

Supplementary Materials: Contribution of Molecular Structure to Self-Assembling and Biological Properties of Bifunctional Lipid-Like 4-(*N*-Alkylpyridinium)-1,4-Dihydropyridines

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Table 1. Toxicity test data of tested 4-(*N*-alkylpyridinium)-1,4-dihydropyridine derivatives **3**, **6**, **7**, and **9–11** on microorganism species; each compound boundary concentration is depicted in mM. Values of IC₅₀ on HT-1080 and MH-22A cell lines are included for comparison and are not included in PCA analyses.

Compound		3	6	7	9	10	11
Number of Propargyl Groups		0	1	2	2	0	1
Alkyl Chain Length in Pyridinium		12	12	2	12	16	16
Compounds		Boundary concentration, mM					
Microorganisms							
<i>P. mirabilis</i>	gram negative	0.001	1	0.1	0.01	0.01	0.0001
<i>M. luteus</i>	gram positive	0.001	0.0001	0.001	0.0001	0.001	0.001
<i>P. aeruginosa</i>	gram negative	0.01	0.01	0.01	0.01	10	0.01
<i>B. subtilis</i>	gram positive	0.01	0.0001	0.1	0.01	0.0001	0.0001
<i>K. pneumoniae</i>	gram negative	0.1	0.1	10	0.1	0.01	10
<i>E. coli</i>	gram negative	0.01	0.001	1	0.0001	0.01	0.01
<i>S. cerevisiae</i>	-	0.001	0.001	1	0.0001	0.0001	0.0001
Cell lines		Cytotoxicity, IC ₅₀ , μM					
HT-1080	-	0.037	0.004	1	0.002	-	-
MH-22A	-	0.015	0.001	1	0.001	-	-

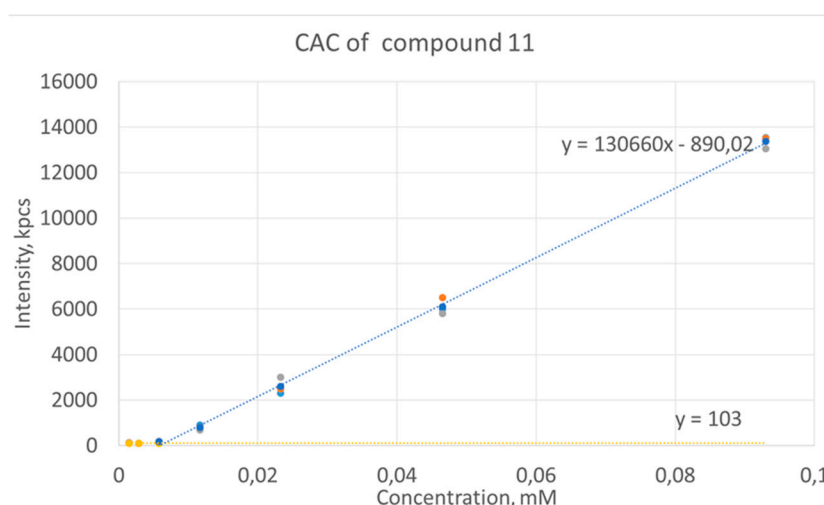


Figure 1. Representative example of determination of critical aggregation concentration (CAC) by DLS method for 4-(*N*-hexadecylpyridinium)-1,4-DHP derivative **11**.

Data of the critical micelle concentration (CAC) was used for data generation of Table 2.