Electronic Supplementary Material (ESI) for Analytical Methods.

Detrimental Impact of Aqueous Mobile Phases in 18F-labelled Radiopharmaceutical Analysis via Radio-TLC

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Supplementary Information

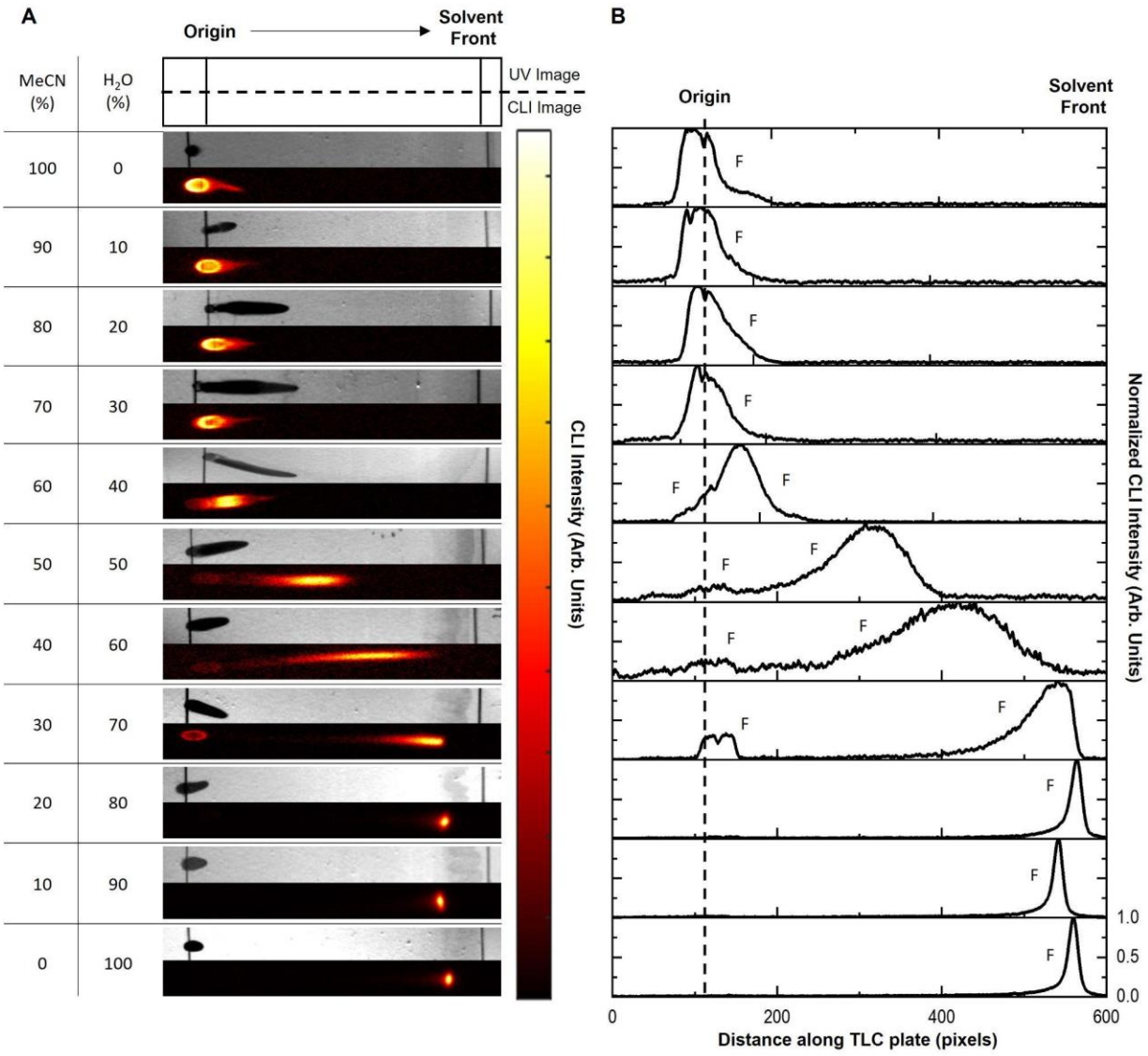
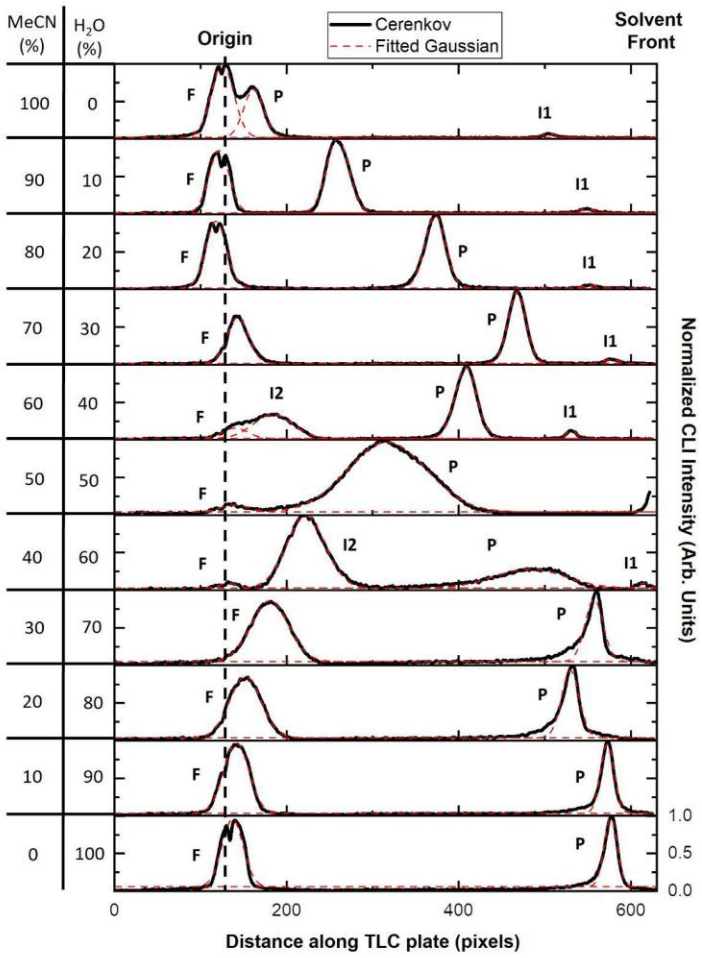


Figure S1. The effect of aqueous mobile phases (MeCN:H_2O) on the migration of [^{18}F]KF/K_{222}. **(A)** For each mobile phase composition, two images are shown: a UV image of the TLC plate spotted with K_2CO_3/K_{222} and stained with I_2 (top) and a CLI image of a TLC plate spotted with [^{18}F]KF/K_{222} (middle). **(B)** TLC chromatograms generated from the CLI images. F denotes [^{18}F]KF/K_{222}.

Table S1. Impact of water composition in aqueous mobile phases (MeCN:H_2O) on the R_f of [^{18}F]KF/K_{222}.

MeCN (%)	H_2O (%)	R_f
100	0	0.0
90	10	0.0
80	20	0.0
70	30	0.0
60	40	0.0, 0.16
50	50	0.0, 0.40
40	60	0.0, 0.53
30	70	0.0, 0.77
20	80	0.88
10	90	0.92
0	100	0.93

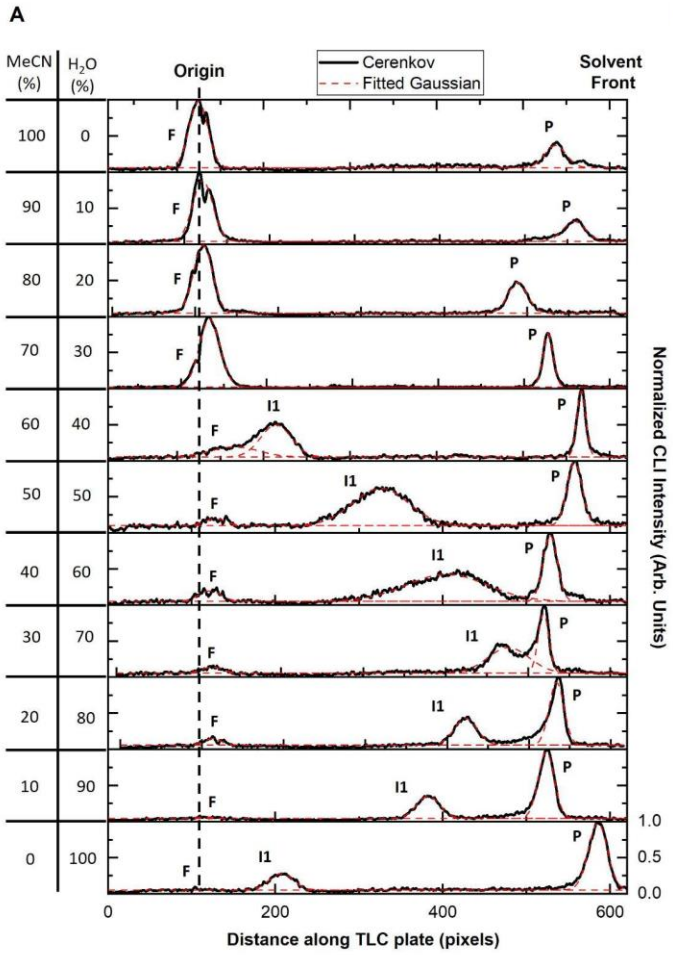
A



B

[18F]fluoride (%)	Impurity (%)	[18F]Fallypride (%)
62	2	36
42	2	56
43	1	56
42	2	56
9	33, 3	55
3	0	96
2	65, 1	32
62	0	38
62	0	38
62	0	38
62	0	38

Figure S2. The adverse impact of water-containing mobile phases in the naive calculation of fluorination efficiency for [^{18}F]Fallypride. **(A)** Chromatograms of samples of [^{18}F]Fallypride/[^{18}F]TBAF separated under different compositions of MeCN:H_2O mobile phases replicated from Figure 3. Chromatograms are annotated with the following naive assignment of bands: F ([^{18}F]fluoride, assumed at origin), P (radiopharmaceutical product, confirmed with the spotting of Fallypride standard); I_i (additional band(s), naively assumed to be impurities). **(B)** The computed proportion of each species based on naive assumptions. The actual proportions of [^{18}F]TBAF and [^{18}F]Fallypride in the samples were 44% and 56%, respectively.

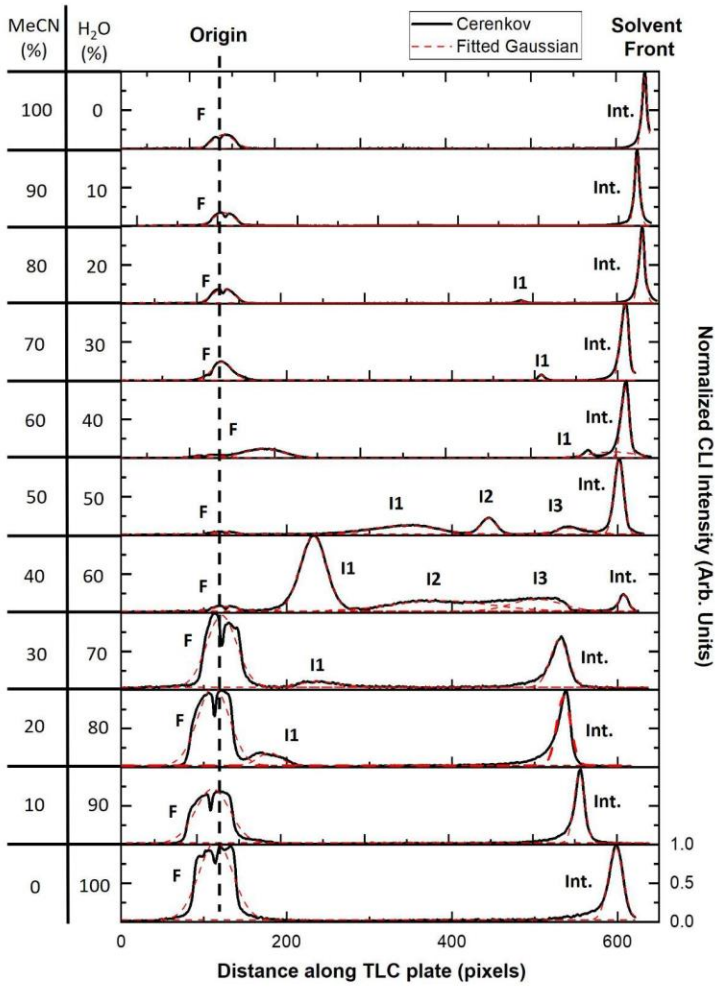


B

[^{18}F]fluoride (%)	Impurity (%)	[^{18}F]FMZ (%)
72	0	28
73	0	27
70	0	30
72	0	28
23	48	29
5	65	30
7	65	28
7	58	35
7	37	56
2	32	66
0	24	76

Figure S3. The adverse impact of water-containing mobile phases in the naive calculation of fluorination efficiency for [^{18}F]FMZ. **(A)** Chromatograms of samples of [^{18}F]FMZ/[^{18}F]TBAF separated under different compositions of MeCN:H_2O mobile phases replicated from Figure 4. Chromatograms are annotated with the naive assignment of bands: F ([^{18}F]fluoride, assumed at origin), P (radiopharmaceutical product, confirmed with the spotting of FMZ standard); I_i (additional band(s), naively assumed to be impurities). **(B)** The computed proportion of species is based on naive assumptions. The samples' actual proportions of [^{18}F]TBAF and [^{18}F]Fallypride were 72% and 28%, respectively.

A



B

[18F]fluoride (%)	Impurity (%)	[18F]FET-Intermediate (%)
39	0	61
39	0	61
38	3	59
35	4	61
6	29, 21	45
3	32, 13, 12	40
3	50, 27, 16	4
67	6	27
67	8	26
71	0	29
71	0	29

Figure S4. The adverse impact of water-containing mobile phases in the naive calculation of fluorination efficiency for [^{18}F]FET-intermediate. **(A)** Chromatograms of samples of [^{18}F]FET-intermediate/[^{18}F]TBAF separated under different compositions of MeCN:H_2O mobile phases replicated from Figure 5. Chromatograms are annotated with the naive assignment of bands: F ([^{18}F]fluoride, assumed at origin), P (radiopharmaceutical product, assumed at the solvent front); I_i (additional band(s), naively assumed to be impurities). **(B)** The computed proportion of species is based on naive assumptions. The actual proportions of [^{18}F]TBAF and [^{18}F]FET-intermediate in the samples were 39% and 61%, respectively.