Electronic Supplementary Material (ESI) for MedChemComm.

Supporting Information

Effects of polar κ receptor agonists designed for the periphery on ATP-induced Ca^{2+} release from keratinocytes

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Table SI1: Comparison of recorded and reported $logD_{7.4}$ values of reference compounds

compound	log $D_{7.4}$ ± SEM (number of experiments)[a)]	log $D_{7.4}$ [b)]
phenazone	0.29 ± 0.11 (n=9)	0.38
propranolol	0.96 ± 0.04 (n=9)	1.26
lidocaine	1.74 ± 0.01 (n=8)	1.71
impiramine	2.26 ± 0.04 (n=8)	2.40
haloperidol	2.87 ± 0.11 (n=9)	2.98
chlorpromazine	3.12 ± 0.01 (n=9)	3.40

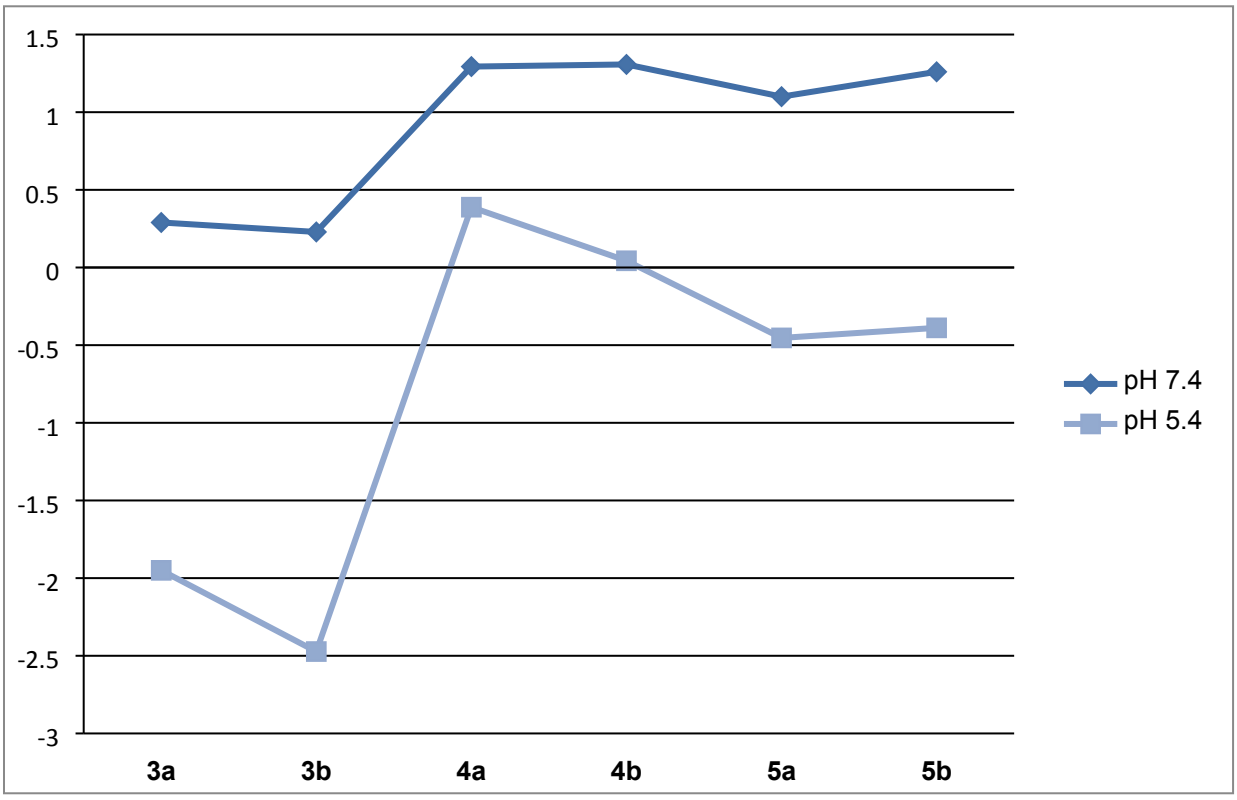
[a)] $logD_{7.4}$ values obtained by shake flask / LC-MS method

[b)] log $D_{7.4}$ taken from literature[1]

Table SI2: ESI source parameters used for the ionization of the test compouds **3a**,**b** - **5a**,**b** and the reference compounds.

Compound	SIM ion [m/z]	fragmentor voltage [V]	dry gas temperature [°C]
3a	396	140	200
3b	412	140	200
4a	454	150	200
4b	470	150	200
5a	488	160	200
5b	504	170	200
phenazone	189	150	350
propranolol	260	150	350
lidocaine	235	150	300
imipramine	281	150	350
haloperidol	376	150	350
chlorpromazine	319	120	260

Figure SI1: logD values determined by distribution between *n*-octanol and MOPS buffer. The upper line shows the development of the $logD_{7.4}$ values and the lower line the $logD_{5.4}$ values.



Reference

1. F. Lombardo, M. Y. Shalaeva, K. A. Tupper, F. Gao, *J. Med. Chem* **2001**, *44*, 2290-2497.