sensors

MDPI

Supplementary Materials for

Fluorescence Spectra of Prototropic Forms of Fluorescein and Some Derivatives and Their Potential Use for Calibration-Free pH Sensing

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Table S1. Designation, supplier, and part numbers.

Part N° in Figure 1	Designation	Supplier/Country	Reference
1	Light emitting diode	Thorlabs, USA, supplier France	M470F3
2	Multimode patch cable	Thorlabs, USA, supplier France	M19L01
3	Variable attenuator	CivilLaser, China	FVA-UV
4	Fluorescence beam splitter Including: Exc. filter #1 Exc. filter #2 Dicroic mirror Em. filter	DORIC Lenses, Canada Semrock, supplier France Optoprim Semrock, supplier France Optoprim Semrock, supplier France Optoprim Semrock, supplier France Optoprim	Custom assembled FF01-457/50-25 FF01-474/27-25 LPD02-488RU-25 LP02-488RU-25
5	Custom patch cable	DORIC Lenses, Canada	Custom assembled
6	Ferule interconnect	Thorlabs, USA, supplier France	ADAF2
7	Custom bare fiber Including: Multimode fiber	DORIC Lenses, Canada Thorlabs, USA, supplier France	CuFG200UEAstom assembled
8	Test solution Containing: NaCl 1M Fluorescein FITC FAM pH adjusted with: Nafion, 50 µm OH- ion exchange resin	 Merck, Sigma Aldrich, Germany, supplier France Merck, Sigma Aldrich, Germany, supplier France MedChemTronica, Sweden MedChemTronica, Sweden IonPower, US Merck, Sigma Aldrich, Germany, supplier France	 CAS: 7647-14-5 CAS: 2321-07-5 CAS: 3326-32-7 CAS: 3301-79-9 NR212 CAS: 39339-85-0
9	Magnetic stirrer	LLG LABWARE, Germany, supplier France	uni*STIRRER* 1
10	pH meter	Hanna Instruments France, France	HI 991001
11	Multimode patch cable	Thorlabs, USA, supplier France	M22L01
12	Spectrometer	Ocean Optics, USA, supplier France	QE Pro ES
13	Computer	Non-applicable	

Table S2. List of parameters for each molecule including starting values for the minimization algorithm.

		Molecule		
Coefficient	**Starting Value**	**Fluorescein**	**FITC**	**FAM**
$\widetilde{K}a_1$	1.00×10^{-2}	9.25×10^{-4}	1.90×10^{-2}	1.54×10^{-2}
$\widetilde{K}a_2$	1.00×10^{-5}	5.66×10^{-6}	5.26×10^{-6}	4.04×10^{-5}
$\widetilde{K}a_3$	1.00×10^{-6}	5.46×10^{-7}	9.43×10^{-7}	2.79×10^{-6}
Aa1	0.28	0.21	0.27	0.23
Aa2	0.44	0.38	0.37	0.32
Aa3	0.47	0.55	0.56	0.53
Ac1	0.23	0.28	0.21	0.10
Ac2	0.30	0.29	0.30	0.26
Ac3	0.74	0.75	0.66	0.80
Ad1	0.41	0.40	0.43	0.45
Ad2	0.08	0.07	0.08	0.04
Ad3	0.73	0.77	0.73	0.67
An1	0.45	0.44	0.43	0.52
An2	0.63	0.67	0.64	0.63
An3	0.32	0.27	0.32	0.30
Ta1	620	467.25	581.37	649.77
Ta2	1000	952.70	985.78	1939.47
Ta3	2768	3080.75	2857.80	3717.31
Tc1	995	1111.72	940.00	1115.80
Tc2	4091	4681.94	4699.53	4551.25
Tc3	2783	2722.59	2952.21	3133.19
Td1	1843	1835.51	1887.99	2194.87
Td2	2978	2744.48	3032.09	3193.47
Td3	1084	1154.68	1236.10	1149.87
Tn1	1108	1129.23	1095.53	1198.29
Tn2	4021	3812.93	3784.18	3724.71
Tn3	1424	1231.79	1536.62	1308.06
Ya1	507	507.33	512.23	513.00
Ya2	518	516.72	523.52	520.97
Ya3	532	523.61	536.07	533.80
Yc1	509	504.95	527.39	508.53
Yc2	570	570.19	565.38	573.55
Yc3	535	536.12	553.71	533.70
Yd1	534	536.59	543.35	533.83
Yd2	565	573.52	578.71	593.04
Yd3	511	511.42	517.58	512.28
Yn1	508	510.47	512.86	511.12
Yn2	544	544.33	552.35	549.95
Yn3	542	543.47	544.51	545.73