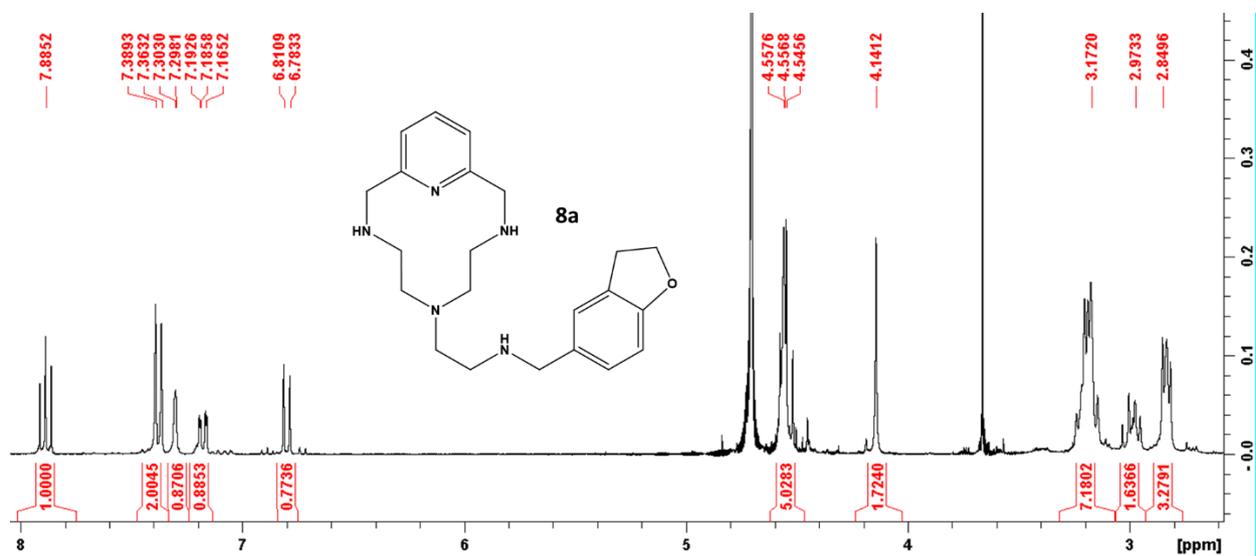
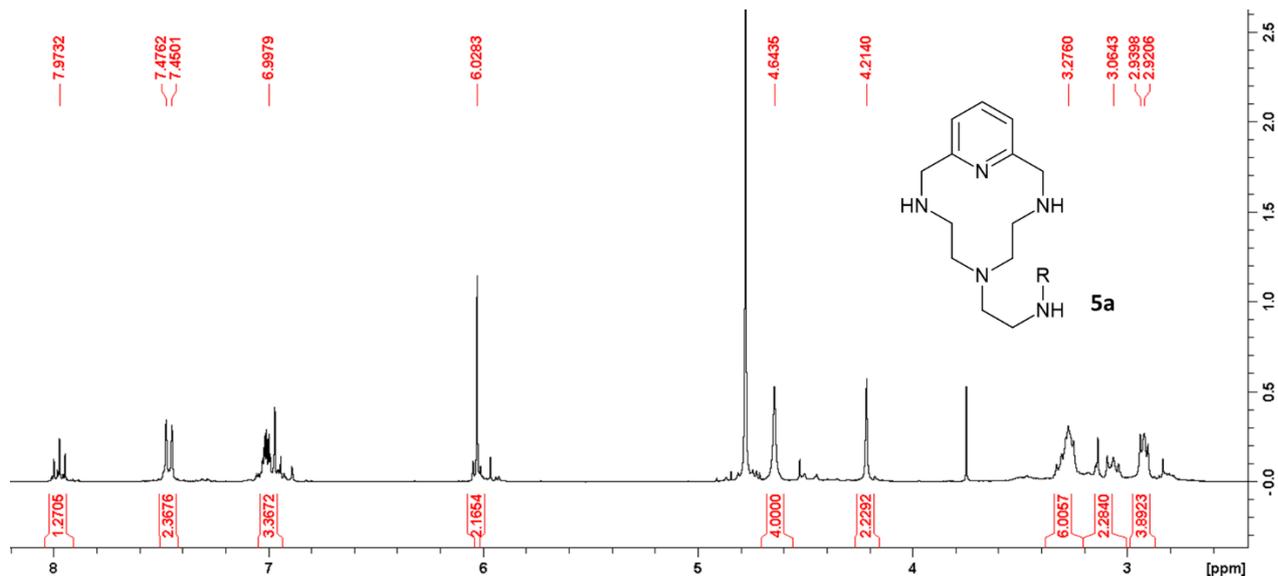


Figure S2. Scheme and X-ray crystallographic structure of **3a**·3HCl.

Slow evaporation of vessels containing a concentrated aqueous solution of **3a**·3HCl yielded white crystals suitable for X-ray diffraction. Analysis of single crystals of the ligand was carried out with an Enraf-Nonius KAPPA CCD single-crystal diffractometer ($\lambda = 0.71073 \text{ \AA}$). CIFs of crystal structures have been deposited with the number 2210255.

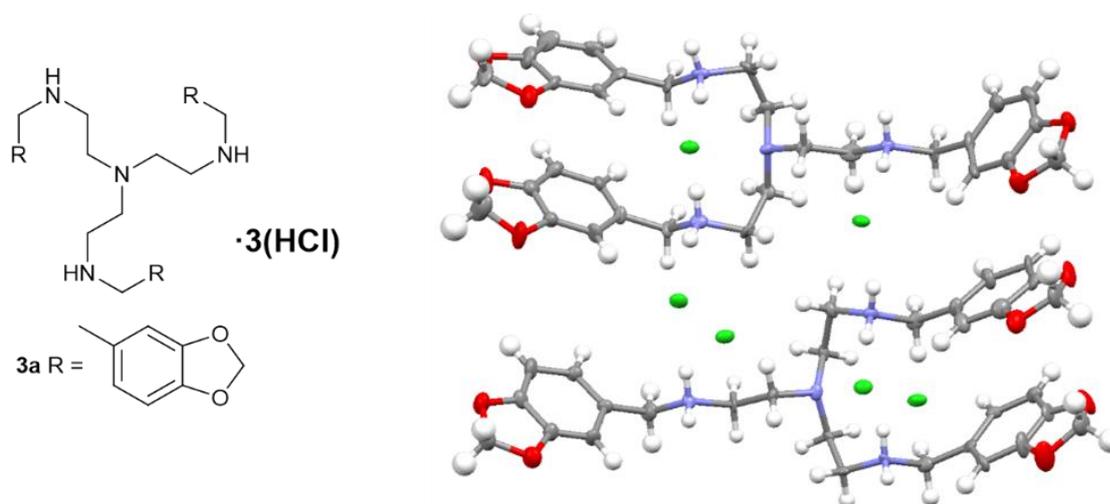


Table S1. Crystal data, data collection parameters, and results of the analysis.

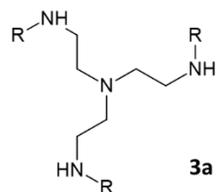
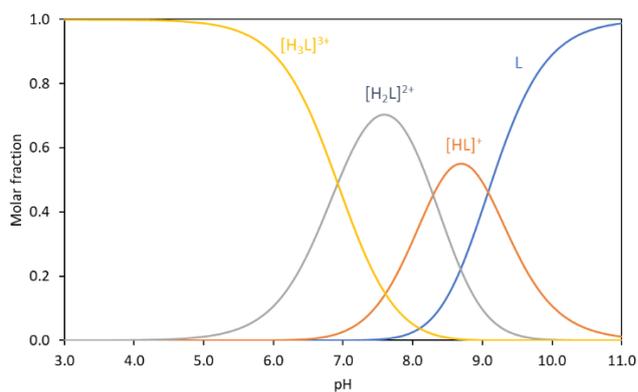
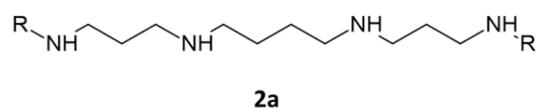
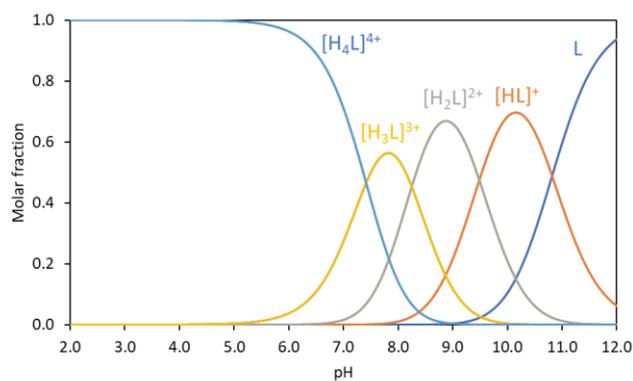
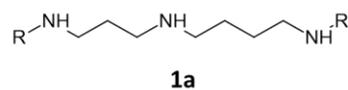
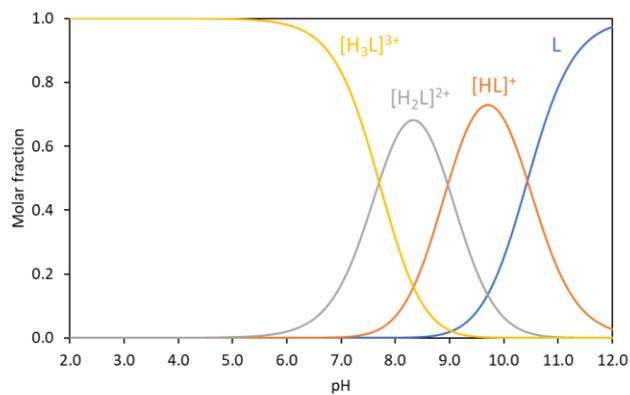
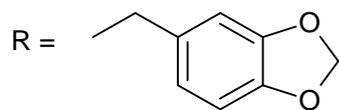
Crystallographic data

Formula	C ₃₀ H ₃₉ Cl ₃ N ₄ O ₆
Formula weight	658.00
Crystal system	triclinic
Space group	P 1
Cell	
<i>a</i> / Å	7.241(4)
<i>b</i> / Å	11.317(7)
<i>c</i> / Å	20.092(13)
α / °	77.11(3)
β / °	87.00(3)
γ / °	76.795(16)
<i>V</i> / Å ³	1562.5(16)
<i>Z</i>	2
<i>T</i> / K	150
size / mm	0.382 × 0.262 × 0.052
<i>F</i> ₀₀₀	692
density / g.cm ⁻³	1.399
R(int)	0.1946
θ_{\max} / deg.	29.982
θ_{\min} / deg.	2.350
reflections	
- collected	58315
- unique	8581
<i>R</i> 1	
- all	0.1221
- $F^2 > 2\sigma_{F^2}$	0.0856
<i>wR</i> 2	
- all	0.2312
- $F^2 > 2\sigma_{F^2}$	0.2007
<i>GoF</i>	1.034
- parameters	777
- constraints	0
- restraints	39

Hydrogen bonds

D--H..A	d(D-A) / Å	d(H..A) / Å	d(D, A) / Å	ang(D,H,A) / °
N2--H2A..Cl3	0.91	2.14	3.033(14)	167
N2--H2B..Cl4[x+1, y, z]	0.91	2.22	3.114(12)	167
N3--H3A..Cl1[x+1, y, z]	0.91	2.15	3.034(10)	163
N3--H3B..Cl2	0.91	2.41	3.189(11)	144
N4--H4A..Cl2	0.91	2.25	3.145(12)	169
N4--H4B..Cl5	0.91	2.22	3.112(11)	166
N6--H6A..Cl1[x, y-1, z]	0.91	2.17	3.077(9)	171
N6--H6B..Cl5	0.91	2.24	3.128(10)	165
N7--H7A..Cl6	0.91	2.29	3.200(10)	173
N7--H7B..Cl4[x, y-1, z]	0.91	2.21	3.106(11)	166
N8--H8A..Cl3	0.91	2.20	3.071(12)	159
N8--H8B..Cl6	0.91	2.40	3.151(12)	140

Figure S3. Molar fraction species distribution diagrams.



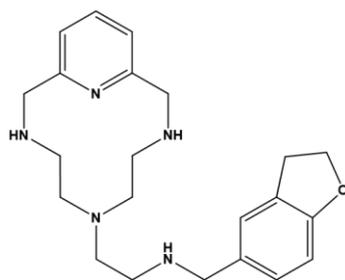
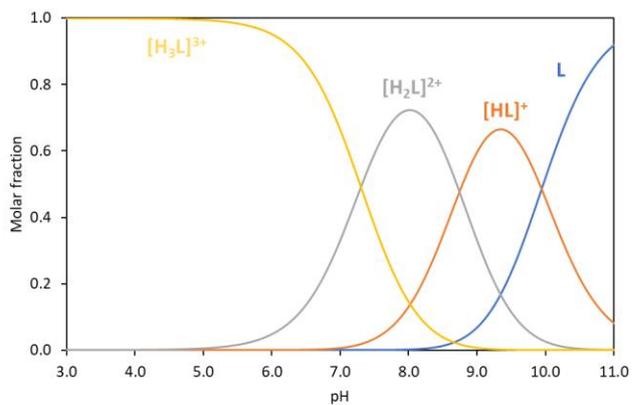
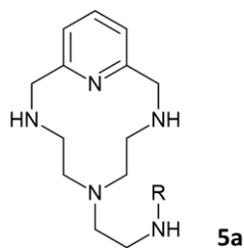
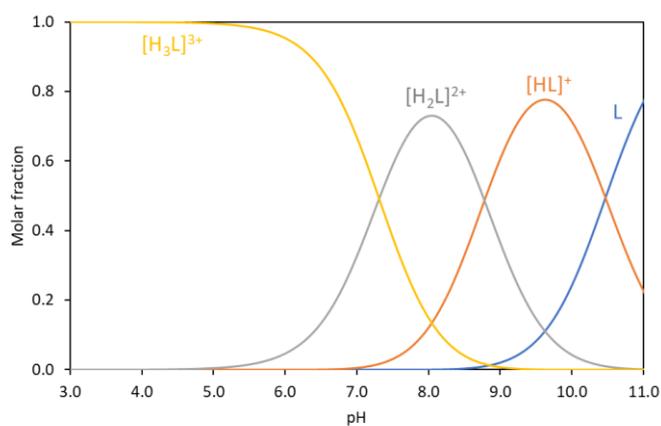
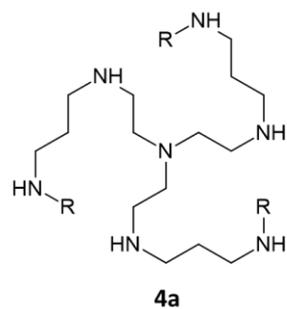
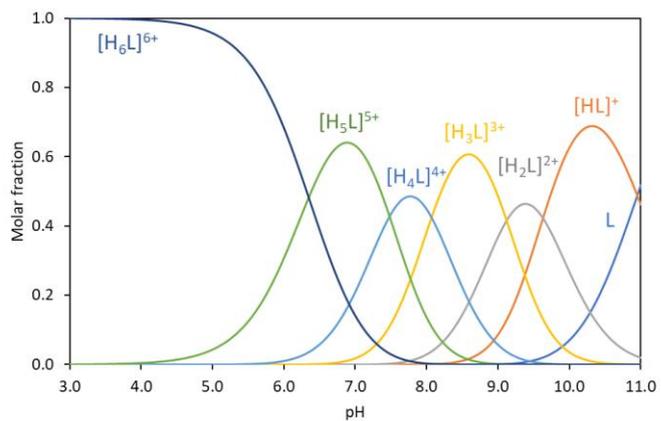


Figure S4. Determination of the minimal microbicidal concentration.

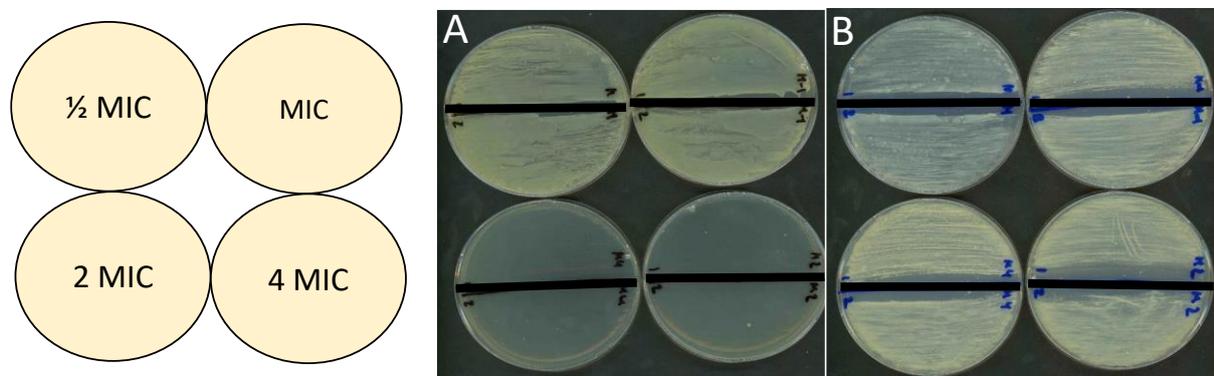
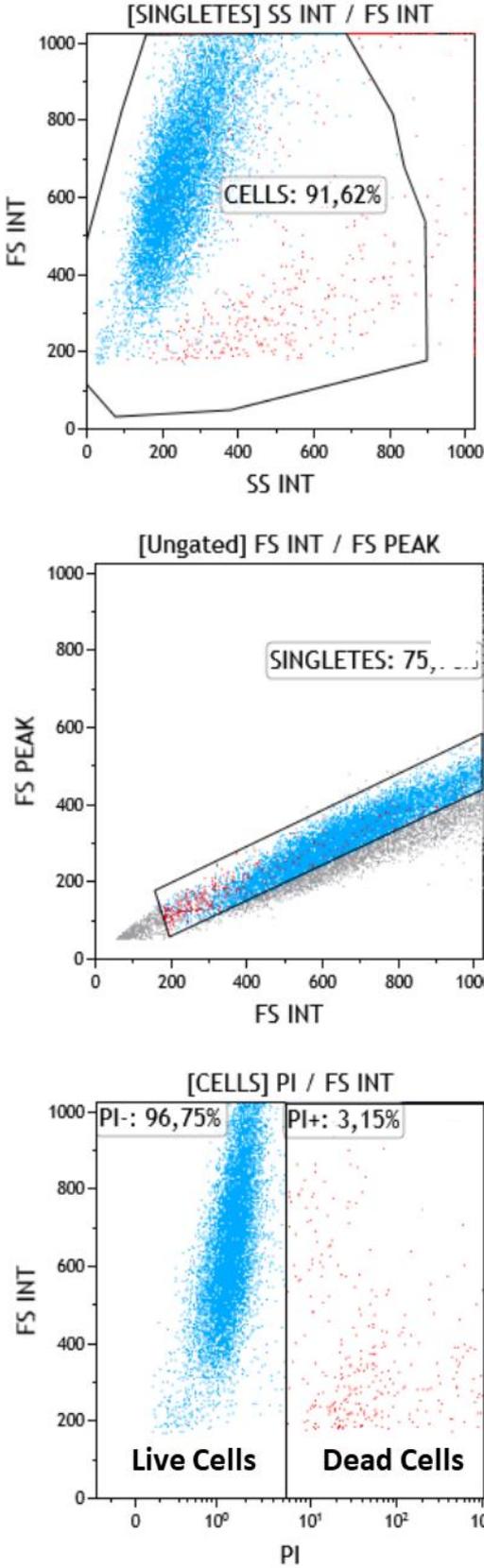


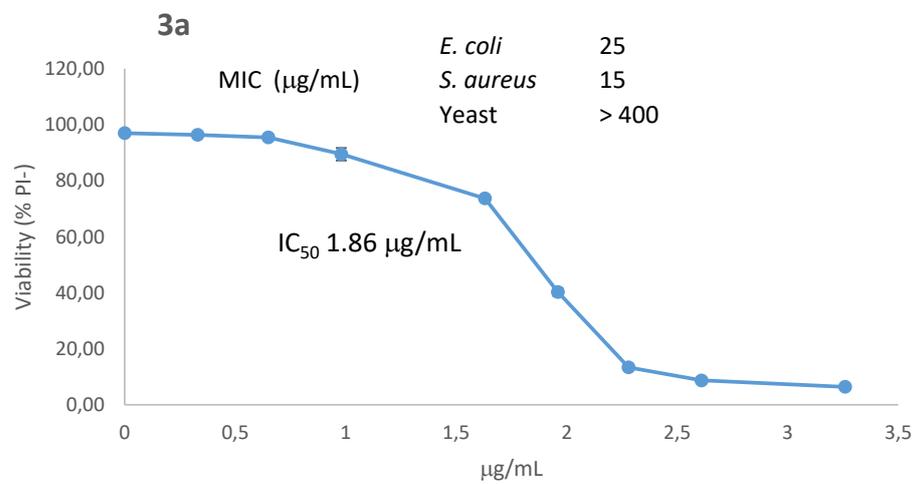
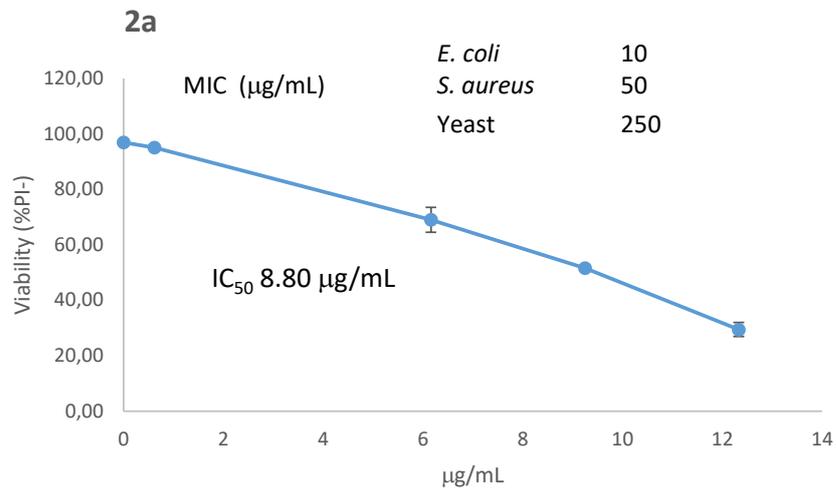
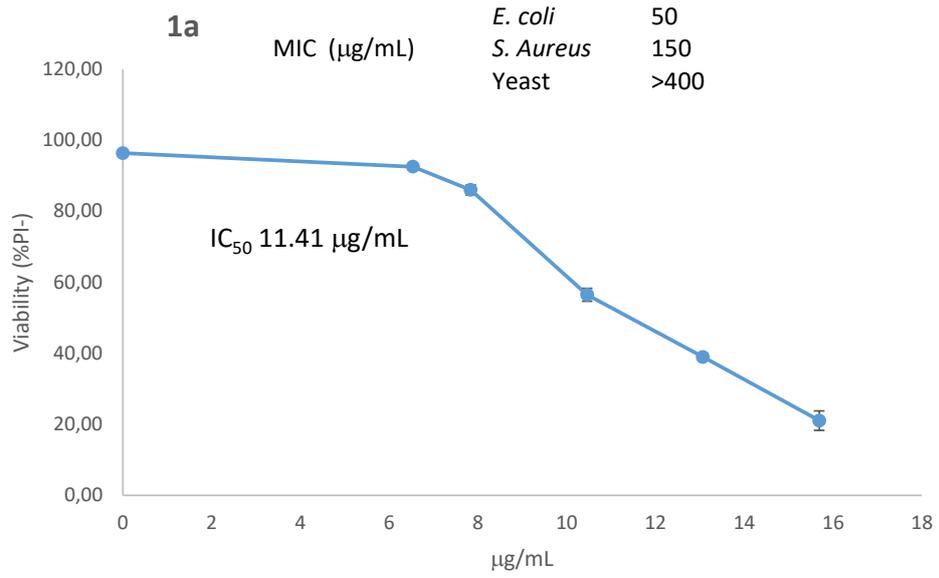
Figure S4. Determination of the minimal microbicidal concentration. On the left, a scheme of the plates used for these experiments is shown. In each sector 30 μ L of a 10-fold dilution of each one of the tubes described in the experimental section were applied. On the right, representative images of the resulting growth in plate are shown. (A) Compound **4a** in *S. aureus*. (B) Compound **4a** in BY4741.

Figure S5. Cytotoxicity determination by FACS.

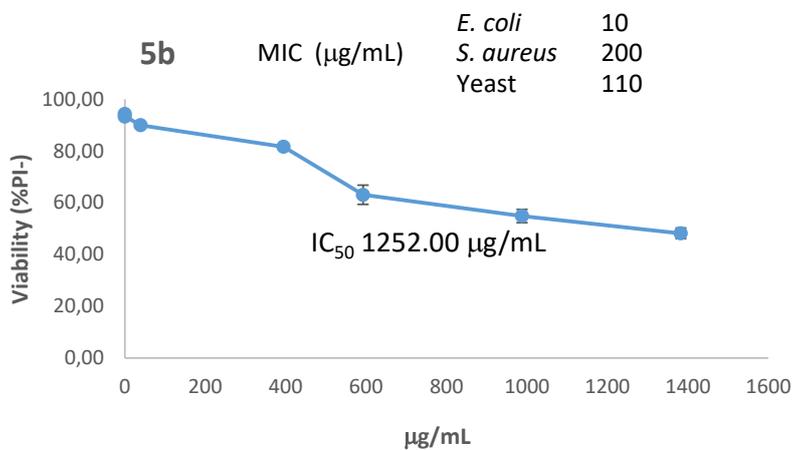
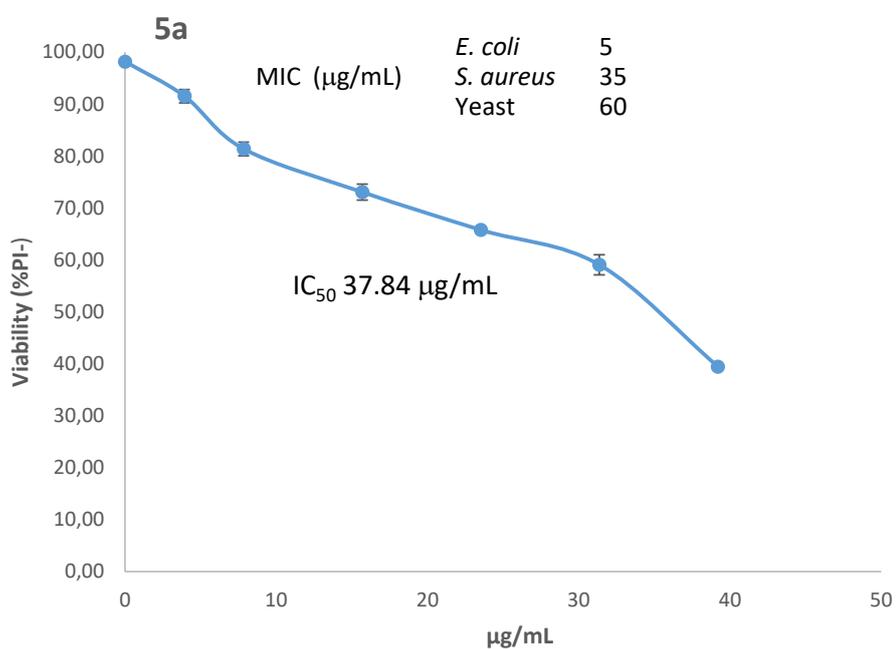
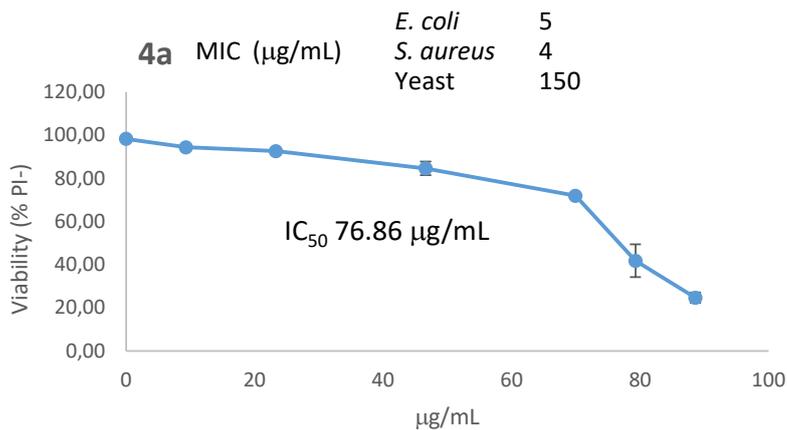
A



B



Bcont



Bcont

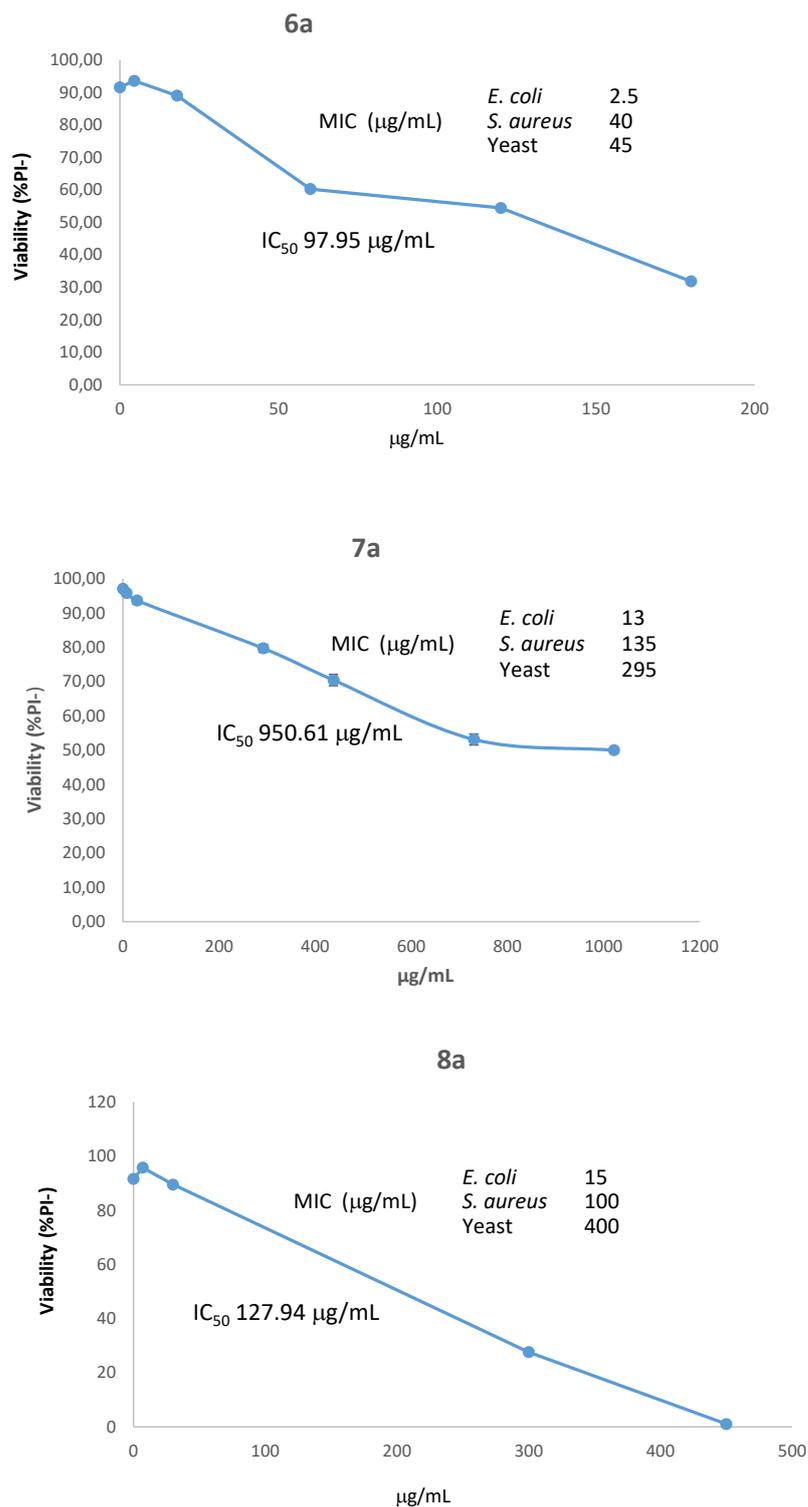


Figure S5. Cytotoxicity determination by FACS. (A) Image of the information provided by these analyses. (B) Graphs showing the variation of the Jurkat cells viability in function of the concentration of the compounds tested.