

Supplementary Information

Modelling ligand depletion for simultaneous affinity and binding site quantification on cells and tissue

Judith Weber¹, Klara Djurberg², Sara Lundsten Salomonsson^{2,3}, Maria Kamprath¹, Aileen Hoehne¹, Hadis Westin², Fernanda Vergara¹, Sina Bondza^{*2,3}

¹ 3B Pharmaceuticals GmbH, Berlin, Germany

² Ridgeview Instruments AB, Uppsala, Sweden

³ Department of Immunology, Genetics and Pathology, Uppsala University, Uppsala, Sweden

*Corresponding author: s.bondza@ridgeviewinstruments.com

Supplementary Tables

Table 1. Cell concentration [cells/mL] for plates used for experiments with varying cell numbers between experiments. Cells were seeded one day prior the experiment. 3 mL cell suspension was used for seeding per plate.

CELL LINE	CELL CONCENTRATION [CELLS/ML]							
	Exp.1	Exp.2	Exp.3	Exp.4	Exp.5	Exp.6	Exp.7	Exp.8
HEK-FAP	1E+06	5E+05	1E+06	5E+05	1E+06	2E+06	1E+06	2E+06
PC3-PIP	1E+06	5E+04	1E+06	5E+05	1E+05	5E+05	n.a.	n.a.

Table 2. HPLC retention times of radiolabeled test compounds

TEST COMPOUND	RETENTION TIME [MIN]
¹¹¹ In-GIPR-TRACER	6.9
¹¹¹ In-FAP-TRACER	7.6
¹¹¹ In-PSMA-TRACER	5.8

Table 3. Parameter intervals for simulation of curves

PARAMETER	LOWER LIMIT	UPPER LIMIT
Log(k _a)	3	6
Log(k _d)	-6	-3
Log(nB)	10	14

Table 4. Concentration series of simulated three association phases data

CONCENTRATION ASSOCIATION 1 (nM)	CONCENTRATION ASSOCIATION 2 (nM)	CONCENTRATION ASSOCIATION 3 (nM)
0.3	1	3
1	3	5
1	10	20
1	3	9
0.3	1	10

Table 5. Concentration series of simulated two association phases data

CONCENTRATION ASSOCIATION 1 (nM)	CONCENTRATION ASSOCIATION 2 (nM)
1	3
1	9
3	9