

Table: Analytical data of the bis(ammonio)alkane compounds.

no.	Anal. (mol wt)	mp (°C)	IR (v, cm ⁻¹)
1b	(C ₃₄ H ₄₈ Br ₂ N ₄ O ₄) C,H,N 736.6	223-226	2960, 1760, 1710, 1610, 1380, 730
1c	(C ₃₆ H ₅₂ Br ₂ N ₄ O ₄) C,H,N 764.7	237-238 (dec.)	2960, 1770, 1710, 1610, 1390, 730
2a	(C ₃₃ H ₄₆ Br ₂ N ₄ O ₄) C,H,N 722.6	239	2950, 1770, 1710, 1405, 1380, 730
2b	(C ₃₅ H ₅₀ Br ₂ N ₄ O ₄) C,H,N 750.6	198-200	2960, 1770, 1710, 1610, 1460, 1380, 720
2c	(C ₃₅ H ₅₀ Br ₂ N ₄ O ₄) C,H,N 750.6	208-210	2940, 1760, 1710, 1610, 1360, 730
3a	(C ₃₄ H ₄₈ Br ₂ N ₄ O ₄) C,H,N 736.6	238	2970, 1765, 1700, 1370, 740
3b	(C ₃₆ H ₅₂ Br ₂ N ₄ O ₄) C,H,N 764.6	119-121	2940, 1760, 1700, 1610, 1380, 870, 740
3c	(C ₃₈ H ₅₆ Br ₂ N ₄ O ₄) C,H,N 792.7	198-200 (dec.)	2960, 1760, 1610, 1380, 1080, 740

Table: ^1H NMR data of the bis(ammonio)alkane compounds (δ (ppm), DMSO- d_6);

s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet.

no.	1b	1c	2a	2b	2c	3a	3b	3c
phth- CH_3	-	-	2.48 (s)	2.48* (s)	2.48* (s)	2.48 (s)	2.48* (s)	2.49 (s)
phth	7.83-7.91 (m)	7.84-7.94 (m)	7.64-7.86 (m)	7.64-7.78; 7.83-7.89 (m)	7.63-7.88 (m)	7.60-7.67 (m) 7.73 (d)	7.63-7.77 (m)	7.65 (d) 7.70 (s) 7.77 (d)
N- CH_2 -	3.49 (m) 3.66 (t)	3.50 (m)	3.64 (m)	3.48 (m) 3.65 (t)	3.50 (m) 3.64 (t)	3.63 (t, 6.3)	3.48 (m) 3.63 (t)	3.49 (m)
N- CH_2 - <u>CH_2</u>	2.06 (m)	-	2.06 (m)	2.07 (m)	2.06 (m)	2.05 (m)	2.05 (m)	-
C(CH_3) $_2$ -	1.23 (s)	1.23 (s)	-	1.22 (s)	1.23 (s)	-	1.22 (s)	1.22 (s)
$\text{CH}_2\text{-N}^+$	3.41 (m)	3.39 (m)	3.36 (m)	3.40 (m)	3.42 (m)	3.42 (m)	3.36 (m) 3.43 (m)	3.43 (m)
$\text{N}^+(\text{CH}_3)_2$	3.03 (s) 3.17 (s)	3.18 (s)	3.02 (s)	3.03 (s) 3.18 (s)	3.04(s) 3.18(s)	3.03 (s)	3.03 (s) 3.18 (s)	3.18 (s)
$\text{N}^+\text{-CH}_2$	3.27 (m) 3.35 (m)	3.27 (m)	3.27 (m)	3.30 (m) 3.33 (m)	3.28 (m)	3.27 (m)	3.28 (m) 3.29 (m)	3.29 (s)
$\text{N}^+\text{-CH}_2$ - <u>CH_2</u>	1.72 (m)	1.77 (m)	1.65 (m)	1.76 (m)	1.72 (m)	1.66 (m)	1.72 (m)	1.78 (m)
$\text{N}^+\text{-CH}_2$ - <u>$\text{CH}_2\text{-CH}_2$</u> -	1.32 (m)	1.29 (m)	1.29 (m)	1.32 (m)	1.32 (m)	1.30 (m)	1.32 (m)	1.35 (m)

*partially hidden by DMSO- d_6 signal

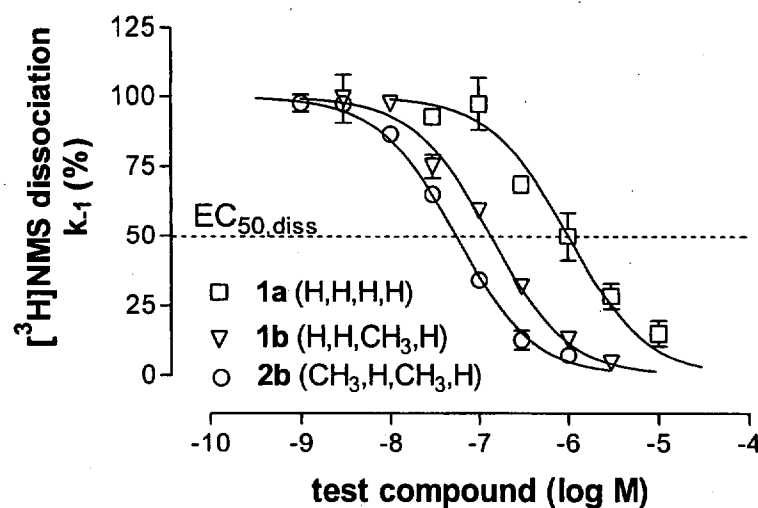


Figure: Concentration/effect-curves for the inhibition of $[^3\text{H}]\text{NMS}$ dissociation by the indicated test compounds. Ordinate: apparent rate constant k_{-1} of $[^3\text{H}]\text{NMS}$ dissociation from muscarinic M_2 receptors expressed as percentage of the control value. Abscissa: concentration of the test compound. Indicated are mean values $\pm$ S.E.M. of three independent experiments. Error bars are not shown when they are smaller than the symbols. Sigmoidal curve fitting. Slope factors n_H were not significantly different from unity ($P > 0.05$, F-test).

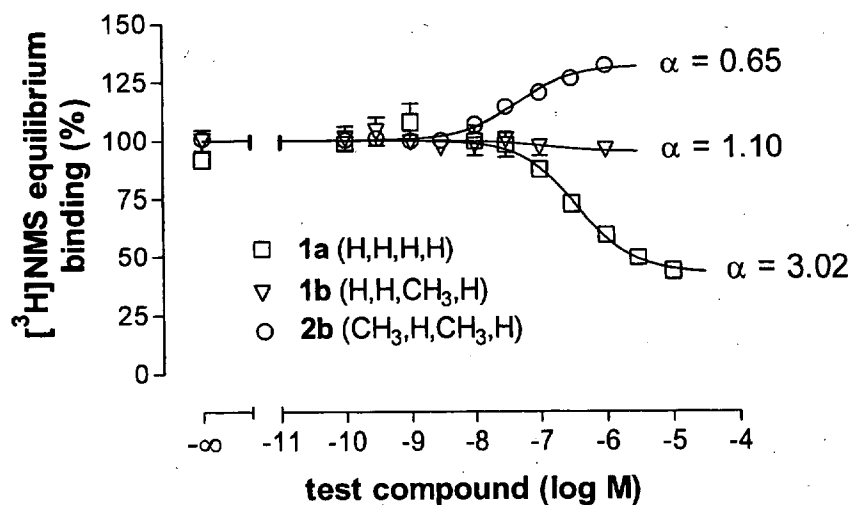


Figure: Effects of the indicated test compounds on the equilibrium binding of [³H]NMS. Ordinate: specific [³H]NMS binding in percent of the control value in the absence of test compound as indicated by the starting value of the binding curve. Abscissa: concentration of the test compound. Indicated are mean values $\pm$ S.E.M. of three independent experiments. Error bars are not shown when they are smaller than the symbols. Curve fitting was based on the ternary complex model of allosteric interactions. α is the factor of cooperativity between the allosteric agent and [³H]NMS.