# Supplementary Materials: Synthesis, Structure and Antimicrobial Properties of Novel Benzalkonium Chloride Analogues with Pyridine Ring

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Table S1. Assignments of characteristic <sup>1</sup>H-NMR and <sup>13</sup>C-NMR signals of P13-P18.

	P13		P14		P15		P16		P17		P18	
	${}^{1}\mathrm{H}$	<sup>13</sup> C	${}^{1}\mathrm{H}$	<sup>13</sup> C	${}^{1}\mathrm{H}$	<sup>13</sup> C	1H	<sup>13</sup> C	${}^{1}\mathrm{H}$	<sup>13</sup> C	${}^{1}\mathrm{H}$	<sup>13</sup> C
Α	8.71	150.65	8.71	150.67	8.70	150.66	8.71	150.68	8.71	150.70	8.71	150.68
В	7.73	127.59	7.72	127.59	7.72	127.58	7.73	127.58	7.73	127.59	7.73	127.58
С	-	136.17	-	136.14	-	136.14	-	136.12	-	136.15	-	136.12
D	5.24	65.58	5.26	65.57	5.25	65.57	5.30	65.49	5.30	65.53	5.30	65.49
Ε	3.34	49.86	3.34	49.86	3.34	49.86	3.35	49.79	3.35	49.82	3.35	49.79
F	3.53	64.06	3.53	64.04	3.52	64.02	3.54	64.02	3.54	64.07	3.54	64.02
G	1.80	31.47	1.80	31.71	1.80	31.77	1.80	31.80	1.80	31.82	1.80	31.80
Ι	0.87	13.92	0.88	14.00	0.88	14.00	0.88	14.02	0.88	14.03	0.87	14.03

Table S2. ESI-MS characteristic *m*/*z* peaks of P13–P18.

Common d	ES	SI(+)MS	ESI(-)MS		
Compound	[M] <sup>+</sup>	[2M + Cl] <sup>+</sup>	[M + 2Cl]-		
P13	249	533	319		
<b>P14</b>	277	589	347		
P15	305	645	327		
P16	333	701	403		
P17	361	757	431		
P18	389	813	459		

-	P13	P14	P15	P16	P17	P18	<b>Proposed Assignments</b>	
	3436	3439	3454	3451	3409	3401	ν <b>Ο</b> –Η	
_	3242	3245	3244	3244	-	3265	ν Ο–Η	
	3057	3063	3062	3062	3053	3054		
	-	3034	3035	3034	3035	-	NСЦ	
	3027	3023	3026	3026	3022	3023	V C-I Iaromatic	
_	3008	3005	-	-	3007	3005		
	2977	2985	2983	2983	2979	2979		
	2957	2952	2950	2949	2952	2953	NC Harris	
	2929	2921	2920	2915	2915	2915	V <b>C</b> - <b>Π</b> aliphatic	
_	2858	2850	2850	2850	2851	2851		
	1623	1619	1619	1619	-	1617	$\nu$ C=N, $\nu$ C=Caromatic	
	1597	1601	1602	1602	1600	1600	$\nu$ C=N, $\nu$ C=Caromatic	
	1562	1564	1564	1564	1565	1564	$\nu$ C=N, $\nu$ C=Caromatic	
	1473	1470	1470	1470	1471	1472	$\delta$ C–Haliphatic	
	1415	1415	1419	1419	1417	1415	δ C=N, C=Caromatic	
	1351	1355	1355	1355	1354	1353	$\delta$ C–Haromatic	
	1222	1227	1227	1227	1228	1228	$\delta$ C–Haromatic	
	1069	1074	1074	1074	1073	1072	$\delta$ C–Haromatic	
	1006	996	998	996	996	996	γ C=N, C=Caromatic	
	728	728	729	728	727	728	$\gamma$ CH <sub>2</sub>	

Table S3. The FT-IR bands and assignments of P13–P18.

#### Copies of Spectra of P13-P18.



# P13, FT-IR, KBr









P14



### P14, ATR IR



# P14, ESI-MS, CH<sub>3</sub>OH





P15



# P15, FT-IR, KBr



# P15, ESI-MS, CH<sub>3</sub>OH







### **P17**



**P17** 









#### Conductometric Study of P14-P18.



	Standard Error
78957,20152	996,01981
39902,77242	1066,76532
0,02027	1,43103E-4
0,00115	1,36593E-4
	78957,20152 39902,77242 <b>0,02027</b> 0,00115















