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Experimental validation of a computationally-designed tiotropium membrane sensor

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Table (1S) Factors and its corresponding levels for quantitative optimisation of membrane sensor and the measure response of randomly ordered experiments.

Experiment No. ^a	Contentious factors			Response
	Ion exchanger	Ionophore	NPOE/PVC ratio	Detection limit
	TFPB (mmol Kg ⁻¹)	CX8 (mmol Kg ⁻¹)	(Total weigh, mg) ^b	(Log[C], mol L ⁻¹) ^c
5	4.5	5	1.0 (595)	-6.60
9	4.0	10	2.0(593)	-6.85
10	4.0	15	1.5(590)	-6.49
3	5.0	15	1.0 (590)	-6.57
2	5.0	5	1.5(595)	-6.67
7	4.0	10	1.0 (593)	-6.75
1	4.0	5	2.0 (595)	-6.55
4	4.5	10	2.0 (593)	-6.85
11	5.0	10	1.5 (592)	-6.80
6	5.0	15	2.0 (590)	-6.57
8	4.5	15	1.5 (590)	-6.52

^aExperiments are arranged in random order of execution

^b values in parentheses are the total weight of NPOE and PVC in milligrams for each experiment.

^c Detection limits were estimated for each sensor at the point where this linear segment of calibration plot intersects with the extrapolated arm of background potential