

Supplementary information

Red-shifted aminated derivatives of GFP chromophore for live-cell protein labelling with lipocalins

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Table S1. Optical properties of synthesized compounds.

		1a	1b	1c	1d	2a	2c	2b	2d	3	4	5	6	7	M739
water	Abs ^a	602 (-) ^c	600 (-) ^c	609 (-) ^c	597 (31500)	532 (32000)	534 (31000)	529 (30500)	539 (33500)	603 (55000)	608 (58500)	529 (31000)	465 (39000) ^a	532 (56500)	520 (53500)
	Em ^b	690 (1.2)	695 (0.6)	710 (0.5)	705 (0.3)	597 (60)	599 (50)	600 (58)	607 (13)	626 (12)	632 (5.1)	615 (0.2)	516 (0.1) ^b	581 (0.4)	563 (3.1)
MeOH	Abs	578 (37000)	587 (35500)	592 (44500)	597 (33500)	525 (41000)	528 (40500)	526 (42000)	529 (45000)	596 (58000)	580 (53000)	516 (33500)	455 (48000)	503 (52500)	505 (48000)
	Em	657(8.6)	678 (3.9)	670 (1.7)	697 (1.5)	591(67)	594 (61)	591 (89)	597 (56)	635 (37)	626 (15)	608 (0.2)	501 (0.3)	576 (0.3)	557 (22)
CH ₃ CN	Abs	567 (33000)	580 (33000)	587 (38000)	582 (30000)	512 (40500)	514 (40500)	512 (41500)	517 (43500)	580 (52000)	545 (45000)	503 (36000)	443 (43000)	488 (49500)	494 (45500)
	Em	677(6.4)	708 (2.1)	715 (1.1)	716 (1.6)	582 (60)	581 (58)	582 (60)	591 (51)	639 (40)	610 (87)	601 (0.2)	492 (0.3)	562 (0.2)	554 (31)
EtOAc	Abs	565 (34000)	579 (32000)	584 (38000)	582 (30500)	514 (42500)	517 (38500)	514 (39000)	518 (44000)	583 (52000)	532 (44000)	496 (37000)	440 (45000)	473 (48500)	492 (47000)
	Em	660 (12)	690 (3.6)	703 (1.8)	702 (2.7)	570 (63)	567 (64)	572 (82)	580 (53)	631 (53)	592 (55)	578 (0.1)	483 (0.4)	543 (0.2)	538 (63)
dioxane	Abs	571 (33500)	583 (31000)	589 (35500)	591 (31000)	519 (40500)	523 (39500)	521 (39500)	524 (43500)	589 (55000)	534 (40000)	495 (33000)	446 (42000)	478 (50500)	497 (51000)
	Em	655 (16)	685 (4.9)	701 (2.6)	696 (4.8)	569 (70)	568 (70)	570 (90)	576 (53)	624 (66)	587 (30)	572 (0.1)	480 (0.5)	541 (0.2)	538 (72)

a – peak maximum in nm (extinction coefficient in (M cm)⁻¹), b – peak maximum in nm (fluorescence quantum yield in %), c - non soluble enough to measure EC correctly

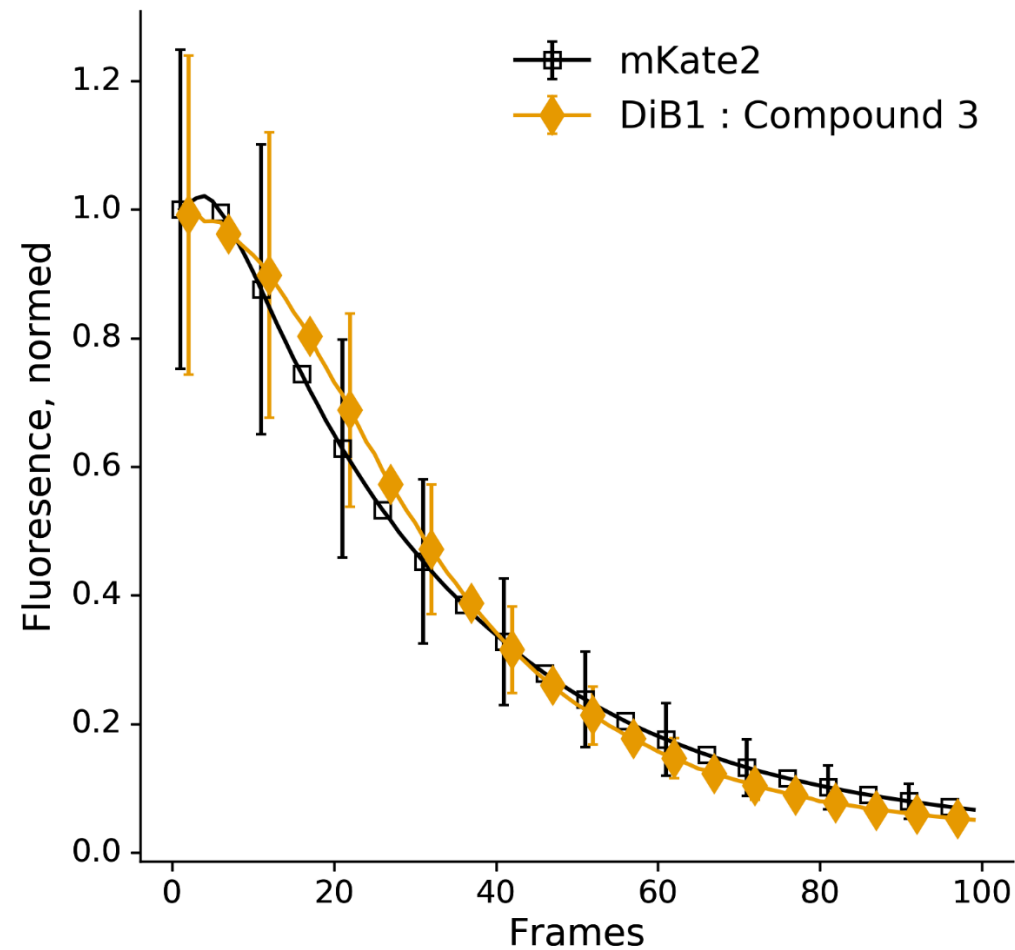


Figure S1. Photostability of DiB1:3 complex in living cells. (Orange line) - photobleaching curves of HEK293T expressing H2B fused with DiB1 and stained with compound **3** in a widefield setup. (black line) - curve for H2B-mKate2 under the same imaging conditions. HEK293T cells expressing H2B fused with the corresponding reporter were imaged 24h after transient transfection in MEM media supplemented with 20mM HEPES. Data points acquired with 40x 0.85NA objective lens at 10s intervals, with 8s bursts of 40 W/cm² green light (pE300 light source, CoolLED) in between the imaging frames. Mean values and standard deviation (n=21 cells) are depicted. Markers are shown for every 5 data points for clarity.

Copies of ^1H and ^{13}C NMR spectra

