SYNTHESIS AND BIOLOGICAL ACTIVITIES OF *N*-[n-(β-D-GLUCOPYRANOSYLOXY)ALKYL]AMINIUM SALTS

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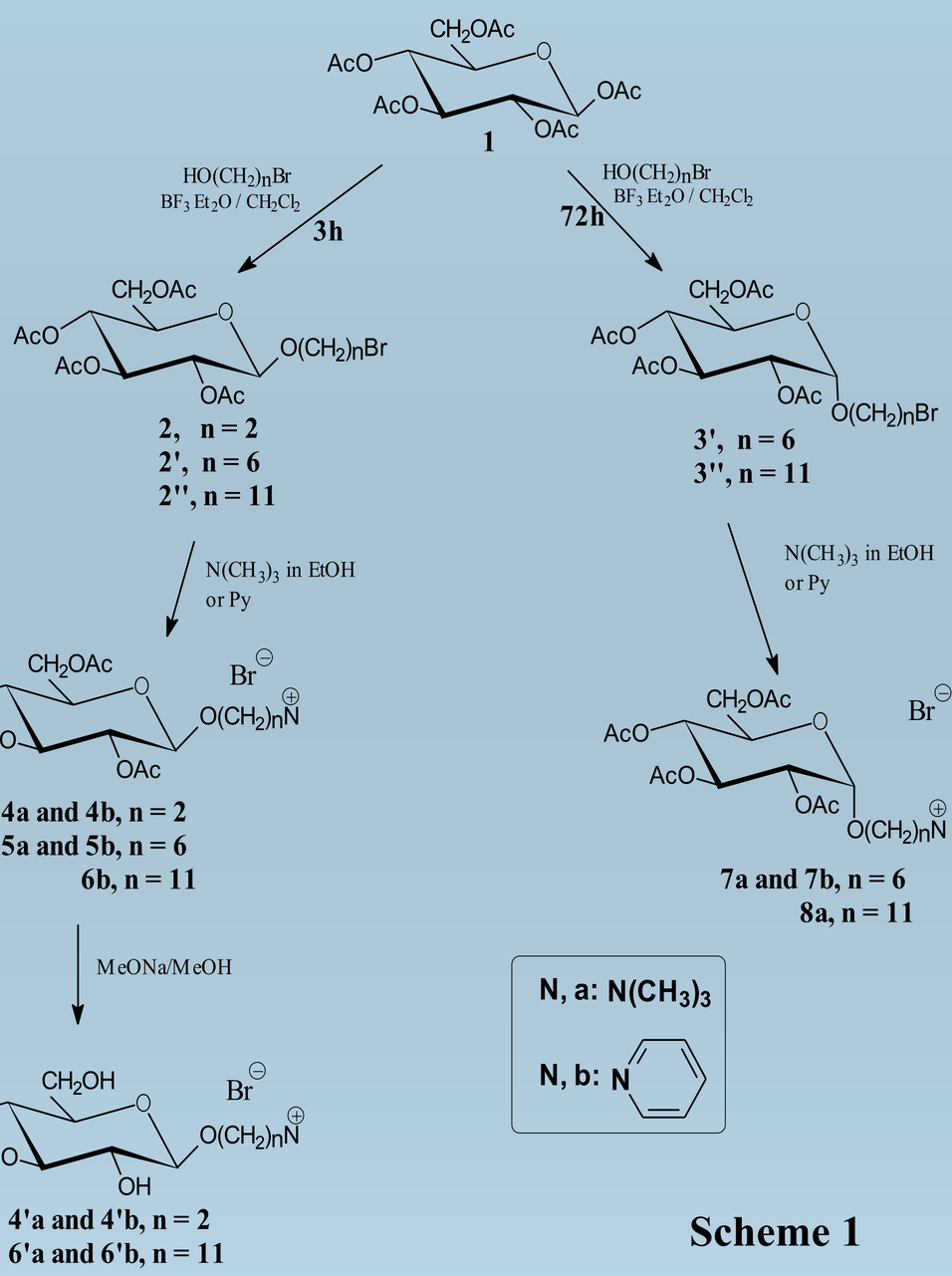
Quaternary ammonium salts (QAS) are extensively used in various applications. They are present in fabric softeners and corrosion inhibitors, they act as fungicides, pesticides and insecticides, they reveal antibacterial and antifungal activities employed in antimicrobial drugs, and they are ingredients of shampoos and hair conditioners. Therefore, global use of QAS in industry, agriculture, healthcare and domestic approaches is doubtless. Although toxicity of some QAS has been reported, majority of these compounds were reported as non-toxic or of low toxicity. Therefore, QAS are generally believed to be safe.

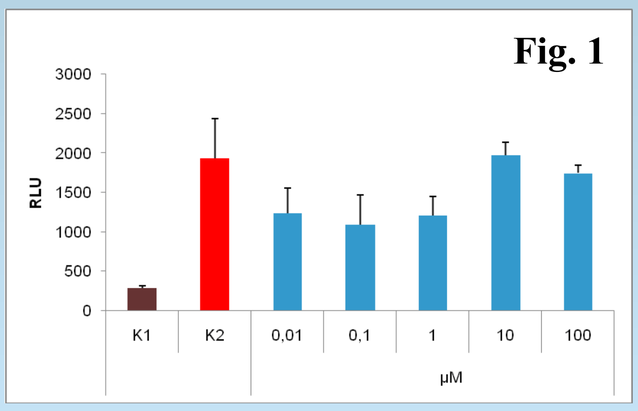
A new series of quaternary ammonium bromides have been synthesized in reaction of (n-bromoalkyl) 2,3,4,6-tetra-*O*-acetyl-β-D-glucopyranoside (n = 2, 6, 11) with two tertiary amines: pyridine and trimethylamine (Scheme 1) according to the Menschutkin's procedure (Menschutkin 1890) gave quaternary ammonium salts (Scheme 1). The structures of isolates were determined by spectral analysis including NMR (Table 1) analyses and X-ray crystallography (Fig. 3, 4). QACs demonstrated mutagenic activity, Fig. 1 for trimethylaminium salts (4a, 4'a) and Fig. 2 for pyridinium salts (4b, 4'b), in bioluminescence mutagenicity assay based on *Vibrio harveyi* A16 strain.



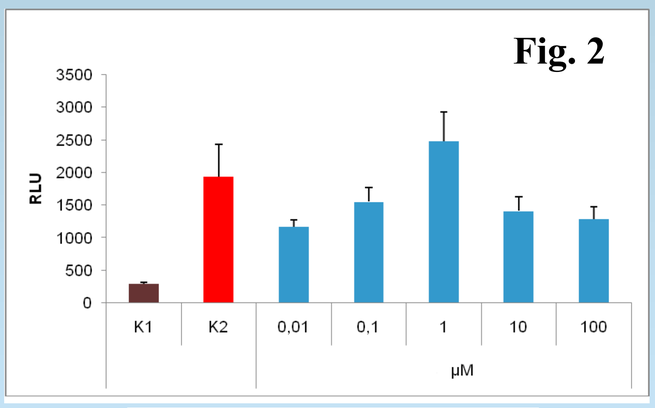
Scheme 1

Table 1. Chemical shifts of sugar protons (ppm) in the ^{1}H NMR spectra for ammonium salts in D_2O solution.

	n	H-1	H-2	H-3	H-4	H-5	H-6	H-6'
4a	**2**	4.90; **d,** 1H	5.03; **dd**, 1H	5.37; **t**, 1H	5.13; **t**, 1H	4.06; **m**, 1H	4.13; **dd**, 1H	4.39; **dd**, 1H
4b	**2**	4.74; **d,** 1H	4.84; **dd**, 1H	5.23; **t**, 1H	4.97; **t**, 1H	3.90; **m**, 1H	4.04; **dd**, 1H	4.23; **dd**, 1H
4'a	**2**	4.46; **d,** 1H	3.26; **t**, 1H	3.44; **q**, 1H	3.34; **t**, 1H	3.42; **dt**, 1H	3.68; **m**, 1H	3.87; **m**, 1H
4'b	**2**	4.38; **d,** 1H	3.18; **t**, 1H	3.27; **dd**, 1H	3.37; **m**, 1H	3.35; **m**, 1H	3.58; **q**, 1H	3.80; **dd**, 1H
5a	**6**	4.78; **d,** 1H	4.88; **dd**, 1H	5.29; **t**, 1H	5.05; **t**, 1H	3.99; **m**, 1H	4.16; **dd**, 1H	4.32; **dd**, 1H
5b	**6**	4.75; **d,** 1H	4.85; **t**, 1H	5.28; **t**, 1H	5.03; **t**, 1H	3.97; **m**, 1H	4.15; **dd**, 1H	4.30; **dd**, 1H
7a	**6**	5.12; **d,** 1H	4.99; **dd**, 1H	5.38; **t**, 1H	5.05; **t**, 1H	4.14; **m**, 1H	4.15; **dd**, 1H	4.30; **dd**, 1H
7b	**6**	5.10; **d,** 1H	4.97; **dd**, 1H	5.36; **t**, 1H	5.04; **t**, 1H	4.15; **m**, 1H	4.13; **dd**, 1H	4.28; **dd**, 1H
6b	**11**	4.48; **d,** 1H	4.95; **m,** 1H	5.18; **dd,** 1H	5.05; **m,** 1H	3.68; **m,** 1H	4.25; **dd,** 1H	4.12; **dd,** 1H
8a	**11**	5.08; **m,** 1H	4.86; **dd,** 1H	5.50; **dd,** 1H	5.60; **m,** 1H	4.03; **m,** 1H	4.11; **dd,** 1H	5.28; **dd,** 1H
6'a	**11**	4.24; **d,** 1H	3.92 – 3.22 **m**, 4H				3.88; **m,** 1H	3.66; **dd,** 1H
6'b	**11**	4.27; **d,** 1H	3.19; **t,** 1H	3.40 – 3.26 **m**, 3H			3.88; **dd,** 1H	3.69; **dd,** 1H



K1 – control 0; **K2** – control MeIQ, 0.1μM



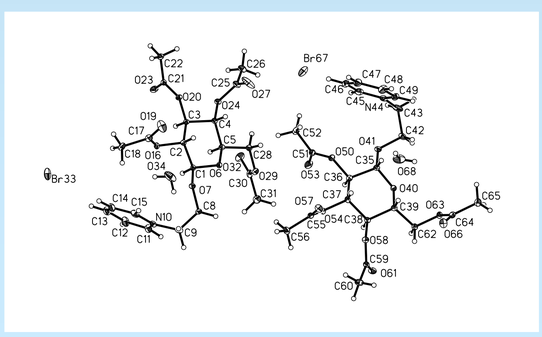


Fig. 3. The X-ray structure of **4b**

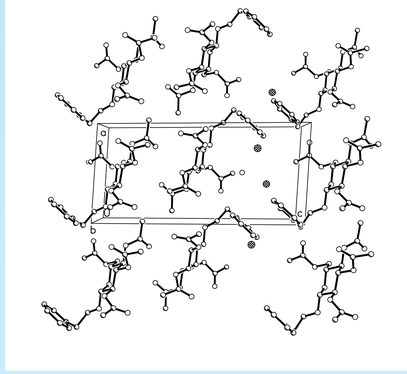


Fig. 4. Molecular packing of **4b**

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