Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information (ESI)

Novel PET-Operated Rosamine Sensor Dyes with Substitution Pattern-Tunable pKa Values and Temperature Sensitivity

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Content:

1. **Synthetic procedure**

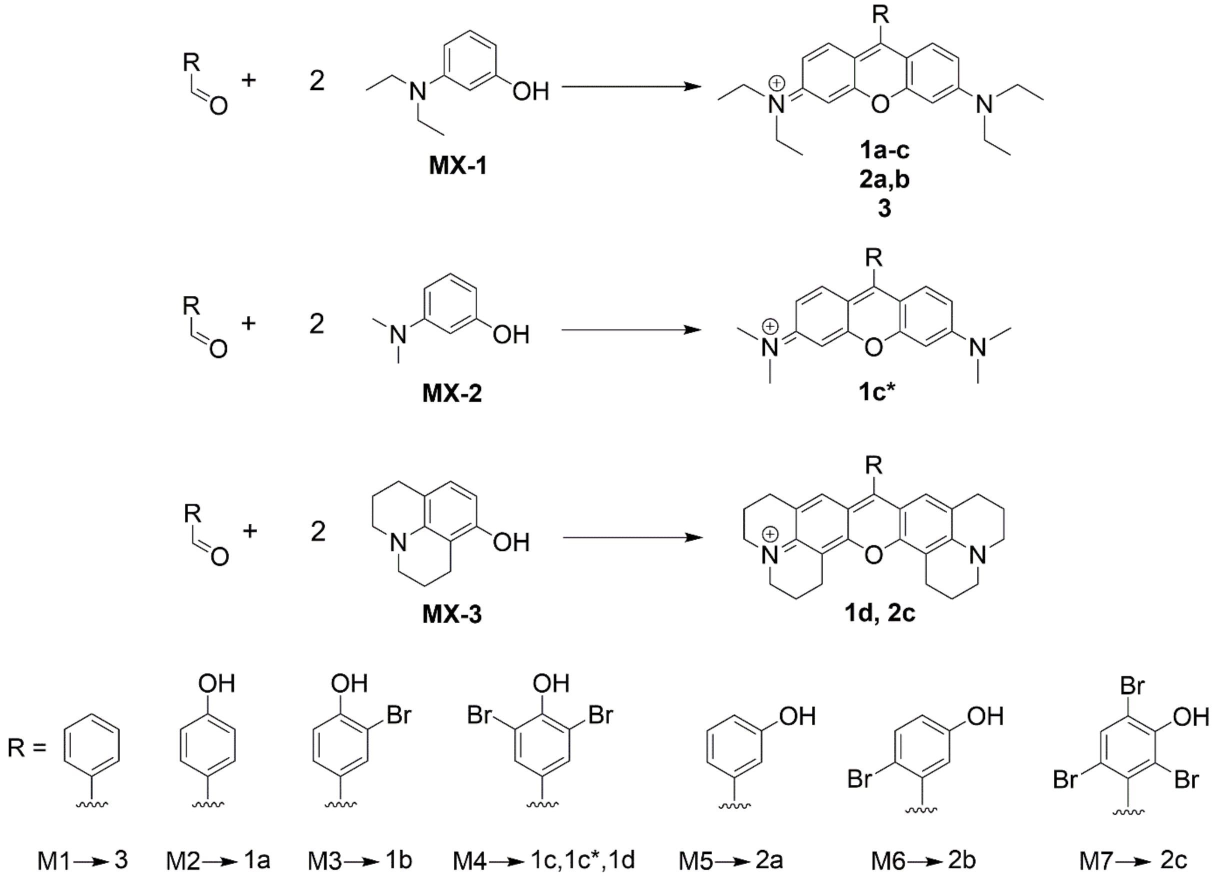


Figure S1: Synthetic route of rosamine dyes.
Reaction conditions: 1) 0.15 eq p-TsOH, propionic acid, 80°C, 2h; 2) 1.1 eq chloranil, rt, 12h.

Synthesis of mono-, di-, and tri-bromo-substituted hydroxybenzaldehyde compounds **M3, M4, M6** and **M7** are described in a previous work.[1]

Rosamines **1a-d**, **2a-c** and **3** were synthesized using differently substituted benzaldehyde derivatives **M1-M7** and the commercially available compounds **MX-1-3**, following the general procedure outlined in Scheme S1. To obtain the desired products in sufficient purity, it was necessary to run several columns (at least 2), followed by extraction with NaCl solution to remove residue propionic acid.

To a solution of the corresponding aldehyde **M1-M7** (1.0 mmol, 1.0 eq.) in 15 mL propanoic acid 3-diethylaminophenol (**MX-1**), 3-dimethylaminophenol (**MX-2**), or 8-hydroxyjulolidine (**MX-3**) (2.0 mmol, 1.5 eq.) and *p*-TsOH (0.15 mmol, 0.15 eq., 26 mg) were added. The solution was protected from light and stirred at 80°C for 2 h. After cooling to room temperature (rt), chloranil (1.5 mmol, 1.5 eq., 370 mg) was added to the reaction mixture that was then stirred overnight at rt. The resulting dark purple solution was evaporated to dryness and the crude product was purified by column chromatography on silica gel (DCM/MeOH, 98/2 to 90/10). The fraction containing the desired product were combined, concentrated and extracted with NaCl solution to yield the desired compound as a purple or violet solid.

Data for **1a**: Compound **1a** was synthesized according to the procedure mentioned above using **M2** (122.5 mg) and **MX-1** (331.3 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **1a** as violet solid (114.1 mg, 27 %).
^{1}H-NMR (500 MHz, CD_3OD): δ = 1.31 (t, J = 7.1Hz, 12H), 3.68 (q, J = 7.1Hz, 8H), 6.95 (d, J = 2.4Hz, 2H), 7.08 (m, 4H), 7.33 (d, J = 8.5Hz, 2H), 7.52 (d, J = 9.6Hz, 2H) ppm.

^{13}C(125MHz, CD_3OD) δ = 11.51, 45.46, 96.02, 113.19, 113.92, 115.50, 122.64, 131.53, 132.10, 155.66, 158.28, 158.40, 159.87 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 415.2380; Found [M]+: 415.2399.

Data for **1b**: Compound **1b** was synthesized according to the procedure mentioned above using **M3** (201.3 mg) and **MX-1** (331.1 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **1b** as violet solid (101.2 mg, 20 %).
^1H-NMR (500 MHz, CD_3OD): δ = 1.32 (t, J = 7.1Hz, 12H), 3.69 (q, J = 7.1Hz, 8H), 6.96 (d, J = 2.5Hz, 2H), 7.10 (dd, ^1J = 9.6Hz, ^2J = 2.5Hz, 2H), 7.16 (d, J = 8.3Hz, 1H), 7.31 (dd, ^1J = 8.3Hz, ^2J = 2.1Hz, 1H), 7.48 (d, J = 9.6Hz, 2H); 7.62 (d, J = 2.1Hz, 1H) ppm.
^{13}C (125MHz, CD_3OD) δ = 11.48, 45.48, 96.06, 110.37, 113.16, 114.12, 116.25, 123.79, 130.39, 131.75, 134.26, 155.72, 156.31, 156.88, 158.23 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 493.1485; Found $[M]^+$: 493.1552.

Data for **1c**: Compound **1c** was synthesized according to the procedure mentioned above using **M4** (280 mg) and **MX-1** (330 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **1c** as violet solid (93 mg, 16 %).
^1H-NMR (500 MHz, CD_3OD): δ = 1.36 (t, J = 7.1Hz, 12H), 3.74 (q, J = 7.1Hz, 8H), 7.02 (d, J = 2.4Hz, 2H), 7.17 (dd, ^1J = 9.6Hz, ^2J = 2.4Hz, 2H), 7.48 (d, J = 9.6Hz, 2H), 7.70 (s, 2H) ppm.
^{13}C(125MHz, CD_3OD) δ = 13.10, 47.16, 97.74, 113.03, 114.89, 116.02, 116.10, 127.26, 133.08, 134.90, 154.71, 155.94, 157.51, 157.54, 159.87 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 573.0570; Found $[M]^+$: 573.0600.

Data for **1c***: Compound **1c*** was synthesized according to the procedure mentioned above using **M4** (281.1 mg) and **MX-2** (275.5 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **1c*** as violet solid (101.9 mg, 19 %).

^1H-NMR (500 MHz, CD_3OD): δ = 3.37 (s, 12H), 7.02 (d, J = 2.5Hz, 2H), 7.17 (dd, ^1J = 9.5Hz, ^2J = 2.5Hz, 2H), 7.49 (d, J = 9.5Hz, 2H), 7.69 (s, 2H) ppm.
^{13}C (125MHz, CD_3OD) δ = 39.61, 96.29, 111.38, 113.36, 114.45, 125.61, 131.14, 133.28, 153.10, 154.97, 157.68, 158.00 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 516.9944; Found $[M]^+$: 516.9935.

Data for **1d**: Compound **1d** was synthesized according to the procedure mentioned above using **M4** (152.8 mg) and **MX-3** (206 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **1d** as violet solid (56.3 mg, 18 %).
^1H-NMR (500 MHz, CD_3OD): δ = 1.97 (t, J = 5.3Hz, 4H), 2.10 (t, J = 5.3Hz, 4H), 2.75 (t, J = 5.7Hz, 4H), 3.05 (t, J = 6.0Hz, 4H), 3.53 (t, J = 5.3Hz, 4H), 3.56 (t, J = 5.3Hz, 4H), 6.87 (s, 2H), 7.51 (s, 2H) ppm.
^{13}C (125MHz, CD_3OD) δ = 19.49, 19.64, 20.46, 27.27, 50.08, 50.59, 105.41, 111.37, 112.68, 124.26, 125.93, 126.16, 132.99, 151.24, 151.37, 152.25, 152.79 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 621.0570; Found [M]+: 621.0671.

Data for **2a**: Compound **2a** was synthesized according to the procedure mentioned above using **M5** (122.5 mg) and **MX-1** (331.5 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **2a** as violet solid (112.1 mg, 27 %).
^1H-NMR (500 MHz, CD_3OD): δ = 1.31 (t, J = 7.1Hz, 12H), 3.68 (q, J = 7.1Hz, 8H), 6.87 (m, 1H), 6.89 (d, J = 7.6Hz, 1H), 6.95 (s, 2H), 7.07 (m, 3H), 7.46 (m, 3H) ppm.
^{13}C (125MHz, CD_3OD) δ = 11.40, 45.41, 95.92, 112.97, 114.00, 116.09, 116.77, 120.24, 129.80, 131.78, 133.28, 155.75, 157.74, 158.17 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 415.2380; Found $[M]^+$: 415.2422.

Data for **2b**: Compound **2b** was synthesized according to the procedure mentioned above using **M6** (202.9 mg) and **MX-1** (331.2 mg) as precursors. Purification by column chromatography on

silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **2b** as violet solid (53.6 mg, 11 %).
^{1}H-NMR (500 MHz, CD_3OD): δ = 1.32 (t, J = 7.1Hz, 12H), 3.70 (q, J = 7.1Hz, 8H), 6.83 (d, J = 2.8Hz, 2H), 6.99 (m, 3H), 7.11 (dd, ^{1}J = 9.5Hz, ^{2}J = 2.4Hz, 2H), 7.25 (d, J = 9.5Hz, 2H), 7.64 (d, ^{1}J = 8.8Hz, 2H) ppm.
^{13}C (125MHz, CD_3OD) δ = 11.31, 45.87, 96.14, 105.36, 114.58, 118.76, 128.61, 131.33, 134.27, 156.03, 158.26 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 493.14852; Found [M]+: 493.1584.

Data for **2c**: Compound **2c** was synthesized according to the procedure mentioned above using **M7** and **MX-3** as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **2c** as violet solid (82.1 mg, 12 %).

^{1}H-NMR (500 MHz, CD_3OD): δ = 2.01 (t, J = 5.3Hz, 4H), 2.14 (t, J = 5.5Hz, 4H), 2.78 (t, J = 6.0Hz, 4H), 3.11 (t, J = 6.3Hz, 4H), 3.56 (t, J = 5.7Hz, 4H), 3.60 (t, J = 5.7Hz, 8H), 6.81 (s, 2H), 7.78 (s, 1H) ppm.
^{13}C (125MHz, CD_3OD) δ = 19.54, 19.63, 20.48, 27.23, 50.14, 50.62, 101.97, 105.47, 111.80, 114.45, 115.36, 124.45, 125.50, 133.12, 134.08, 151.35, 152.58, 153.61 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 698.96750; Found [M]+: 698.9999.

Data for **3**: Compound **3** was synthesized according to the procedure mentioned above using **M1** (106.2 mg) and **MX-1** (330.5 mg) as precursors. Purification by column chromatography on silica gel using DCM/MeOH (98/2 to 90/10) as eluent gave compound **3** as violet solid (119.1 mg, 30 %).
^{1}H-NMR (500 MHz, CD_3OD): δ = 1.32 (t, J = 7.1Hz, 12H), 3.69 (q, J = 7.1Hz, 8H), 6.99 (s, 1H), 7.09 (dd, ^{1}J = 9.5Hz, ^{2}J = 1.7Hz, 2H), 7.38 (d, J = 9.5Hz, 2H), 7.49 (m, 2H), 7.68 (m, 3H) ppm.
^{13}C (125MHz, CD_3OD) δ = 11.50, 45.53, 96.09, 113.20, 114.18, 128.70, 129.42, 130.08, 131.80, 132.25, 155.86, 157.70, 158.29 ppm.
MS (ESI-TOF) m/z calculated for $[M]^+$ 399.2431; Found $[M]^+$: 399.2450.

2. Data and Spectra from Optical Spectroscopy

Table S1: Equation used for sigmoidal curve fitting of pH titration experiments and fitting parameters using normalized and integrated fluorescence emission spectral data ($\int_{550nm}^{700nm} Emission$). The p$K_a$ value was determined from log X_0.

Model	Dose response
Equation 1	$y = A1 + \frac{A2 - A1}{1 + 10^{(logX_o - X)p}}$

Dye	A1	A2	*log X_0*	p	R^2
3_1	-	-	-	-	-
3_2	-	-	-	-	-
3_3	-	-	-	-	-
1a_1	-0.00153 ± 0.01152	0.99307 ± 0.008	8.99409 ± 0.02238	-1.04077 ± 0.06009	0.99797
1a_2	-0.0023 ± 0.0025	0.99698 ± 0.00183	8.98378 ± 0.00557	-0.99819 ± 0.01405	0.99993
1a_3	0.00161 ± 0.00551	0.99169 ± 0.00367	8.99118 ± 0.01076	-1.05934 ± 0.02795	0.99959
1b_1	-0.00452 ± 0.00688	0.9871 ± 0.00677	7.35013 ± 0.01854	-0.92596 ± 0.03303	0.99974
1b_2	-0.00694 ± 0.00577	0.99151 ± 0.0052	7.37477 ± 0.01441	-0.88797 ± 0.02344	0.99981
1b_3	-0.00444 ± 0.00433	0.99258 ± 0.00385	7.36961 ± 0.01139	-0.92499 ± 0.01948	0.99991
1c_1	0.00531 ± 0.00703	1.00062 ± 0.00961	5.54975 ± 0.0191	-0.99844 ± 0.04353	0.99934
1c_2	0.00135 ± 0.00365	1.00412 ± 0.00546	5.49847 ± 0.01193	-0.90259 ± 0.02171	0.99984
1c_3	0.0029 ± 0.00511	0.99983 ± 0.00757	5.49417 ± 0.01644	-0.93257 ± 0.02911	0.99964
2a_1	-0.0074 ± 0.01092	0.97579 ± 0.00648	9.42156 ± 0.02378	-0.97041 ± 0.04784	0.99899
2a_2	-0.0057 ± 0.01448	0.98093 ± 0.00886	9.41741 ± 0.03109	-0.99741 ± 0.06554	0.99813
2a_3	-0.00619 ± 0.00439	0.99178 ± 0.00304	9.4333 ± 0.00961	-0.91641 ± 0.01805	0.99982
2b_1	-0.00474 ± 0.00566	0.99181 ± 0.00328	8.69353 ± 0.0113	-0.91921 ± 0.02133	0.99984
2b_2	-0.00781 ± 0.00718	0.98311 ± 0.00447	8.70158 ± 0.01414	-0.90209 ± 0.02316	0.99968
2b_3	-0.0087 ± 0.00829	0.9846 ± 0.00549	8.70638 ± 0.01799	-0.89107 ± 0.02883	0.99954
1c*_1	0.00339 ± 0.00633	0.99253 ± 0.00922	5.4789 ± 0.02134	-0.79734 ± 0.02734	0.99932
1c*_2	0.00687 ± 0.0064	0.9866 ± 0.00809	5.4624 ± 0.01814	-0.90459 ± 0.03179	0.99935
1c*_3	0.00406 ± 0.01189	0.97976 ± 0.01519	5.47075 ± 0.03566	-0.87098 ± 0.05412	0.99779
1d_1	0.00183 ± 0.00673	1.00705 ± 0.00876	5.85981 ± 0.02282	-0.77618 ± 0.0279	0.99951
1d_2	0.00464 ± 0.00802	0.99972 ± 0.01027	5.87754 ± 0.02879	-0.82544 ± 0.03879	0.99926
1d_3	0.00222 ± 0.0067	1.00509 ± 0.00773	5.87255 ± 0.02003	-0.78119 ± 0.02684	0.99958
2c_1	0.02014 ± 0.0032	0.9904 ± 0.00277	5.11658 ± 0.00824	-1.0997 ± 0.02157	0.99981
2c_2	0.01504 ± 0.01215	1.00333 ± 0.01239	5.13842 ± 0.04425	-0.69362 ± 0.04765	0.99797
2c_3	0.02637 ± 0.02076	1.0122 ± 0.02166	5.17115 ± 0.04877	-0.8743 ± 0.07554	0.99721

2.1. Absorption and emission spectra of the pH-titration (triplicate measurement) of the synthesized dyes (1µmol/L) in a water-methanol mixture (H_2O/MeOH 2/1 vol%) containing borate-citrate buffer (25mM)

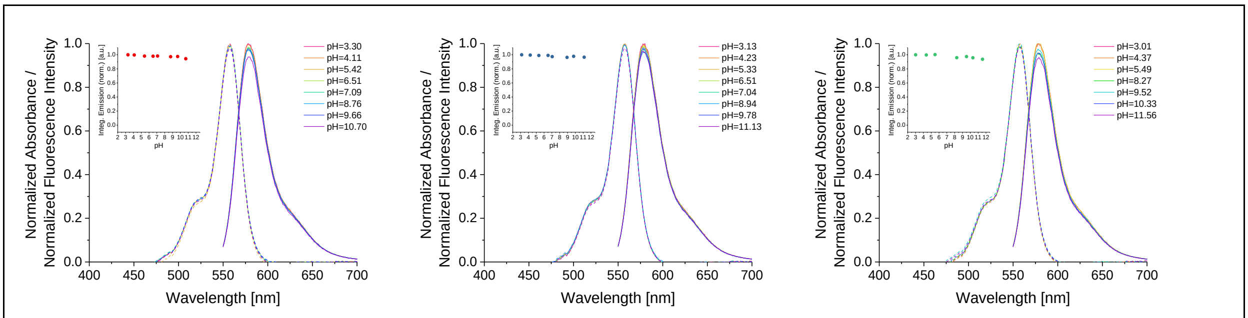


*Figure S2: pH-titration of **3** as triplicate measurement.*

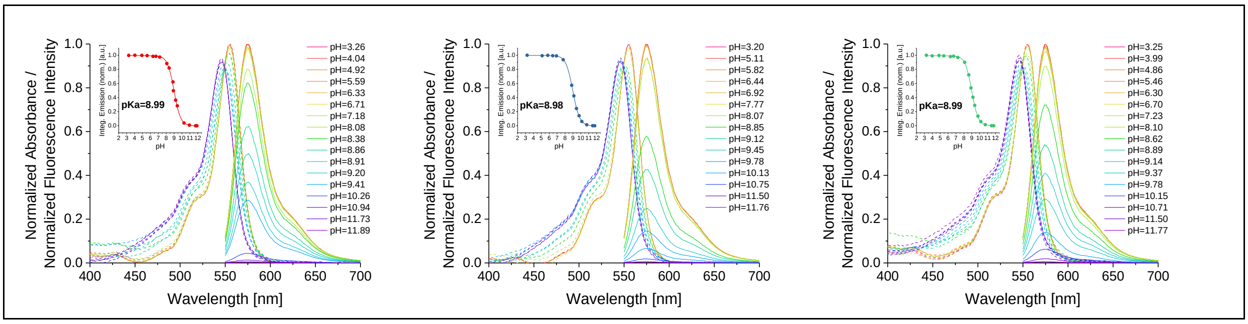


*Figure S3: pH-titration of **1a** as triplicate measurement.*

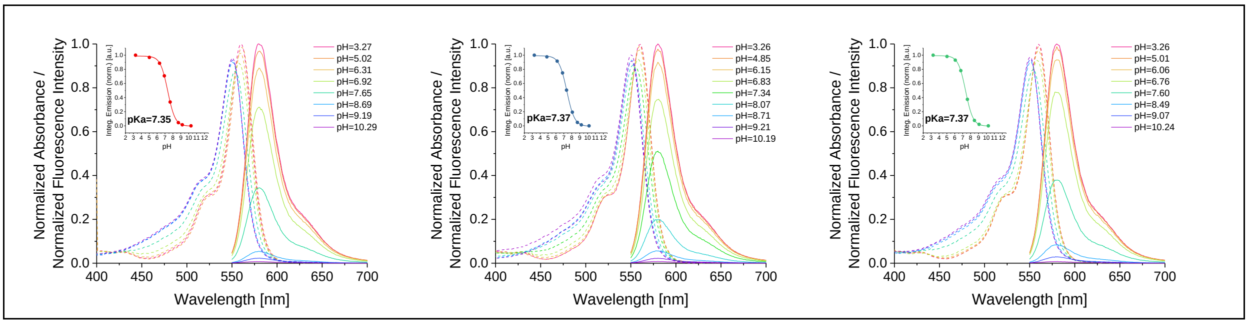


*Figure S4: pH-titration of **1b** as triplicate measurement.*

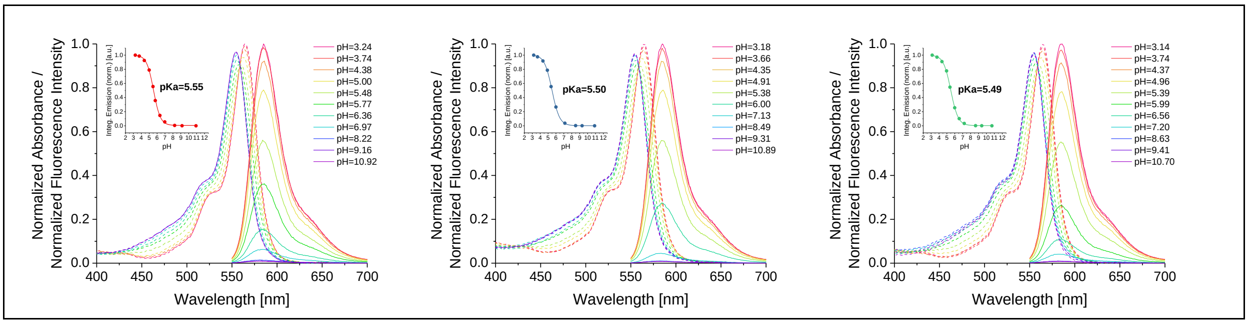


*Figure S5: pH-titration of **1c** as triplicate measurement.*

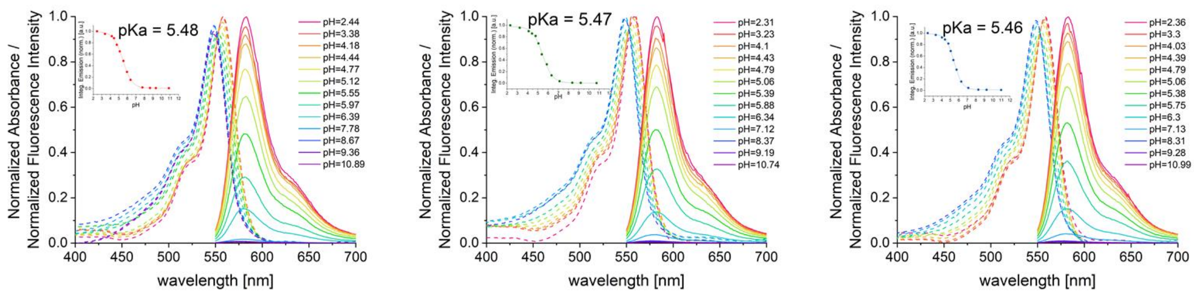


*Figure S6: pH-titration of **1c*** as triplicate measurement.*

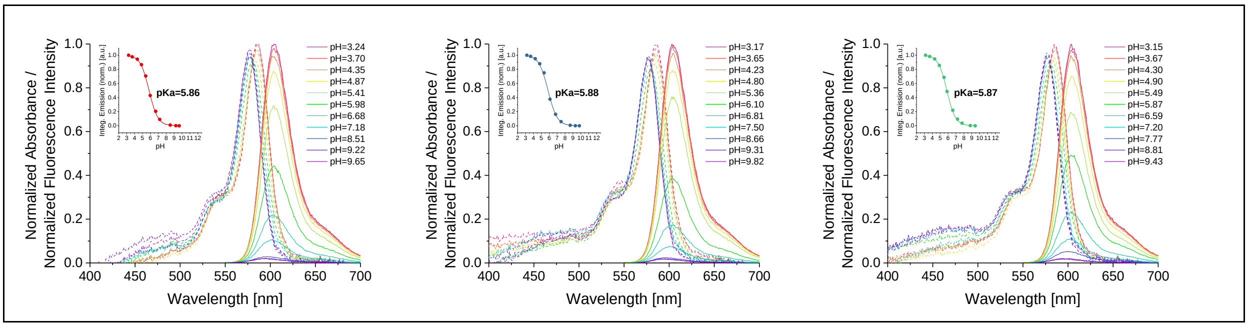


*Figure S7: pH-titration of **1d** as triplicate measurement.*

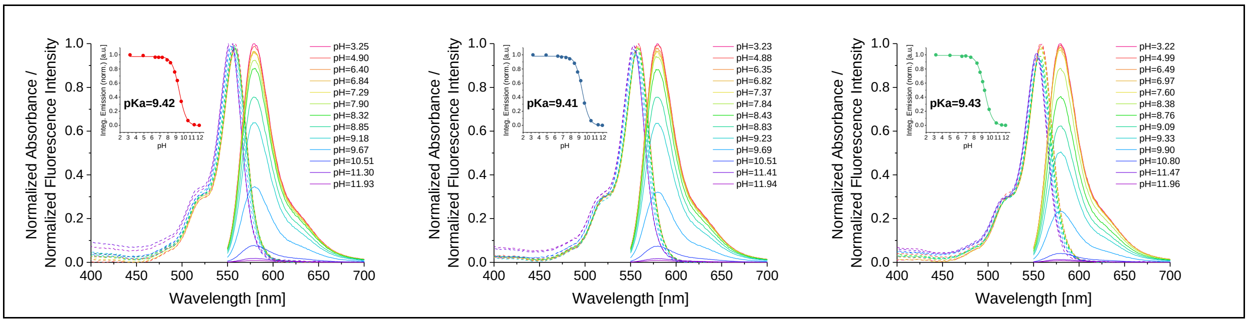


*Figure S8: pH-titration of **2a** as triplicate measurement.*

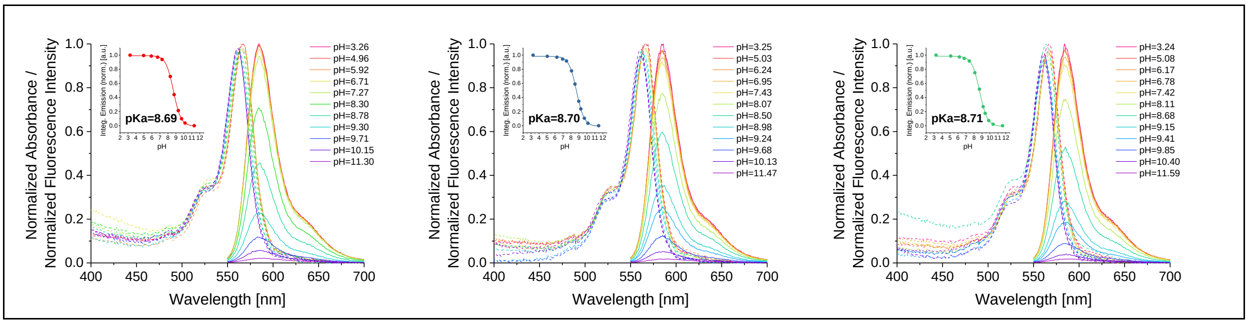


*Figure S9: pH-titration of **2b** as triplicate measurement.*

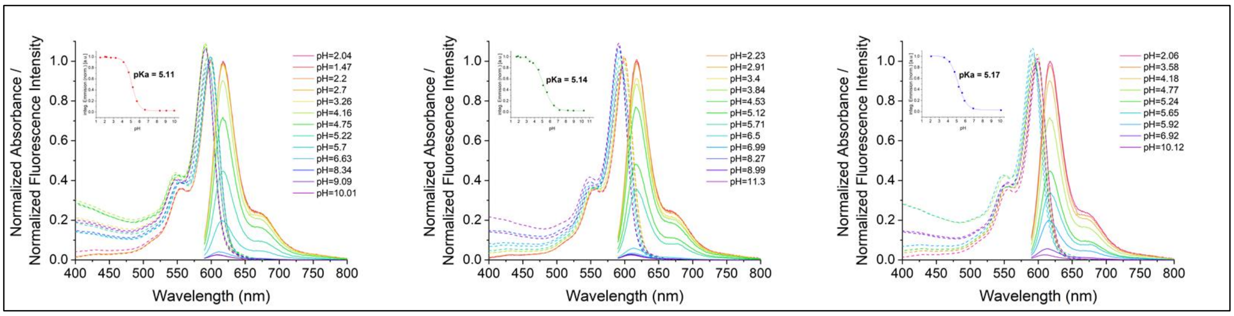


*Figure S10: pH-titration of **2c** as triplicate measurement.*

2.2. pH-titration curves of 1c (1µmol/L) in a water-methanol mixture (H_2O/MeOH 2/1 vol%) containing borate-citrate buffer (25mM) at 20°C and 40°C

Table S2: Fitting parameters using normalized and integrated fluorescence emission spectral data ($\int_{550nm}^{700nm} Emission$).

Dye	A1	A2	*log X_0*	p	R
1c_20°C	0.00135 ± 0.00365	1.00412 ± 0.00546	5.49847 ± 0.01193	-0.90259 ± 0.02171	0.99984
1c_40°C	0.00151 ± 0.0106	1.01258 ± 0.01644	5.48016 ± 0.03214	-0.91341 ± 0.05795	0.99892

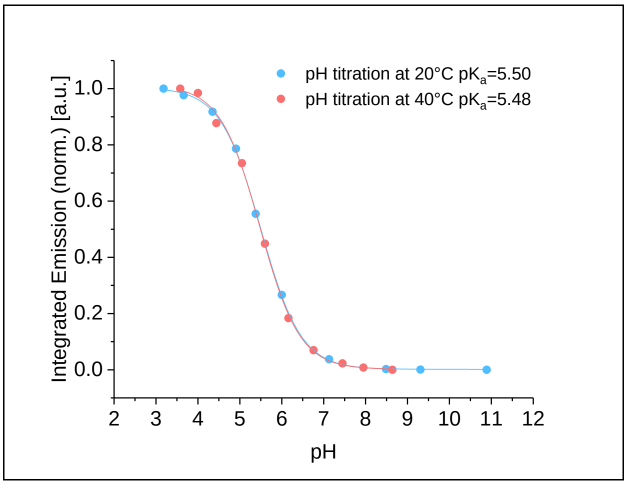


*Figure S11: pH-titration curves of **1c** at 20°C and at 40°C.*

2.3. Reversibility of the switching between protonated and deprotonated form of the dyes (1µmol/L) in a water-methanol mixture (H_2O/MeOH 2/1 vol%) containing borate-citrate buffer (25mM)

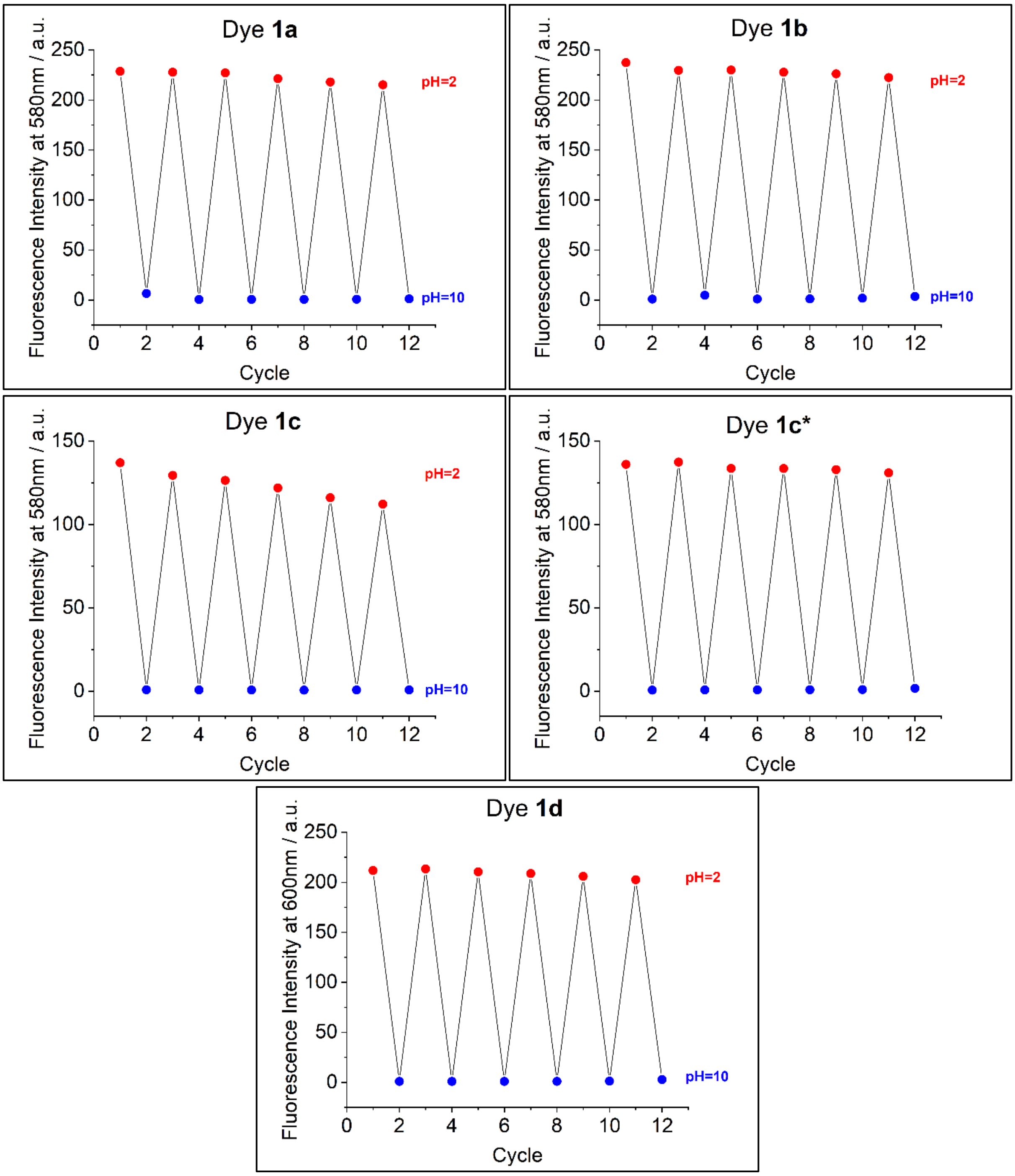


*Figure S12: pOH-derived dyes **1a**, **1b**, **1c**, **1c*** and **1d**.*

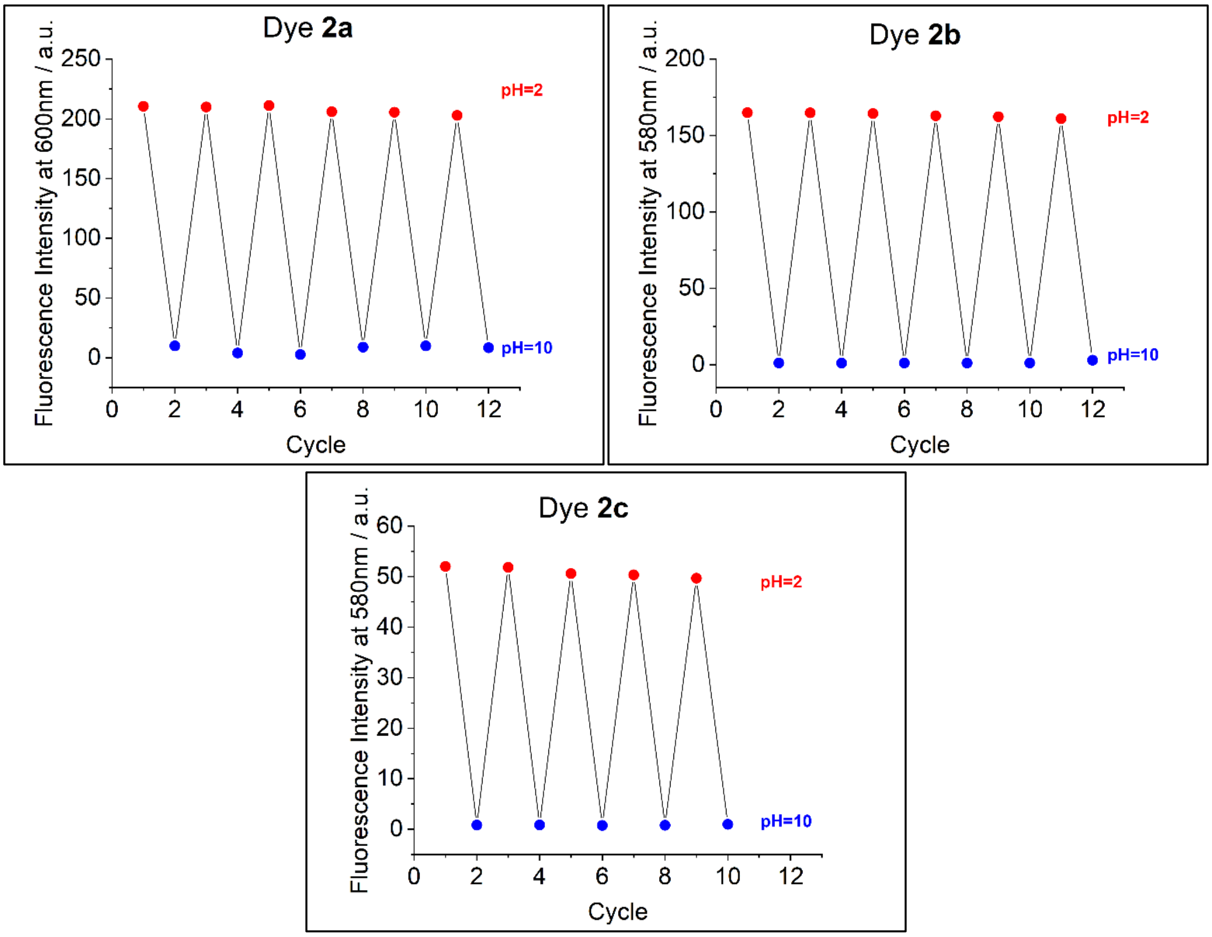


*Figure S13: mOH-derived dyes **2a**, **2b** and **2c.***

2.4. Absorption and emission spectra of the temperature dependence (averaged triplicate measurement) of the dyes 1c, 1d, 2b , 2c (1µmol/L) in a water-methanol mixture (H2O/MeOH 2/1 vol%) containing borate-citrate buffer (25mM)

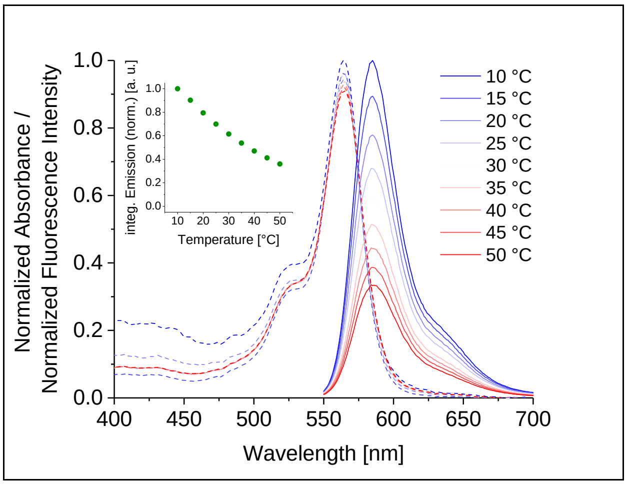


Figure S14: Temperature sensitivity of ***1c****.*

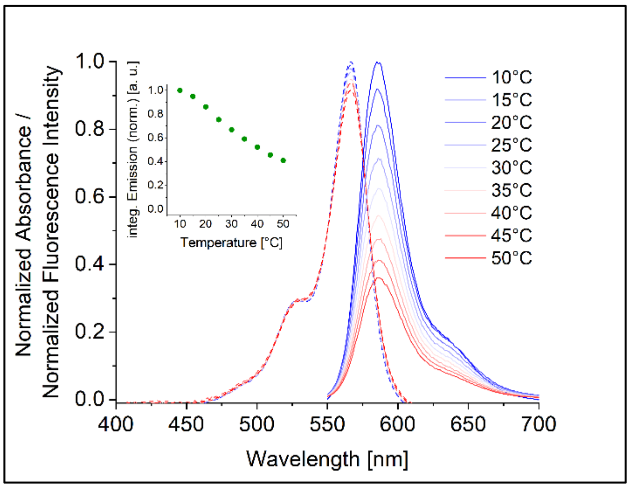


Figure S15: Temperature sensitivity of ***2b****.*

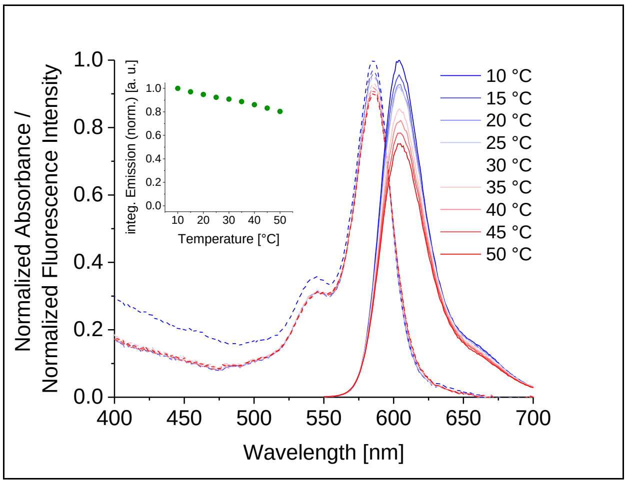


Figure S16: Temperature sensitivity of ***1d****.*

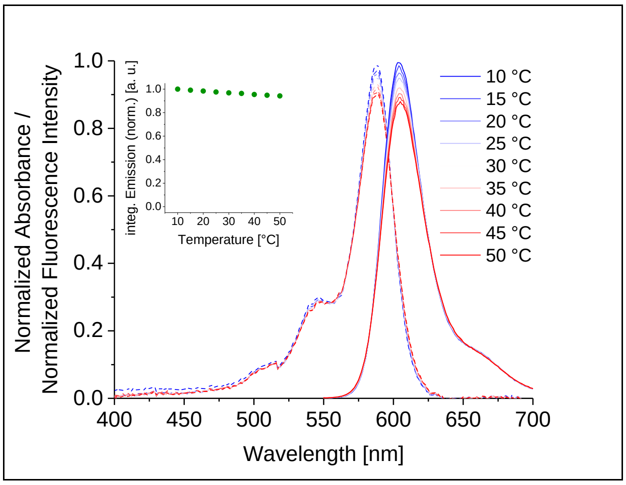


*Figure S17: Temperature sensitivity of **2c**.*

2.5. Fluorescence decay curves of the synthesized dyes (1µmol/L) in methanol (averaged triplicate measurement).

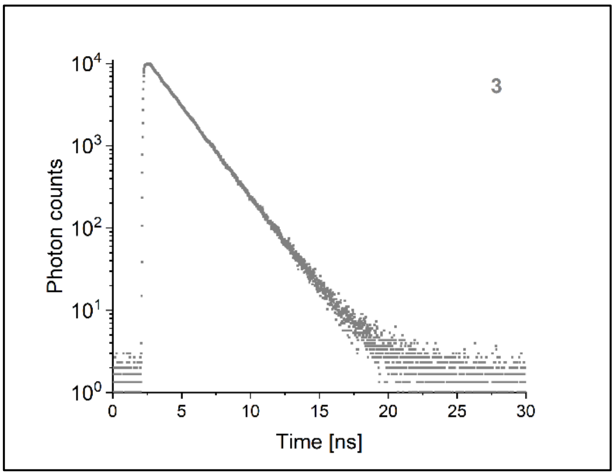


*Figure S18: Fluorescence decay curves of **3**.*

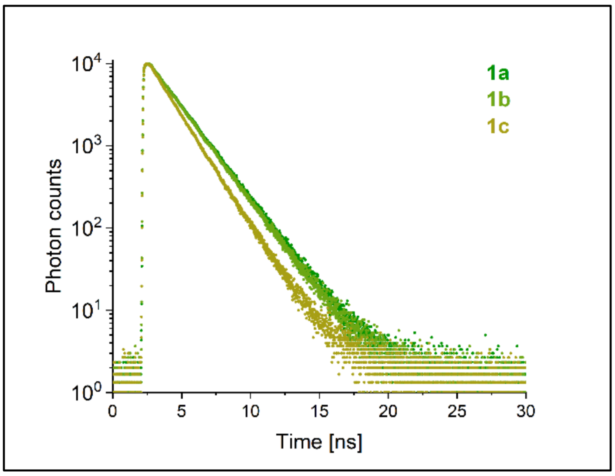


*Figure S19: Fluorescence decay curves of pOH derived compounds **1a**, **1b**, **1c**.*

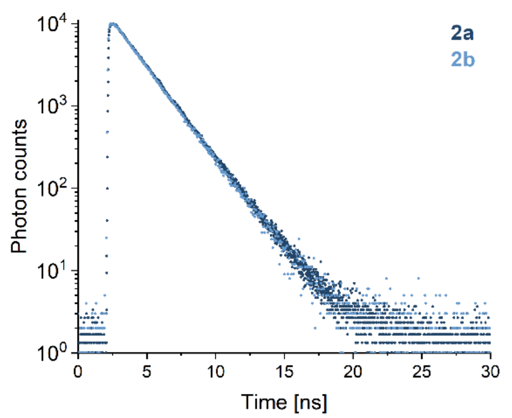


*Figure S20: Fluorescence decay curves of mOH derived compounds **2a**, **2b**.*

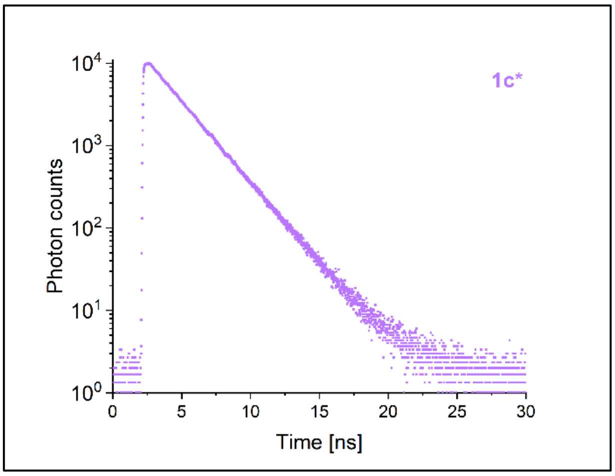


*Figure S21: Fluorescence decay curves of **1c***.*

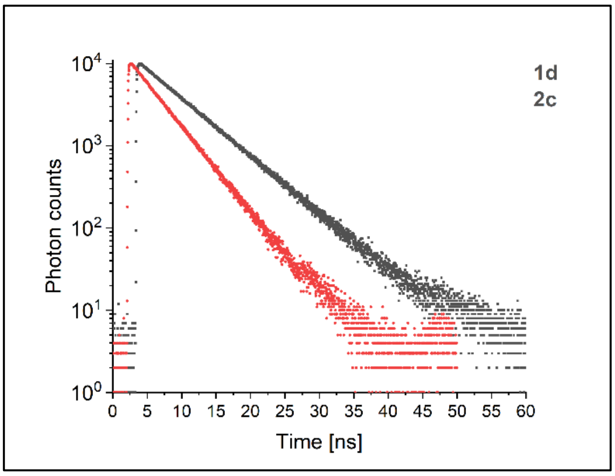


*Figure S22: Fluorescence decay curves of Rhod 101-derived compounds **1d**, **2c**.*

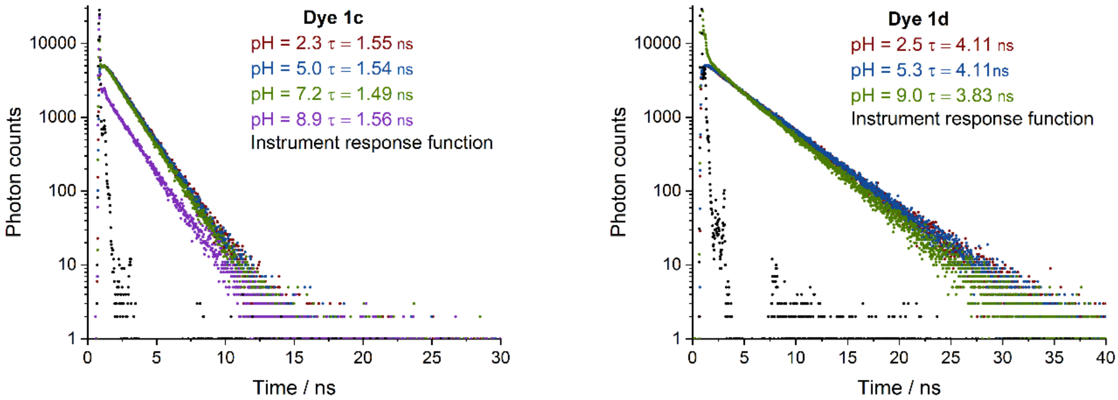
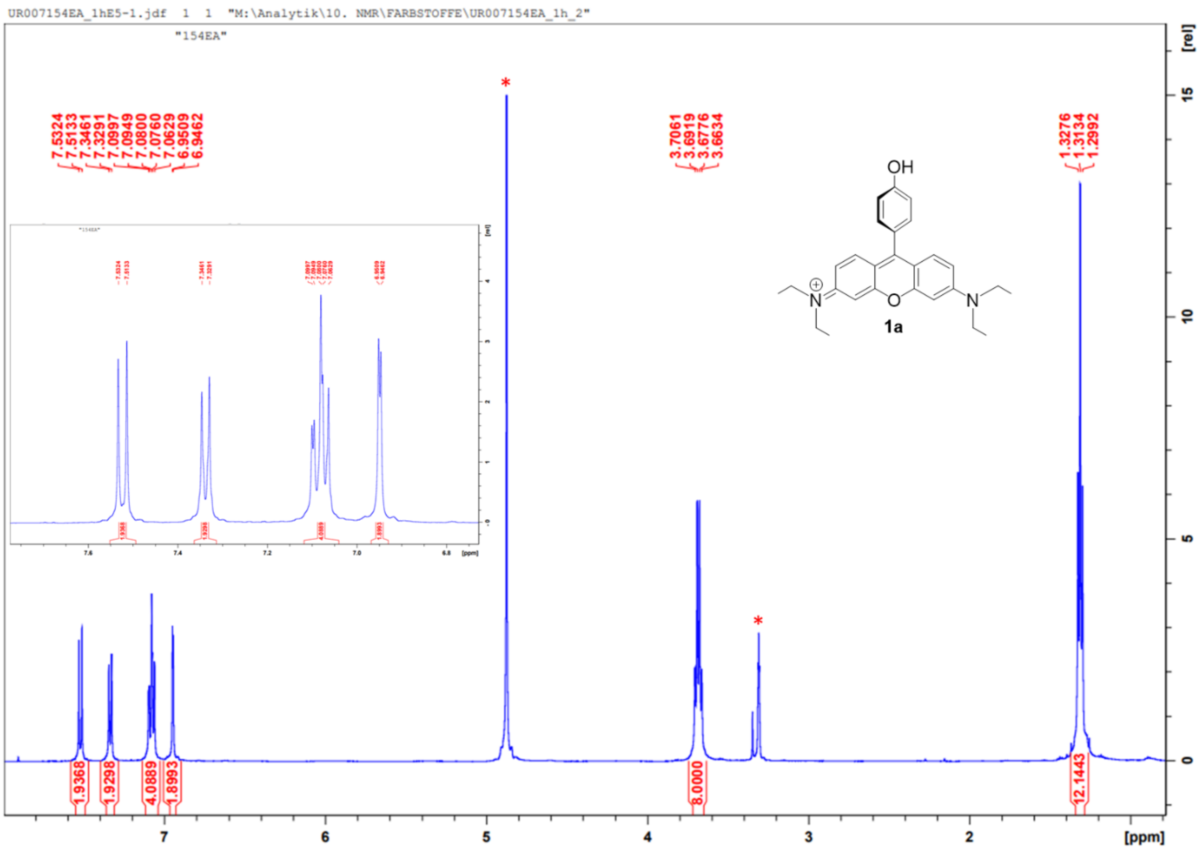
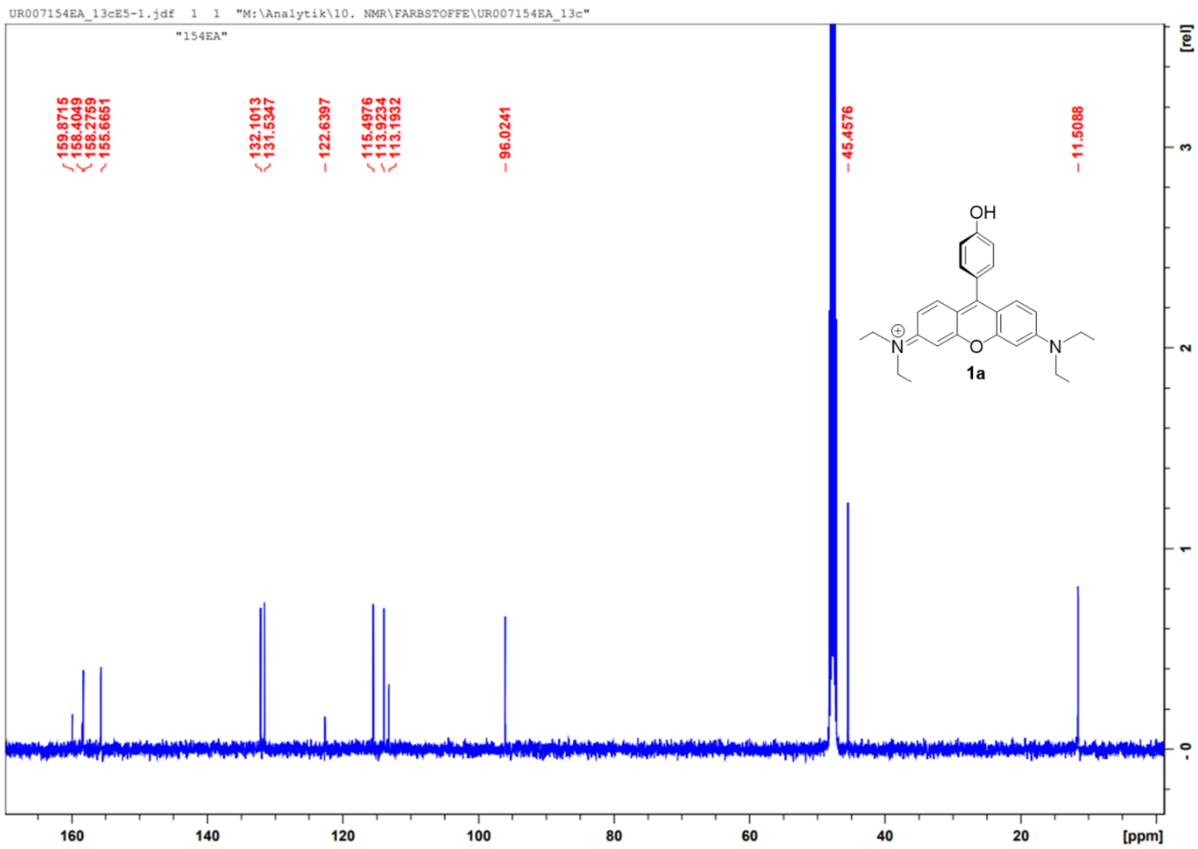


*Figure S23: pH dependence of the fluorescence decay kinetics exemplary shown for dye **1c** and **1d**.*

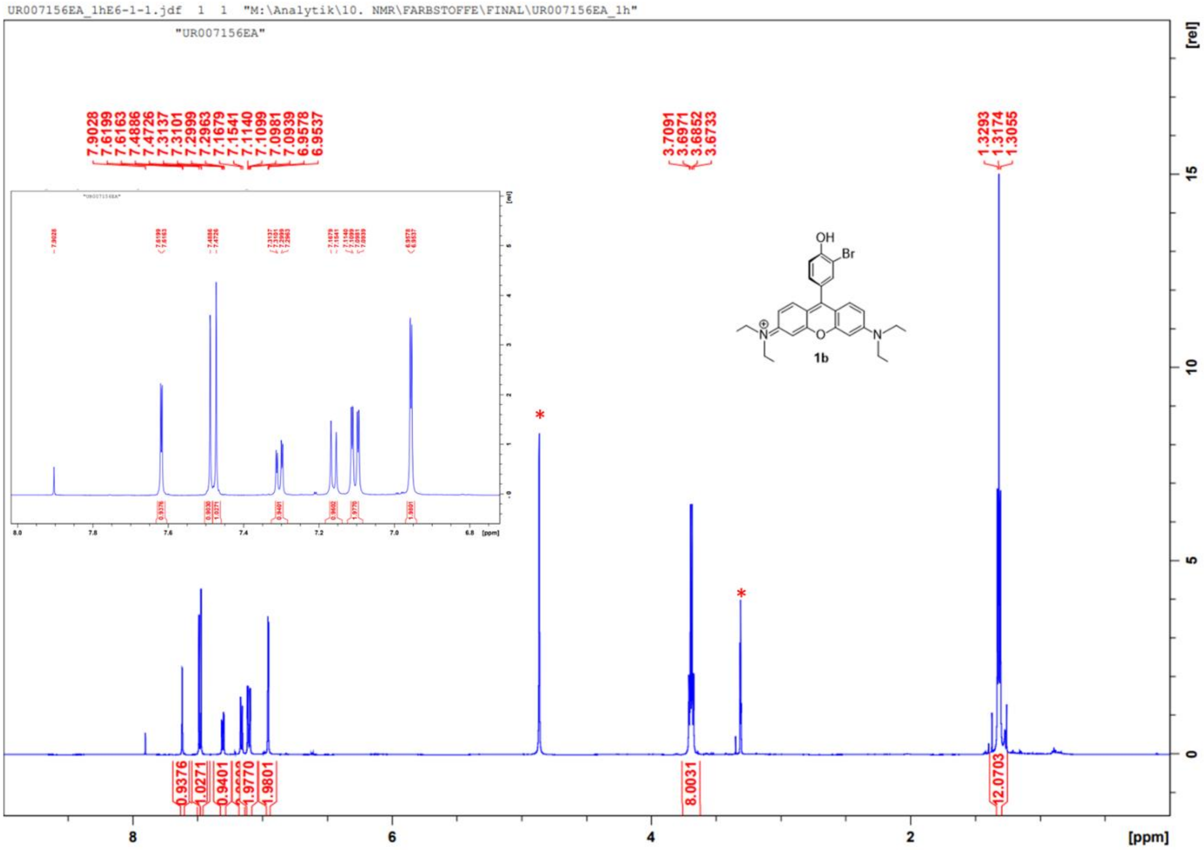
3. NMR spectra

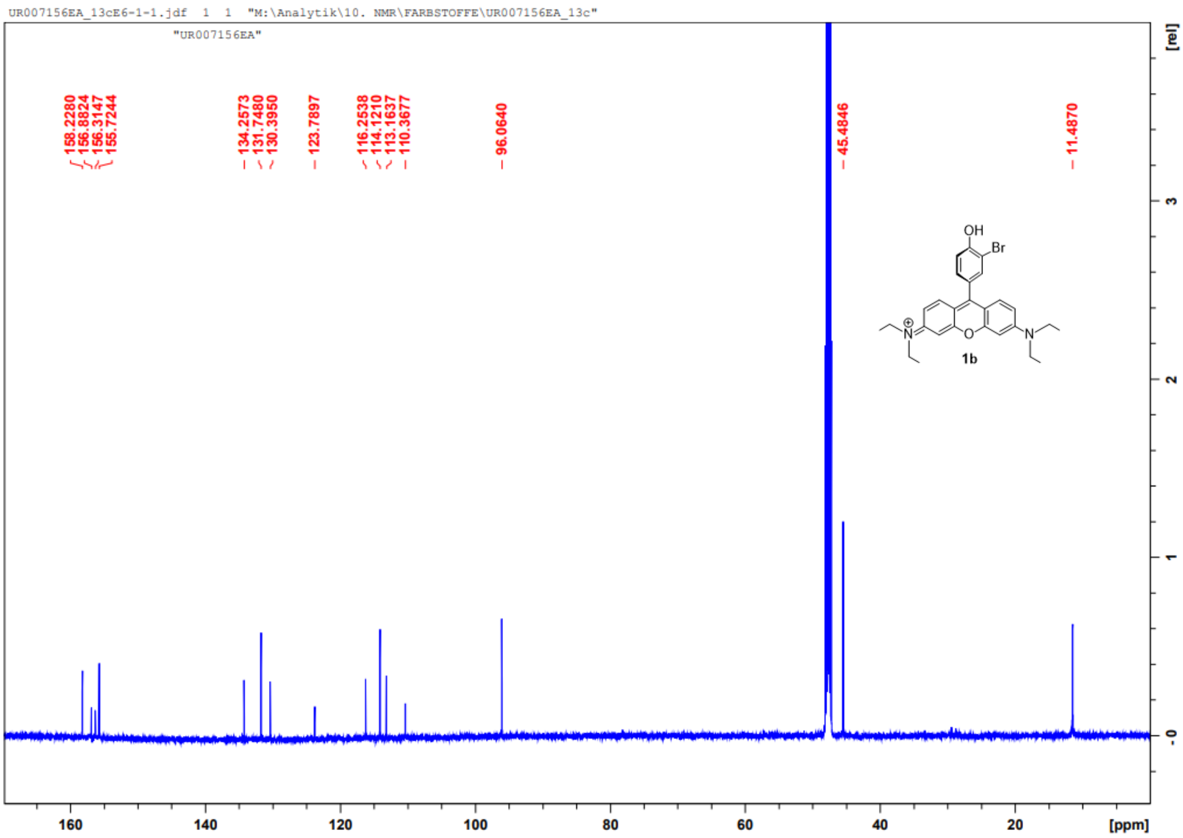
Compound 1a



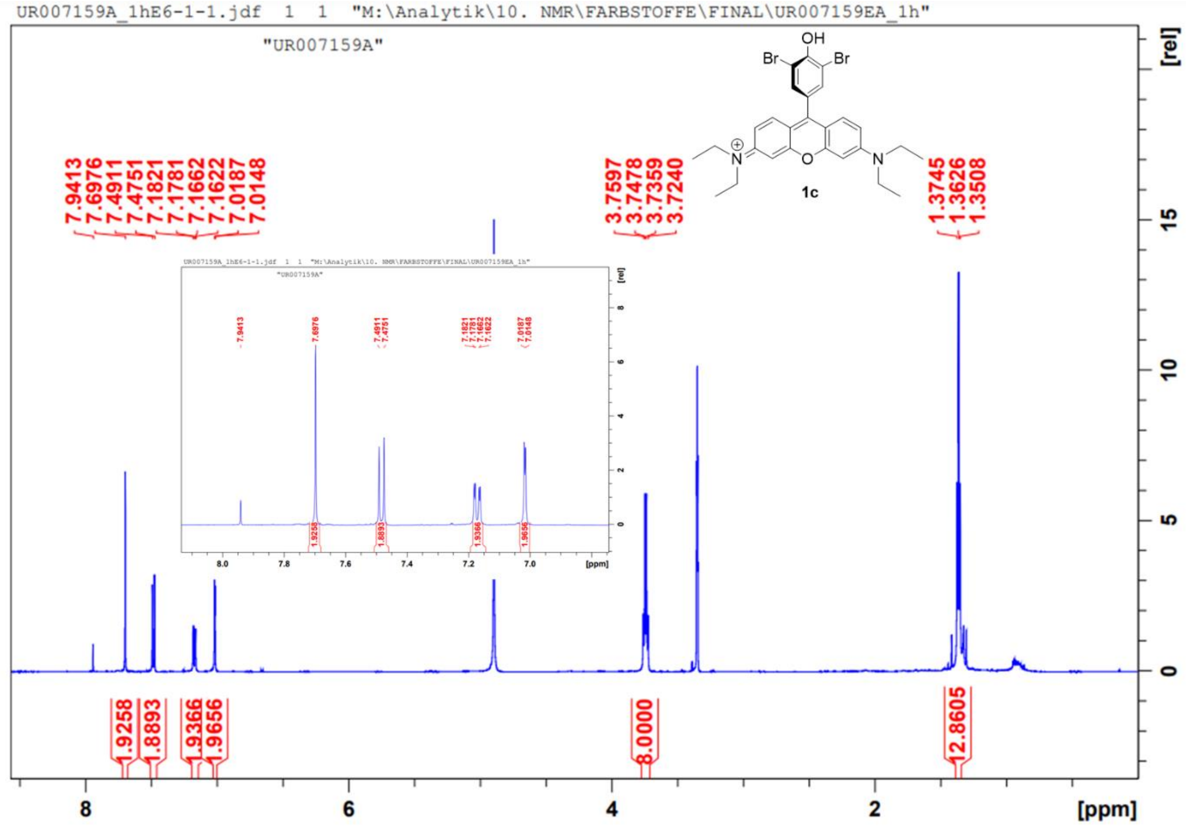


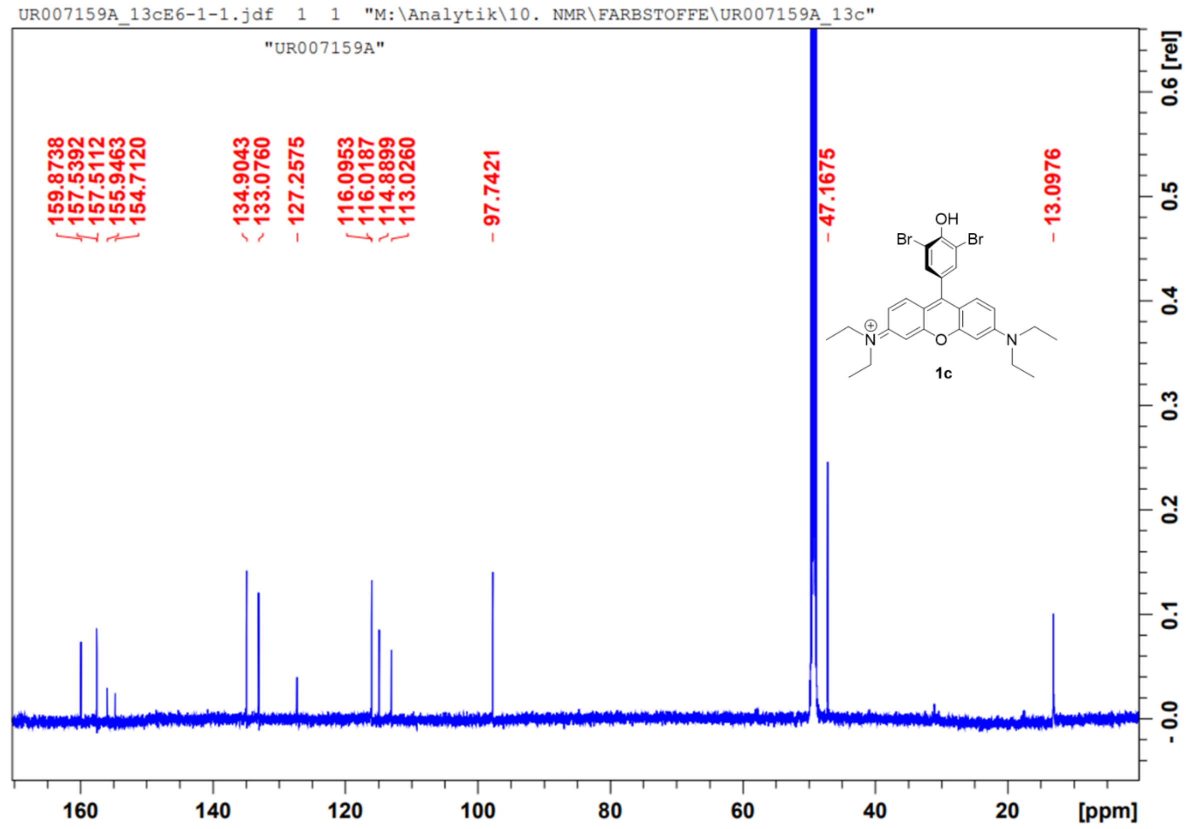
Compound 1b


UR007156EA_1hE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\FINAL\UR007156EA_1h"
"UR007156EA"
7.9028
7.6199
7.6163
7.4886
7.4726
7.3137
7.3101
7.2999
7.2963
7.1679
7.1541
7.1140
7.1099
7.0981
7.0939
6.9578
6.9537
3.7091
3.6971
3.6852
3.6733
1.3293
1.3174
1.3055
OH
Br
N
O
1b
0.9376
1.0271
0.9401
1.9770
1.9801
8.0031
12.0703
[rel]
[ppm]

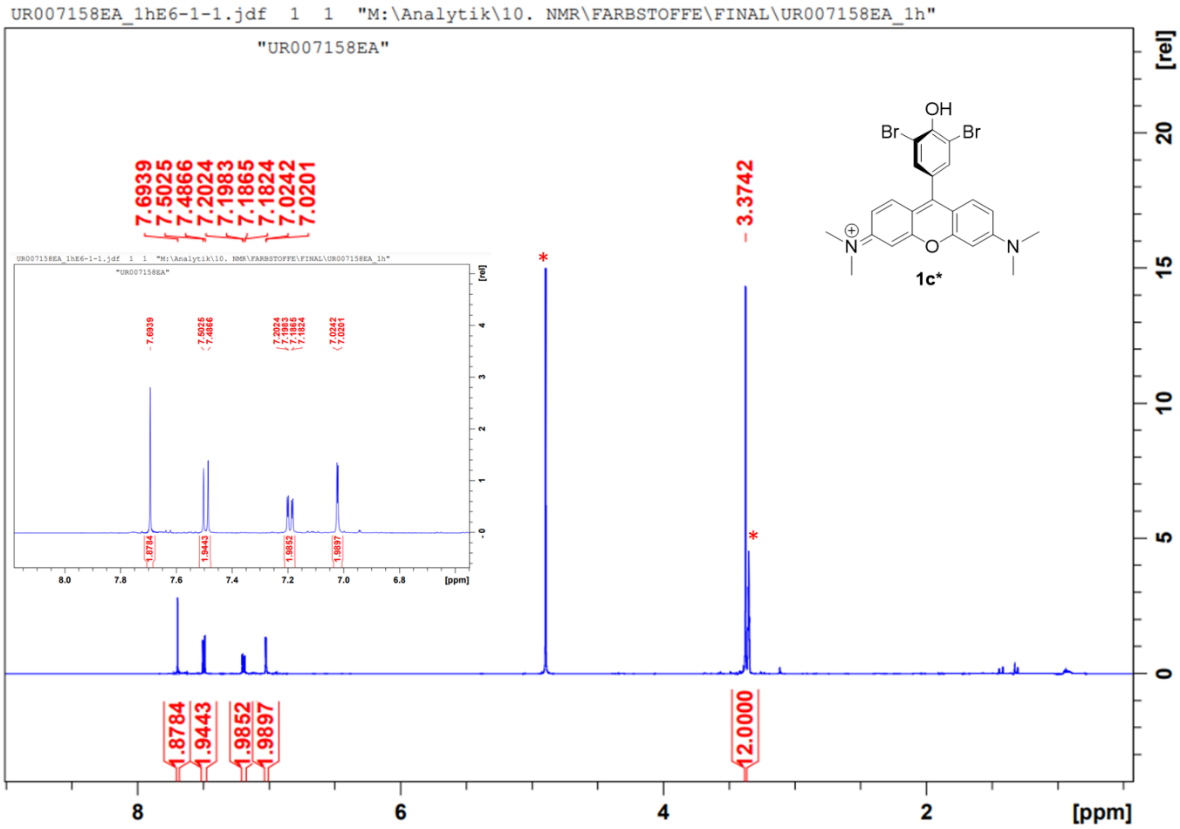

UR007156EA_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007156EA_13c"
"UR007156EA"
158.2280
156.8824
156.3147
155.7244
134.2573
131.7480
130.3950
123.7897
116.2538
114.1210
113.1637
110.3677
96.0640
45.4846
11.4870
OH
Br
N
O
1b
[rel]
[ppm]

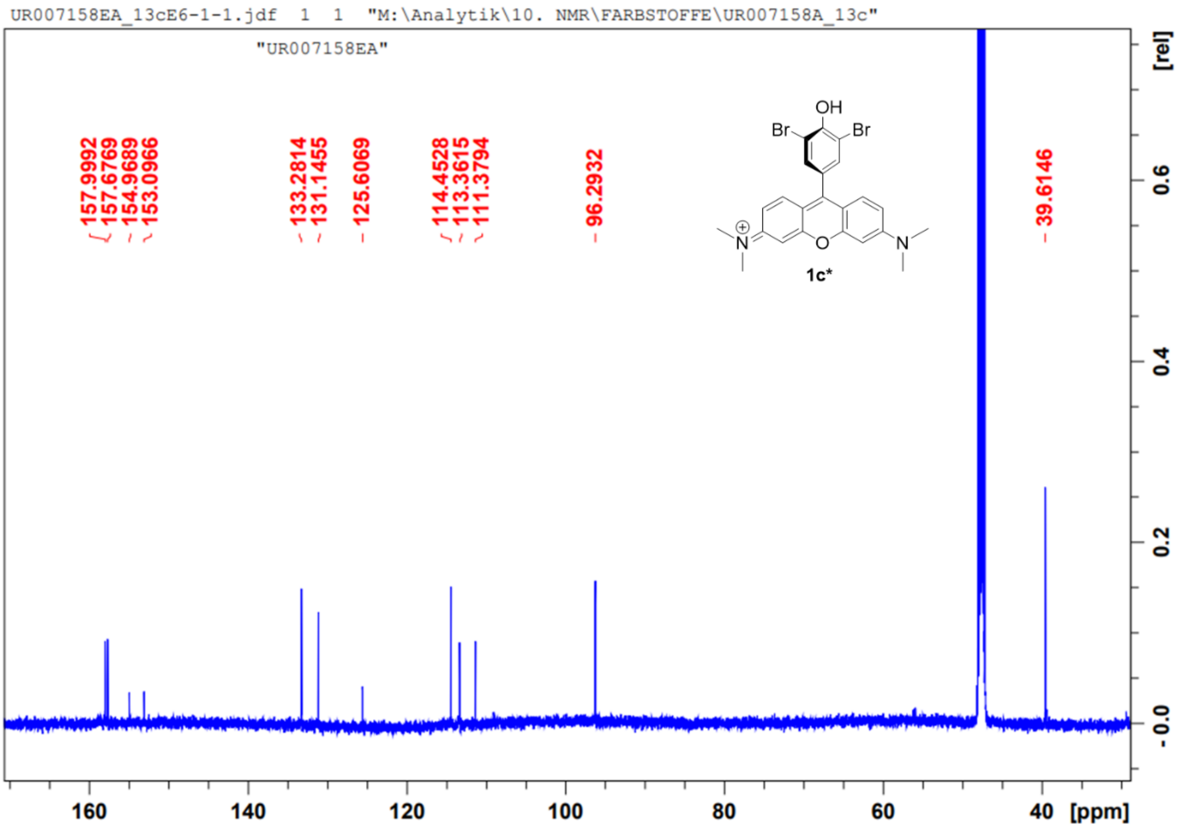
Compound 1c


UR007159A_1hE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\FINAL\UR007159EA_1h"
"UR007159A"
7.9413
7.6976
7.4911
7.4751
7.1821
7.1781
7.1662
7.1622
7.0187
7.0148
3.7597
3.7478
3.7359
3.7240
1.3745
1.3626
1.3508
1c
1.9258
1.8893
1.9366
1.9656
8.0000
12.8605
[rel]
[ppm]

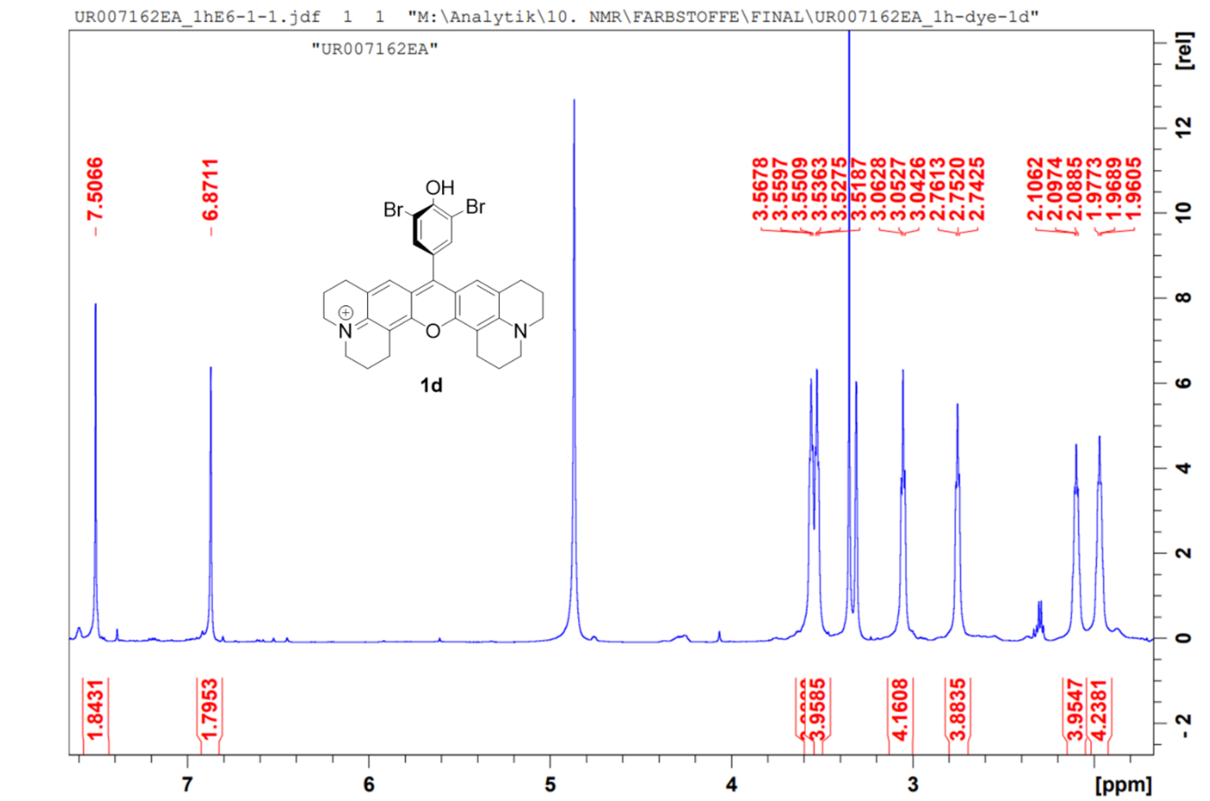

UR007159A_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007159A_13c"
"UR007159A"
159.8738
157.5392
157.5112
155.9463
154.7120
134.9043
133.0760
127.2575
116.0953
116.0187
114.8899
113.0260
97.7421
47.1675
13.0976
1c
[rel]
[ppm]

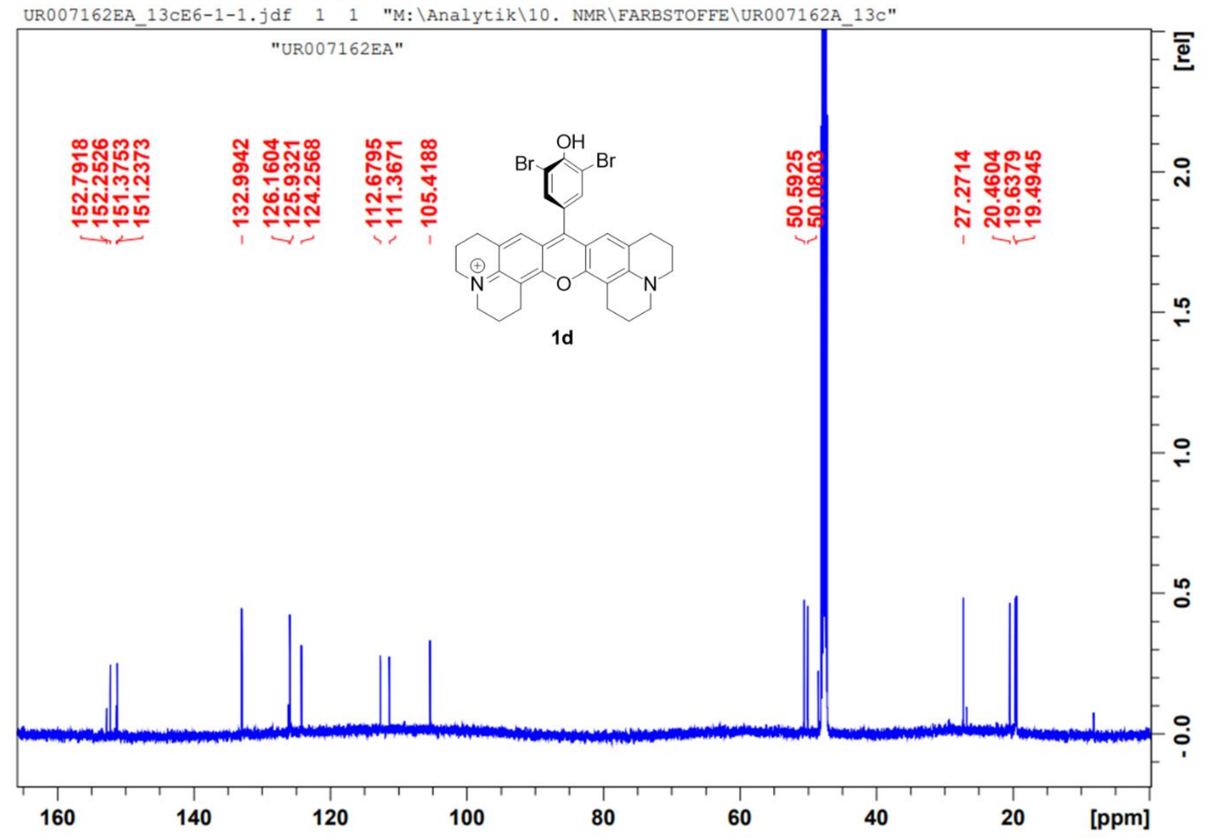
Compound 1c*


UR007158EA_1hE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\FINAL\UR007158EA_1h"
"UR007158EA"
7.6939
7.5025
7.4866
7.2024
7.1983
7.1865
7.1824
7.0242
7.0201
3.3742
1.8784
1.9443
1.9852
1.9897
12.0000
1c*
[rel]
[ppm]

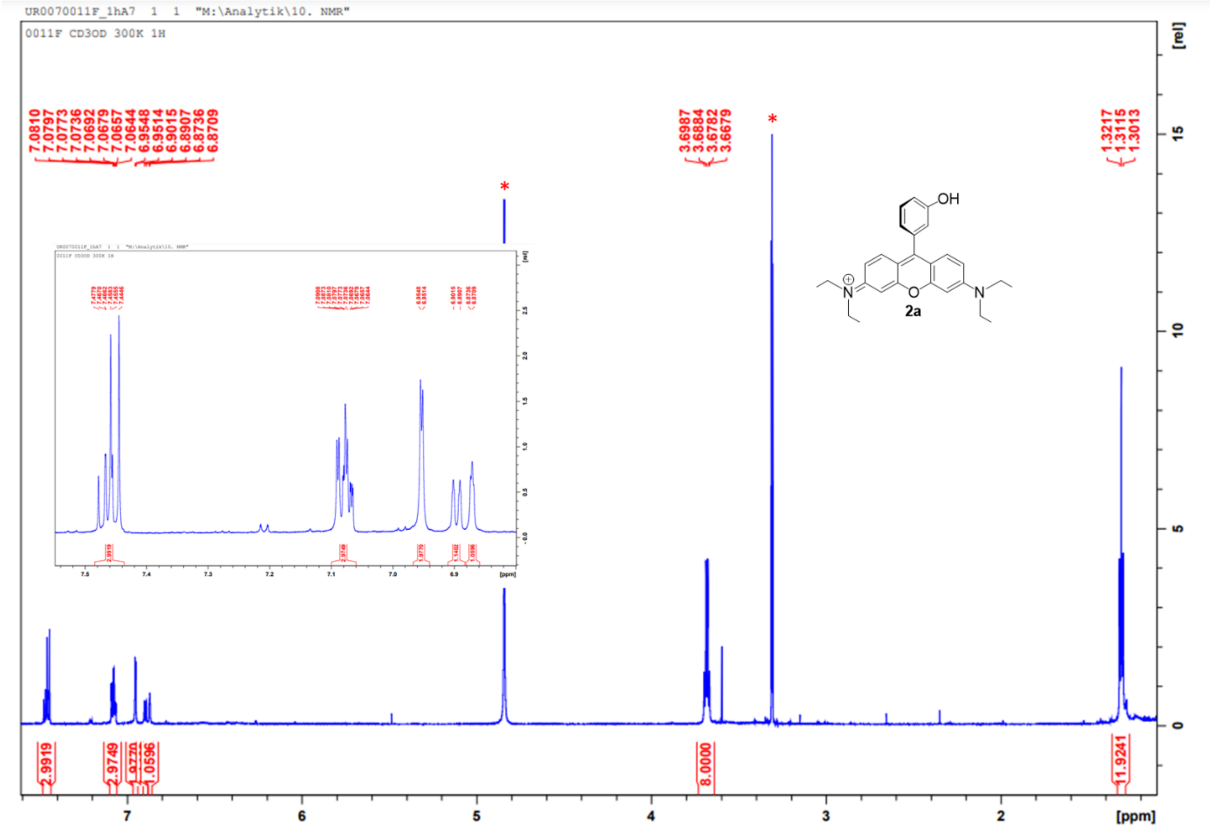

UR007158EA_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007158A_13c"
"UR007158EA"
157.9992
157.6769
154.9689
153.0966
133.2814
131.1455
125.6069
114.4528
113.3615
111.3794
96.2932
39.6146
1c*
[rel]
[ppm]

Compound 1d

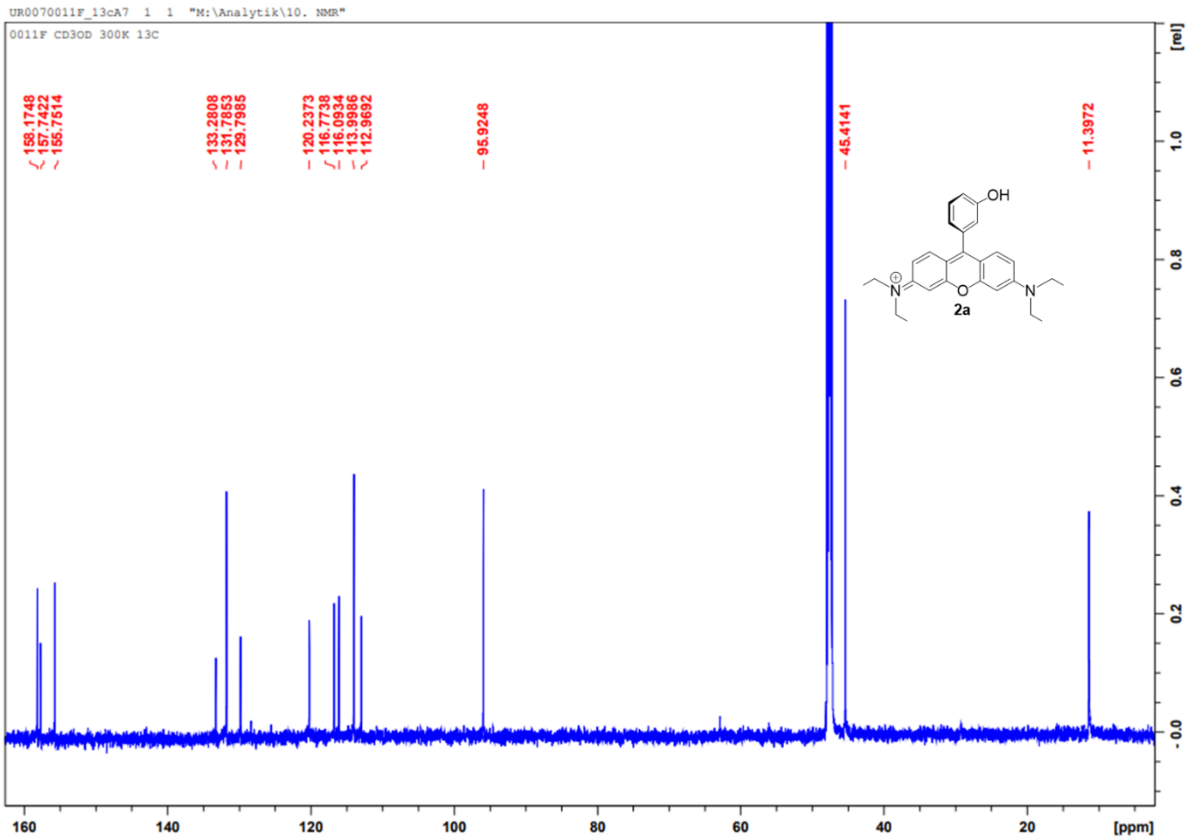

UR007162EA_1hE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\FINAL\UR007162EA_1h-dye-1d"
"UR007162EA"
7.5066
6.8711
3.5678
3.5597
3.5509
3.5363
3.5275
3.5187
3.0628
3.0527
3.0426
2.7613
2.7520
2.7425
2.1062
2.0974
2.0885
1.9773
1.9689
1.9605
OH
Br
Br
N
O
N
1d
1.8431
1.7953
3.9585
4.1608
3.8835
3.9547
4.2381
[rel]
[ppm]


UR007162EA_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007162A_13c"
"UR007162EA"
152.7918
152.2526
151.3753
151.2373
132.9942
126.1604
125.9321
124.2568
112.6795
111.3671
105.4188
50.5925
50.0803
27.2714
20.4604
19.6379
19.4945
OH
Br
Br
N
O
N
1d
[rel]
[ppm]

Compound 2a

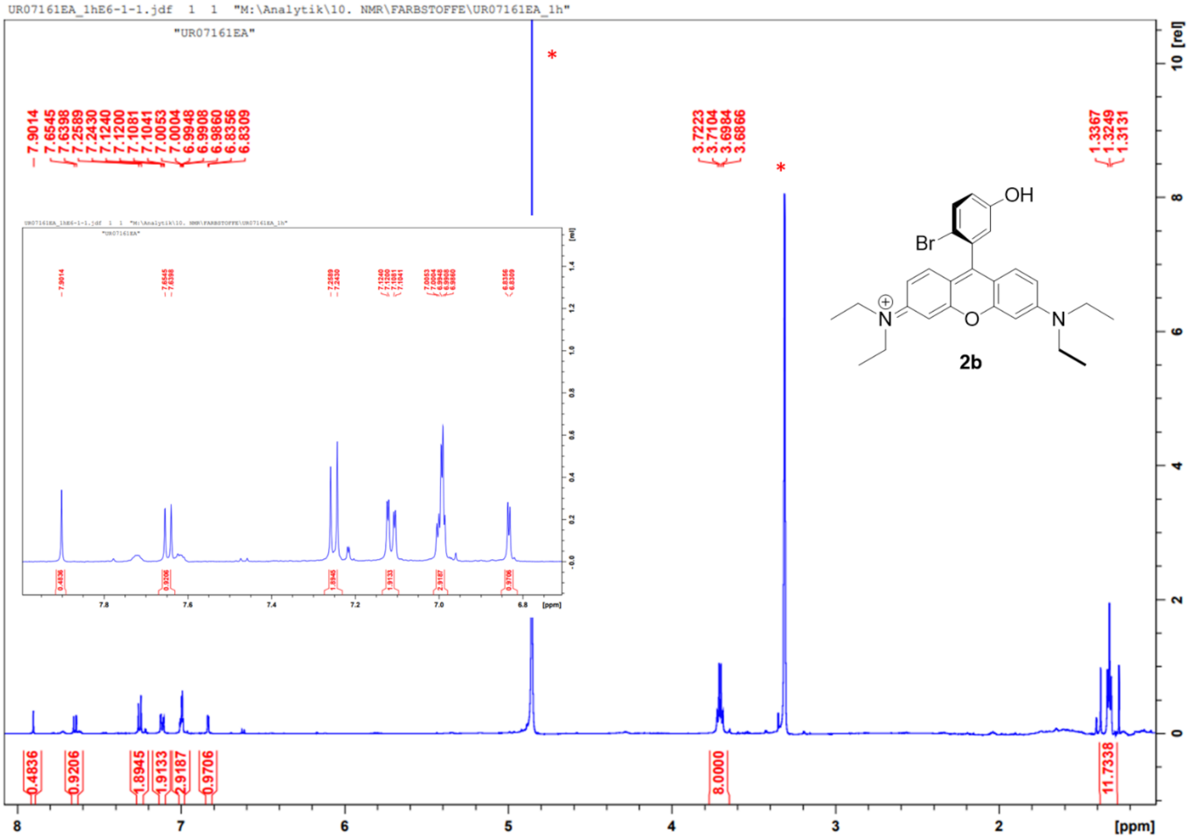


UR0070011F_1hA7 1 1 "M:\Analytik\10. NMR"
0011F CD3OD 300K 1H
7.0810
7.0797
7.0773
7.0736
7.0692
7.0679
7.0657
7.0644
6.9548
6.9514
6.9015
6.8907
6.8736
6.8709
3.6987
3.6884
3.6782
3.6679
1.3217
1.3115
1.3013
OH
N
O
2a
2.9919
2.9749
.9270
1.0596
8.0000
11.9241
[rel]
[ppm]

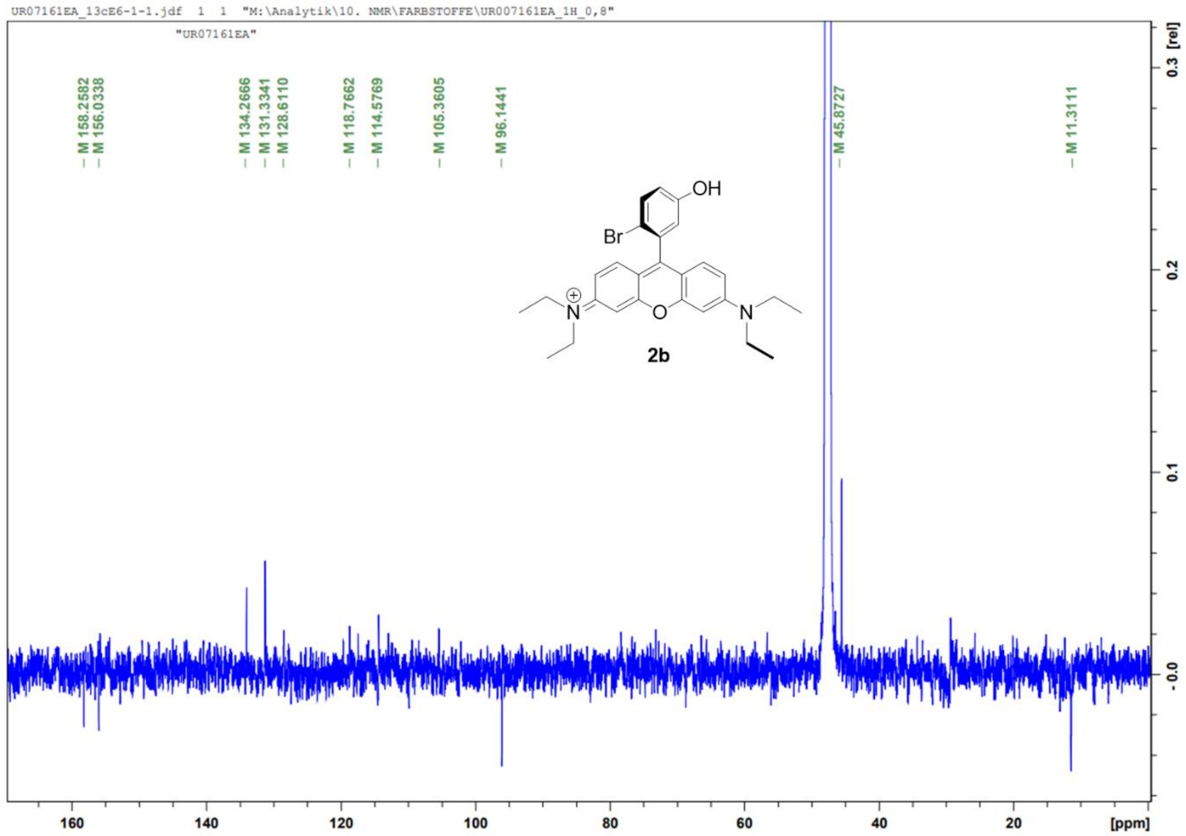


UR0070011F_13cA7 1 1 "M:\Analytik\10. NMR"
0011F CD3OD 300K 13C
158.1748
157.7422
155.7514
133.2808
131.7853
129.7985
120.2373
116.7738
116.0934
113.9986
112.9692
95.9248
45.4141
11.3972
OH
N
O
2a
[rel]
[ppm]

Compound 2b

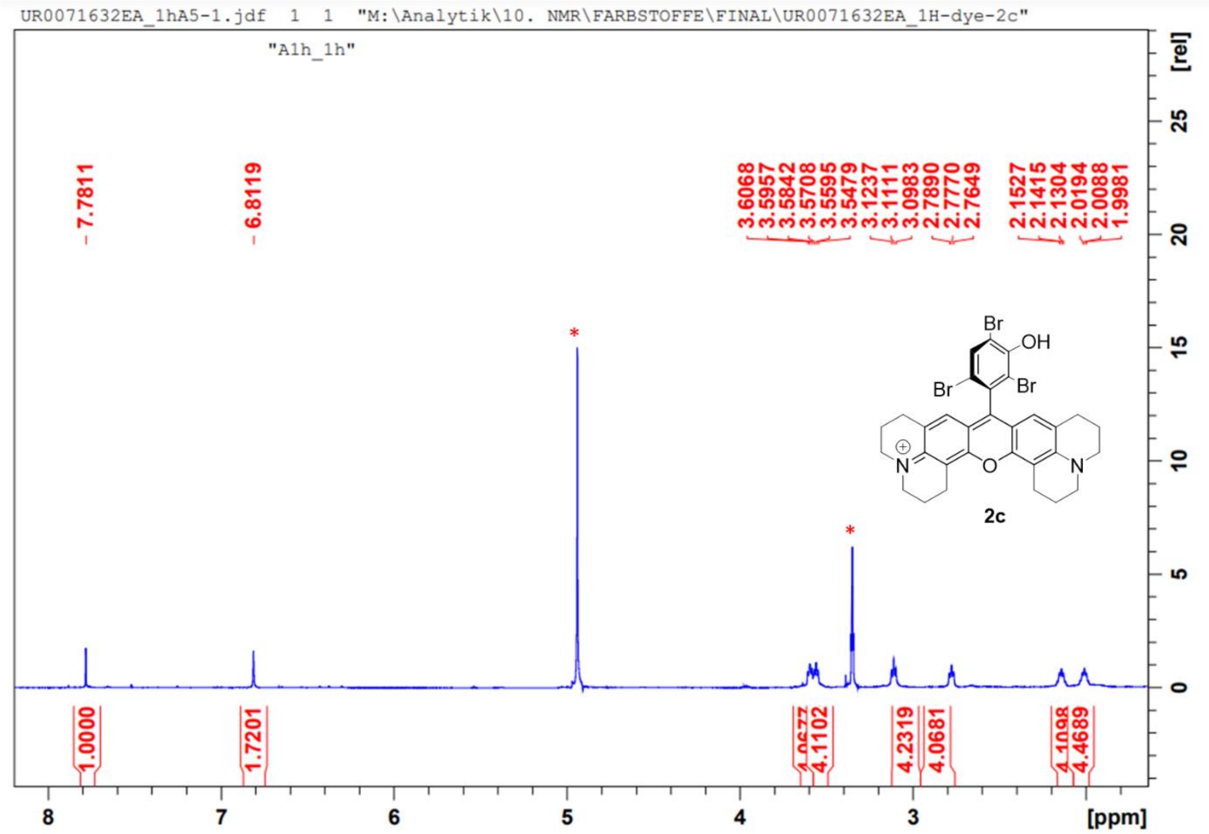


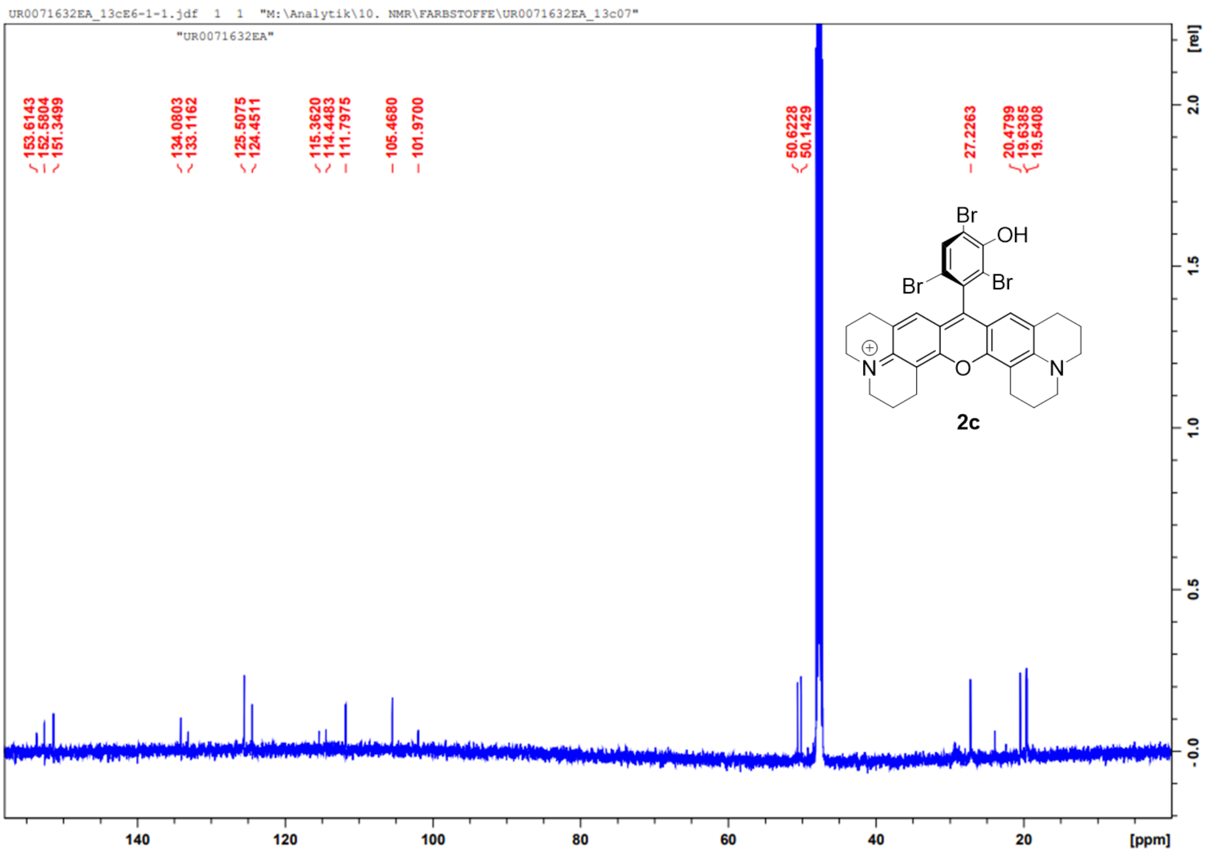
UR07161EA_1hE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR07161EA_1h"
"UR07161EA"
7.9014
7.6545
7.6398
7.2589
7.2430
7.1240
7.1200
7.1081
7.1041
7.0053
7.0004
6.9948
6.9908
6.9860
6.8356
6.8309
3.7223
3.7104
3.6984
3.6866
1.3367
1.3249
1.3131
OH
Br
N
O
N
2b
0.4836
0.9206
1.8945
1.9133
2.9187
0.9706
8.0000
11.7338
[ppm]
[rel]



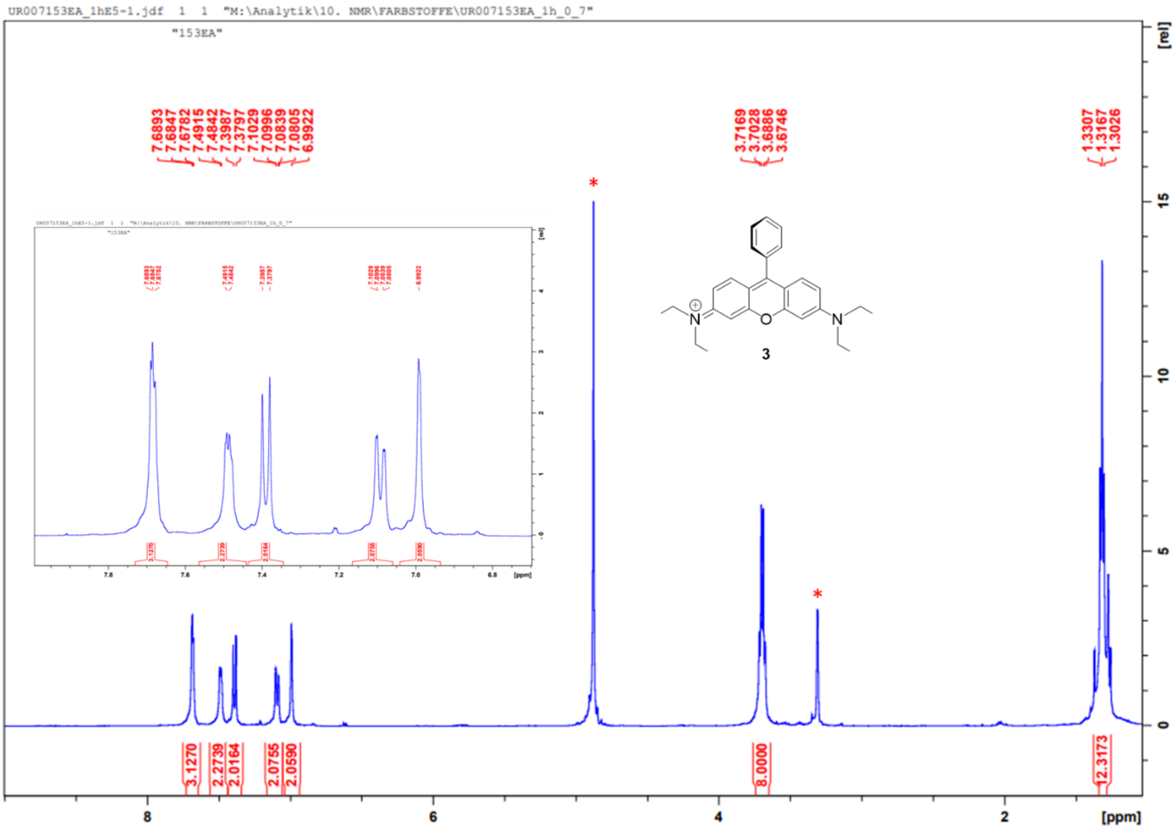
UR07161EA_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007161EA_1H_0,8"
"UR07161EA"
M 158.2582
M 156.0338
M 134.2666
M 131.3341
M 128.6110
M 118.7662
M 114.5769
M 105.3605
M 96.1441
M 45.8727
M 11.3111
OH
Br
N
O
N
2b
[ppm]
[rel]

Compound 2c


UR0071632EA_1hA5-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\FINAL\UR0071632EA_1H-dye-2c"
"A1h_1h"
7.7811
6.8119
3.6068
3.5957
3.5842
3.5708
3.5595
3.5479
3.1237
3.1111
3.0983
2.7890
2.7770
2.7649
2.1527
2.1415
2.1304
2.0194
2.0088
1.9981
1.0000
1.7201
4.1102
4.2319
4.0681
4.4689
2c
[ppm]
[rel]


UR0071632EA_13cE6-1-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR0071632EA_13c07"
"UR0071632EA"
153.6143
152.5804
151.3499
134.0803
133.1162
125.5075
124.4511
115.3620
114.4483
111.7975
105.4680
101.9700
50.6228
50.1429
27.2263
20.4799
19.6385
19.5408
2c
[ppm]
[rel]

Compound 3



UR007153EA_1hE5-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007153EA_1h_0_7"
"153EA"
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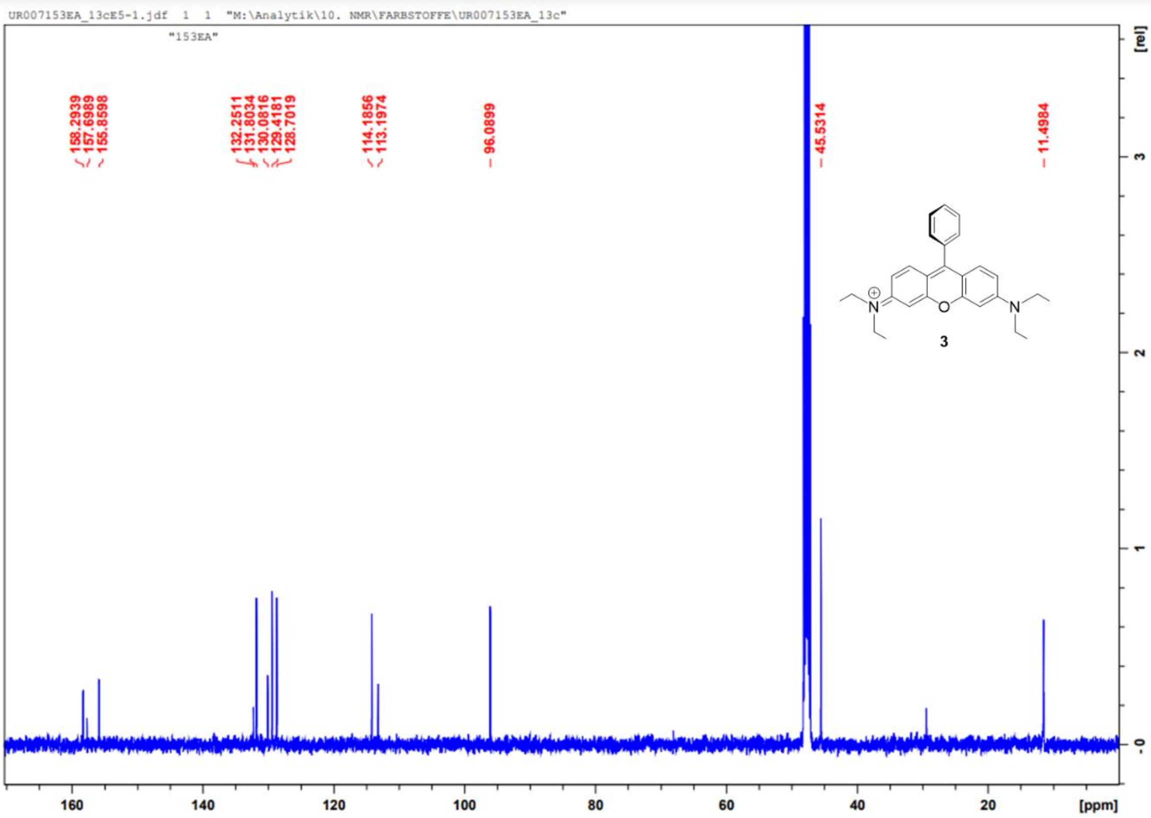
7.6847
7.6782
7.4915
7.4842
7.3987
7.3797
7.1029
7.0996
7.0839
7.0805
6.9922
3.7169
3.7028
3.6886
3.6746
1.3307
1.3167
1.3026
3
3.1270
2.2739
2.0164
2.0755
2.0590
8.0000
12.3173
8
6
4
2
[ppm]
[rel]
0
5
10
15



UR007153EA_13cE5-1.jdf 1 1 "M:\Analytik\10. NMR\FARBSTOFFE\UR007153EA_13c"
"153EA"
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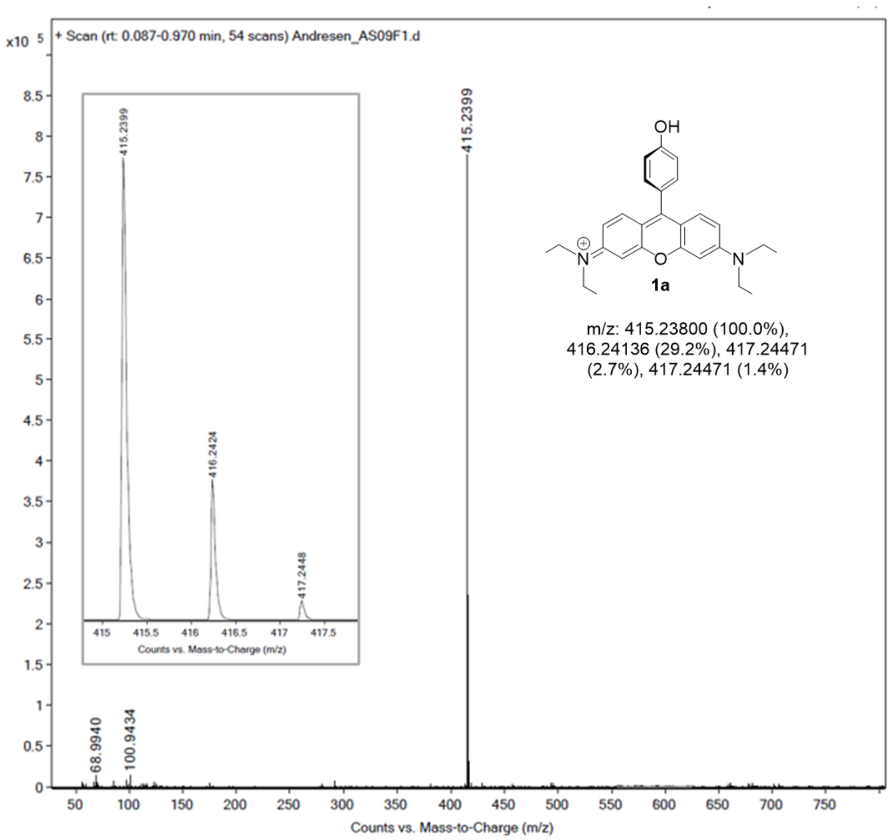
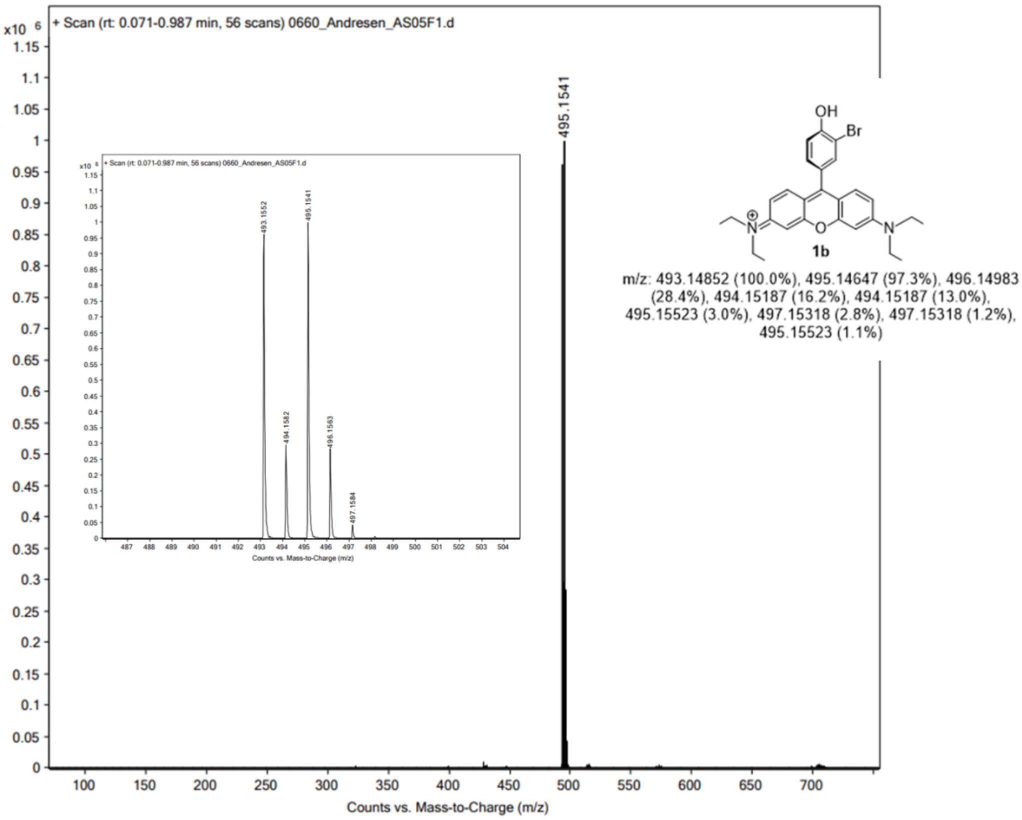
157.6989
155.8598
132.2511
131.8034
130.0816
129.4181
128.7019
114.1856
113.1974
96.0899
45.5314
11.4984
3
160
140
120
100
80
60
40
20
[ppm]
[rel]
0
1
2
3

Mass spectra

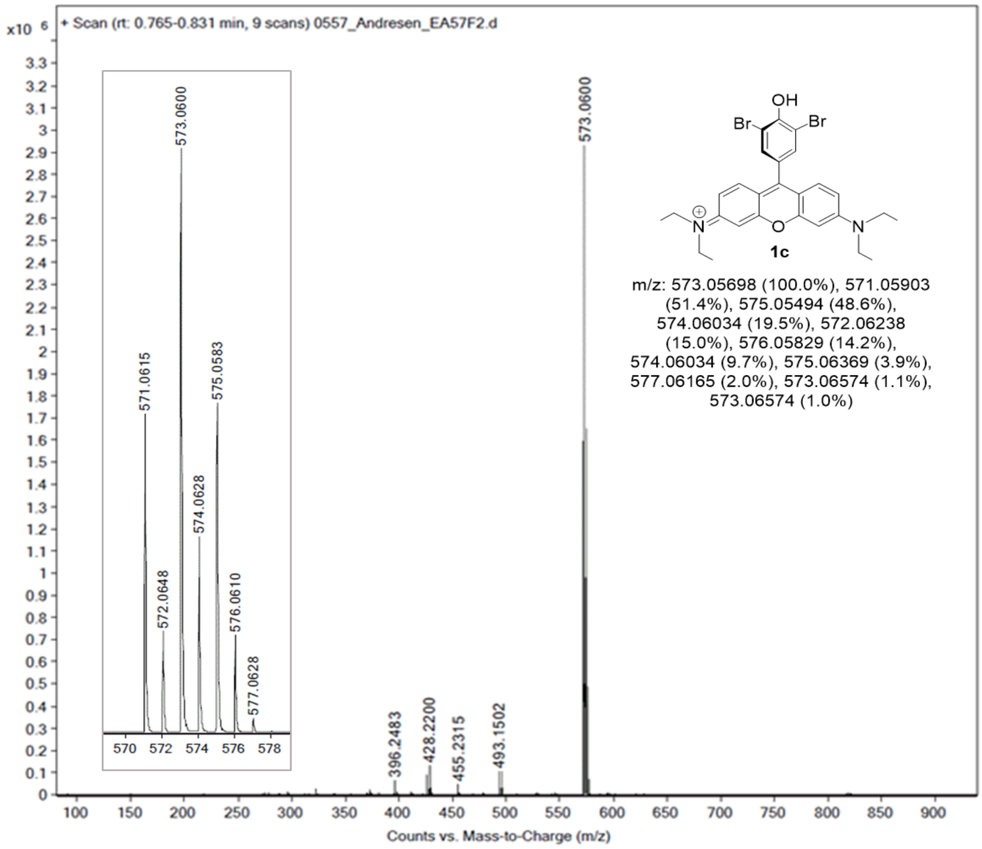
Compound 1a



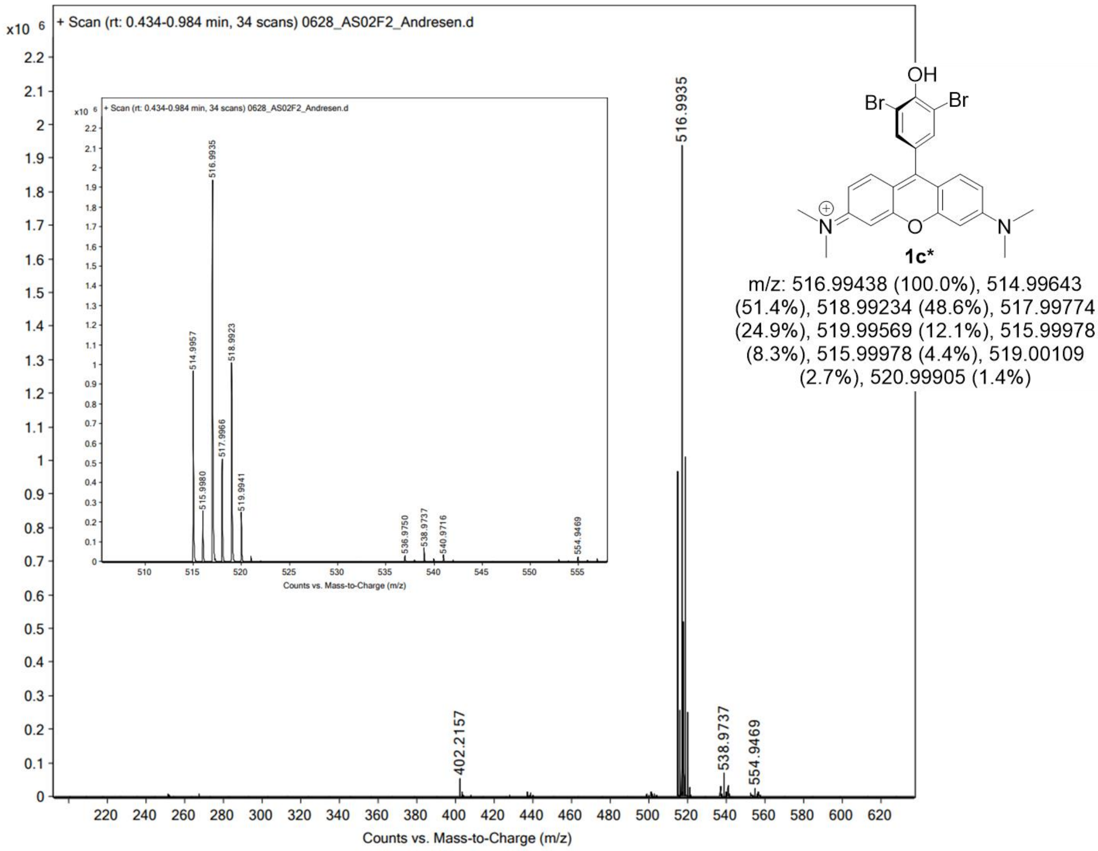
Compound 1b



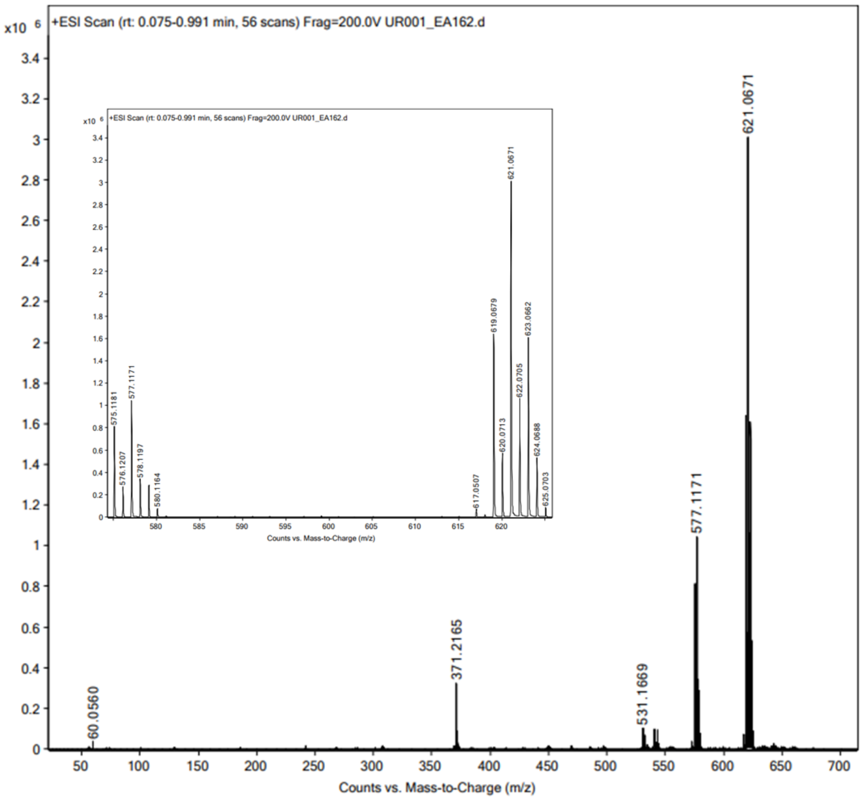
Compound 1c

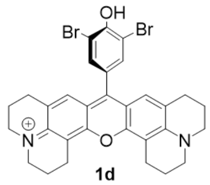


Compound 1c*



Compound 1d

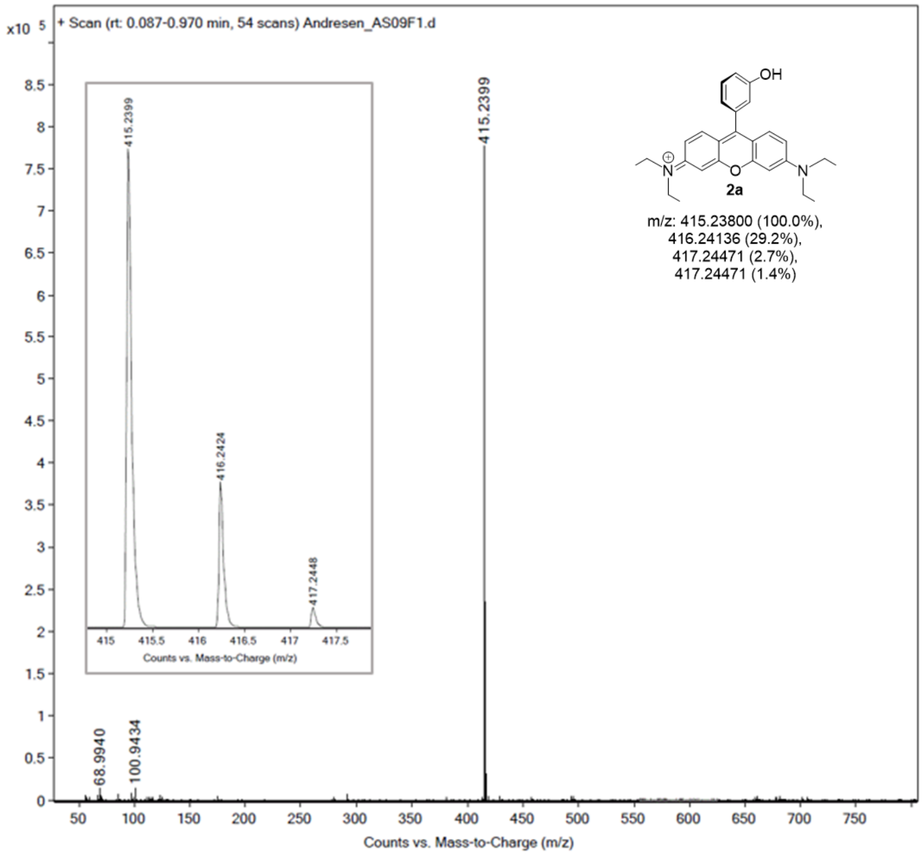




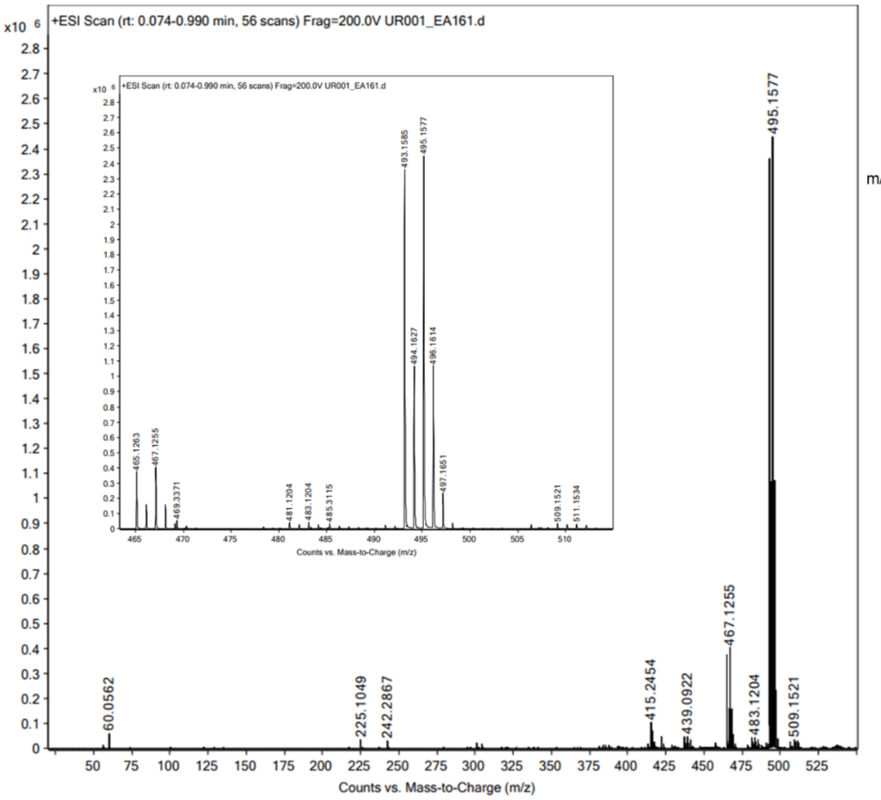
1d

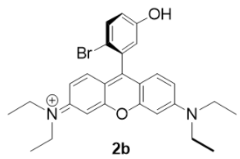
m/z: 621.05698 (100.0%), 619.05903 (51.4%), 623.05494 (48.6%), 622.06034 (33.5%), 620.06238 (16.7%), 624.05829 (16.3%), 623.06369 (2.8%), 625.06165 (2.6%), 623.06369 (2.6%), 621.06574 (1.5%), 621.06574 (1.3%)

Compound 2a



Compound 2b

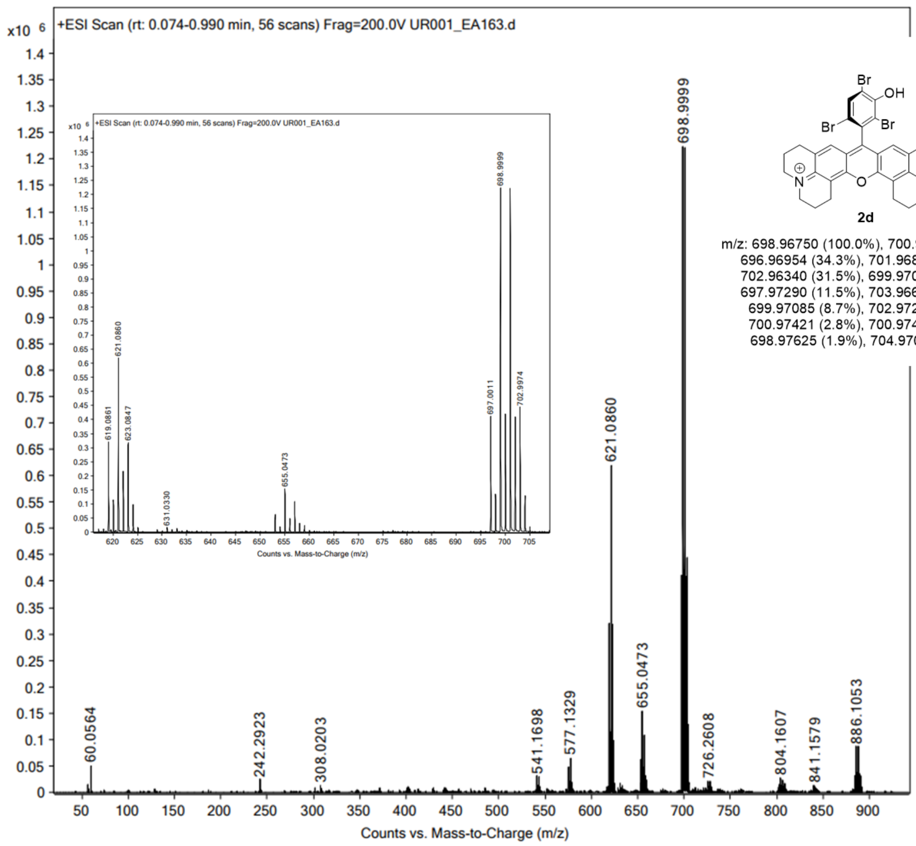




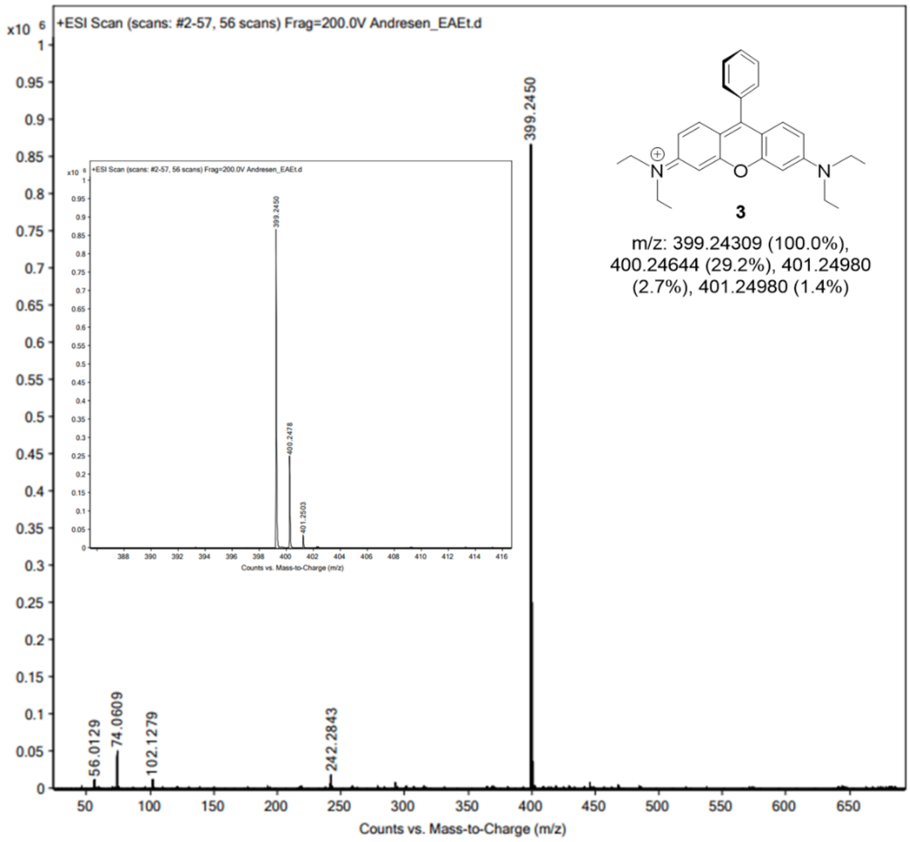
2b

m/z: 493.14852 (100.0%), 495.14647 (97.3%), 496.14983 (28.4%), 494.15187 (16.2%), 494.15187 (13.0%), 495.15523 (3.0%), 497.15318 (2.8%), 497.15318 (1.2%), 495.15523 (1.1%)

Compound 2c



Compound 3



5. References:

1. S. Radunz, H. R. Tschiche, D. Moldenhauer and U. Resch-Genger, *Sensors and Actuators B: Chemical*, 2017, **251**, 490-494.