Three-State Fluorescence of a 2-Functionalized Pyrene-Based RNA-Label

Supporting Information

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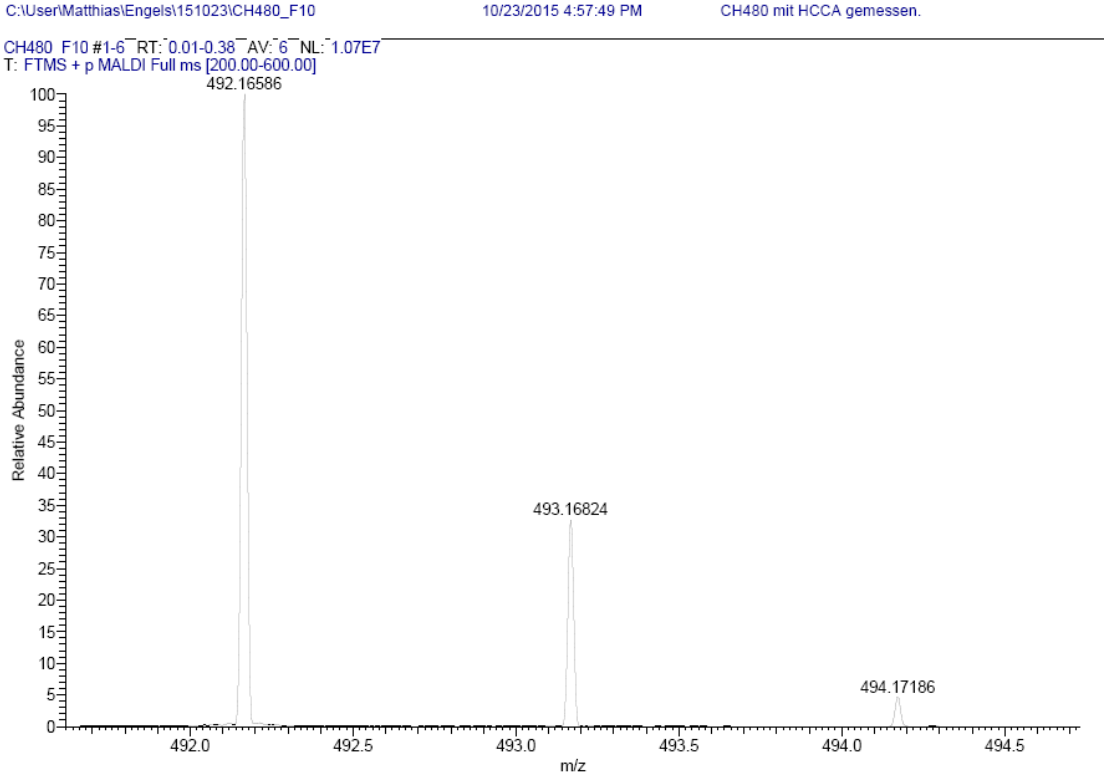
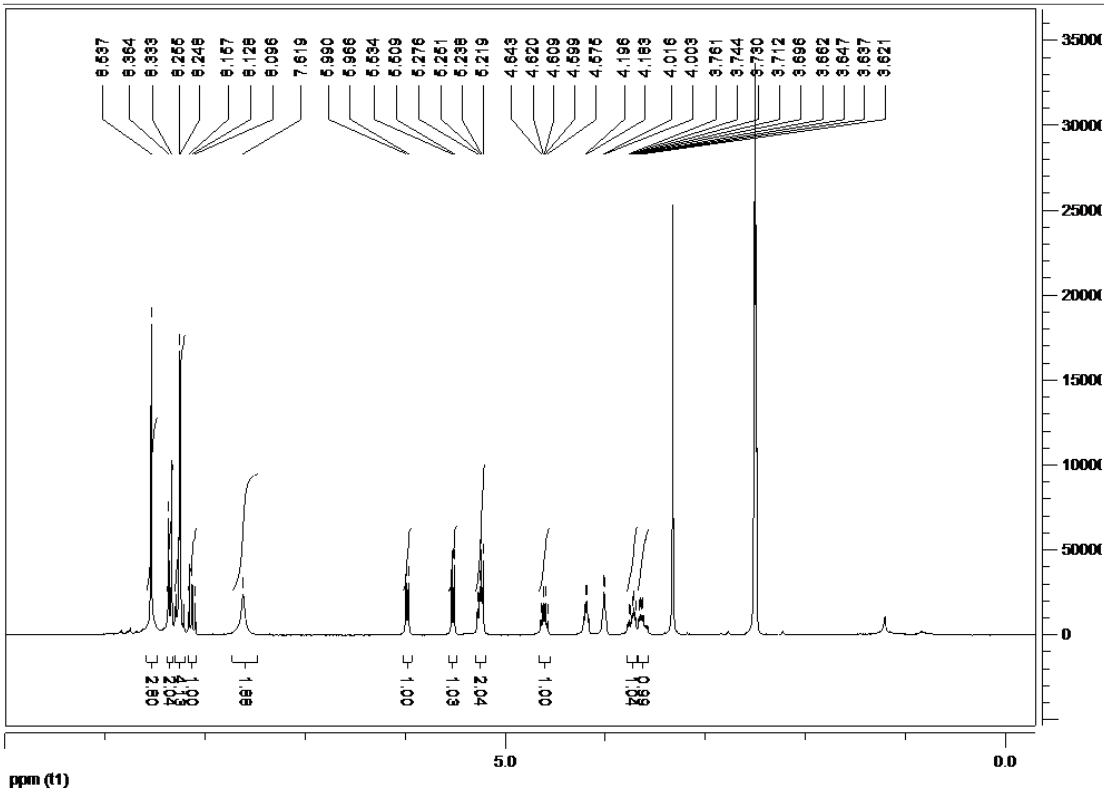
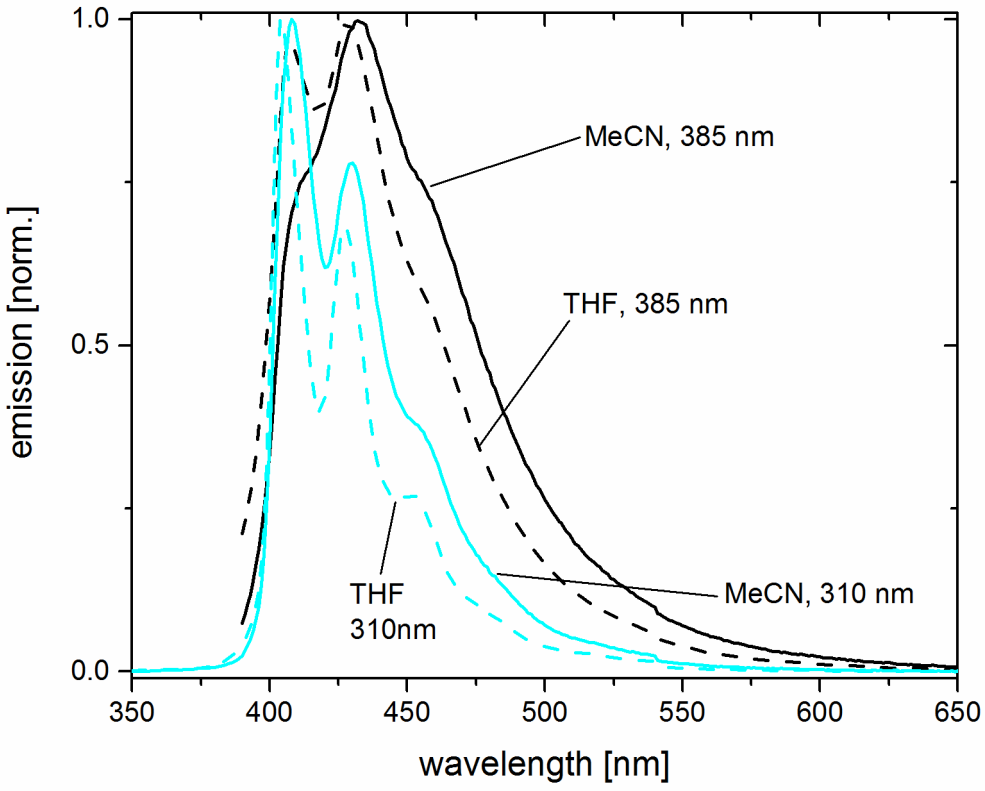
Supporting Figure S1. Mass spectrometry and 1H-NMR of 2PyA in DMSO-d6





Supporting Figure S2. Excitation dependence of 2PyA emission in THF and MeCN



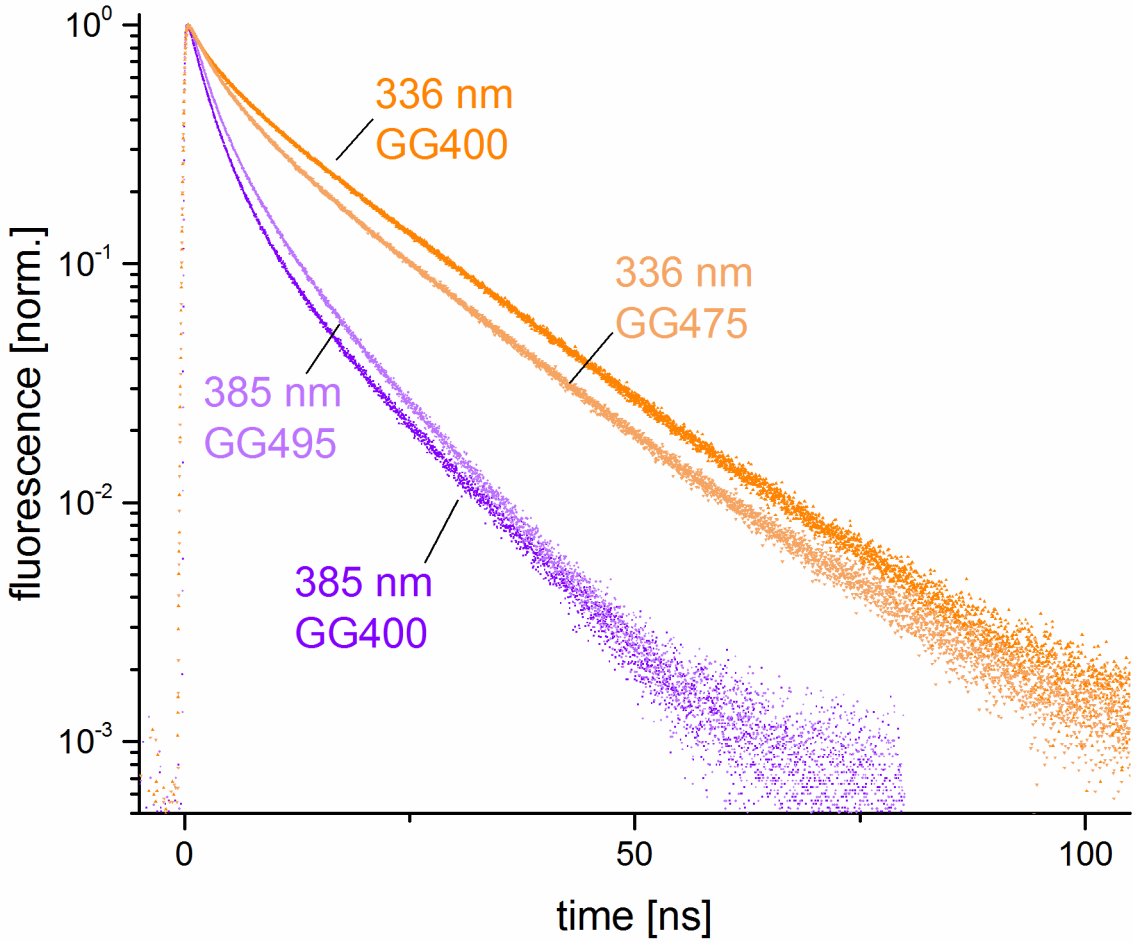
Supporting Table S1. Excitation dependence of the time resolved 2PyA fluorescence

λ_{exc}/nm	τ_1/ns[a]	n_1/%[b]	τ_2/ns[a]	n_2/%[b]	τ_3/ns[a]	n_3/%[b]	χ^2
385	1.6	23	4.6	40	12.4	37	1.1
370	1.5	17	4.6	43	11.7	40	1.1
360	1.2	13	4.3	44	11.7	43	1.2
336	0.8	2	4.4	12	15.8	86	1.1
310	1.1	2	5.1	11	16.0	87	1.1

[a] uncertainty: 0.3 ns

[b] uncertainty: 1 %

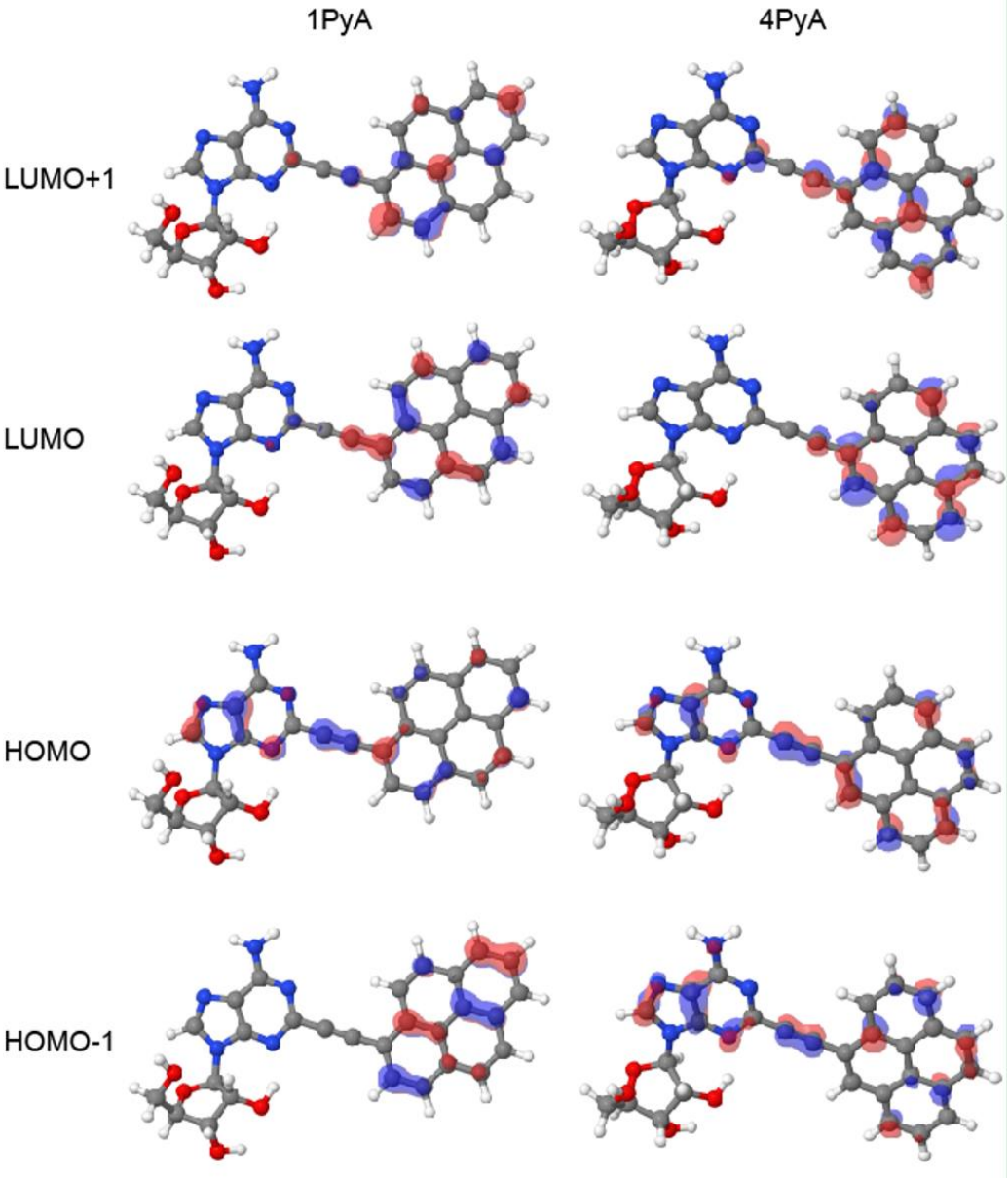
Supporting Figure S3. Emission-filter dependence of the time resolved 2PyA fluorescence



Supporting Table S2. Excitation dependence of the time resolved 2PyA fluorescence

λ_{exc}/nm	filter	τ_1/ns[a]	n_1/%[b]	τ_2/ns[a]	n_2/%[b]	τ_3/ns[a]	n_3/%[b]	τ_{av}/ns	χ^2
385	GG400	1.6	23	4.6	40	12.4	37	6.7	1.1
	GG495	2.0	26	5.7	40	12.1	35	7.0	1.2
336	GG400	0.8	2	4.4	12	15.8	86	14.1	1.1
	GG475	1.3	4	5.1	21	15.5	74	12.7	1.1

Supporting Figure S4. MOs of 1PyA and 4PyA calculated with Turbomole (cc2, def2-TZVP)



Supporting Table S3. Distances for pairs of atoms in 2PyA for different electronic states in coplanar and twisted geometry.

atoms	S_n , n =	distance / Å (change relative to coplanar S_0 / %)	
		coplanar	twisted
C2 ↔ C2$^{\#}$	0	4.07	4.06 (-0.25)
	1	4.00 (-1.72)	4.05 (-0.49)
	2	4.05 (-0.49)	4.06 (-0.25)
C2$^{\#}$ ↔ C7$^{\#}$	0	7.04	7.01 (-0.43)
	1	7.06 (+0.28)	7.05 (+0.14)
	2	7.05 (+0.14)	7.05 (+0.14)
N7 ↔ C2	0	4.04	4.01 (-0.74)
	1	4.02 (-0.50)	4.01 (-0.74)
	2	4.01 (-0.74)	4.00 (-0.99)
N7 ↔ C7$^{\#}$	0	15.15	15.07 (-0.53)
	1	15.10 (-0.33)	15.11 (0.26)
	2	15.11 (0.26)	15.12 (-0.20)