SUPPORTING INFORMATION

Direct Observation of Guanine Photo-Oxidation from New Potential Anticancer Drugs Via Ultrafast Electron Transfer

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Experimental Section

The investigated compounds **A**-**C** were synthesized for previous studies.[1–4] Spectral and photophysical measurements were carried out in ETN (1 mM EDTA, 10 mM Tris-HCl, 10 mM NaCl) aqueous buffered solutions at pH 7.2. Ethylenediaminetetraacetic acid (EDTA), tris(hydroxymethyl)aminomethane hydrochloride (Tris-HCl), and NaCl were purchased from Sigma-Aldrich. Adenosine-5'-triphosphate (ATP), Cytidine-5'-triphosphate (CTP), Guanosine-5'-triphosphate (GTP) and Thymidine-5'-triphosphate (TTP) were purchased from Sigma-Aldrich.

Absorption spectra were measured with a Cary 4E (Varian) spectrophotometer, while fluorescence spectra, with appropriate corrections for the instrumental response, were detected by a FluoroMax-4P spectrofluorimeter (HORIBA Scientific) operated by FluorEssence. The fluorescence quantum yields (ϕ_F, experimental error ± 10%) of dilute solutions (1×10^{-6} M) of the dyes alone and in the presence of ca. 5 mM nucleotides were obtained exciting each sample at the relative maximum absorption wavelength by employing tetracene (ϕ_F = 0.17 in air-equilibrated cyclohexane) as reference compound.[5] Fluorescence lifetimes were measured through an Edinburgh Instrument 199S spectrofluorometer equipped with the single photon counting technique. A LED centered at 450 nm was used as the light source (temporal resolution = 0.5 ns). The experimental error on the fluorescence lifetimes is ± 10%.

Spectrophotometric and fluorimetric titrations were performed by adding increasing volumes of ATP and GTP stock solutions (C ≈ 5 mM) into the cuvette containing the solution of the studied compounds. The initial volume was 2 mL and the total volume of nucleotides added at the end of the titration ranged from 1.2 and 1.6 mL. After mixing nucleotides with the investigated compounds at every addition, it was observed that equilibrium was quickly reached, allowing spectra to be recorded after waiting a standard time of 5 minutes. Each absorption spectrum was multiplied for the relative dilution factor, while emission spectra were corrected by taking into account the changes in absorbance at the excitation wavelength after every addition. Fluorescence data were processed by means of non-linear fitting to a modified Stern-Volmer equation[1] which gave values for the binding constants (K) between each compound and ATP or GTP.

$$\frac{Area_F}{Area_{F,0}} = \frac{1 + \Delta Area_F \times K[Nucleotide]}{1 + K[Nucleotide]} \qquad \text{eq. 1}$$

The determination of ϕ_F for the ATP/compound or GTP/compound complexes was conducted by comparison of the emission spectra of the free ligand ($Area_{F,0}$), used as internal standard, and that of the bound molecule recorded after each addition of nucleotide during the titration ($Area_F$) corrected for the fraction of absorbed light: $\Phi_{F,complex} = \frac{Area_F}{Area_{F,0}} \times \Phi_{F,0}$.

Ultrafast time-resolved transient absorption and fluorescence up-conversion measurements were carried out by using Helios and Halcyone setups (Ultrafast System), already described elsewhere.[6,7] Femtosecond excitation pulses at 400 nm of ca. 40 fs were generated by using an amplified Ti:sapphire laser system. In the transient absorption setup, the pump pulses were passed through a chopper that cut out every second pulse and collimated to the sample in a 2 mm quartz cuvette. Probe pulses for optical measurements were produced by passing a small portion of 800 nm light to an optical delay line with a time window of 3200 ps and focusing it into a 2 mm thick sapphire crystal to generate a white-light continuum in the 450–800 nm range. The white light was focused onto the sample and the differential absorbance (ΔA) in the presence and absence of pump excitation was revealed by a CCD detector at each delay. In the up-conversion setup, the 400-nm pulse excites the sample whereas the fundamental laser beam acts as the "gate" light, after passing through a delay line, which is then summed to the sample emission promoting the up-conversion process in a motorized BBO crystal. The time resolution is about 200 fs while the spectra resolution is 1.5 nm. All the measurements were carried out under magic-angle conditions. Solutions of compounds **A**-**C** in the presence of the nucleotides at ca. 5 mM were prepared in ETN buffer. To avoid photoproduct interferences, the solutions were stirred during the experiments and photodegradation was checked

by recording the absorption spectrum of the samples before and after the measurements. Transient absorption and broadband fluorescence up-conversion data were analyzed using Surface Xplorer PRO (Ultrafast Systems) software, which allows performing singular value decomposition of the 3D surface into principal components (spectra and kinetics) and global analysis (giving lifetimes and Decay Associated Spectra (DAS) of the detected transients). Species Associated Spectra (SAS) were calculated by performing target analysis according to a parallel model for the free and complexed dyes by means of GloTarAn software.[8]

Laser flash photolysis (Edinburgh LP980) experiments were performed upon excitation at 355 nm (third harmonic of a Quanta-Ray/ INDI Nd:YAG laser, Spectra Physics) with nanosecond time-resolution (pulse width 7 ns and laser energy < 1 mJ per pulse) coupled with a PMT for signal detection. The excitation at 355 nm was the pump-pulse while a pulsed xenon lamp was used to probe the absorption properties of the produced excited states. All measurements were performed by purging the sample with pure molecular nitrogen.

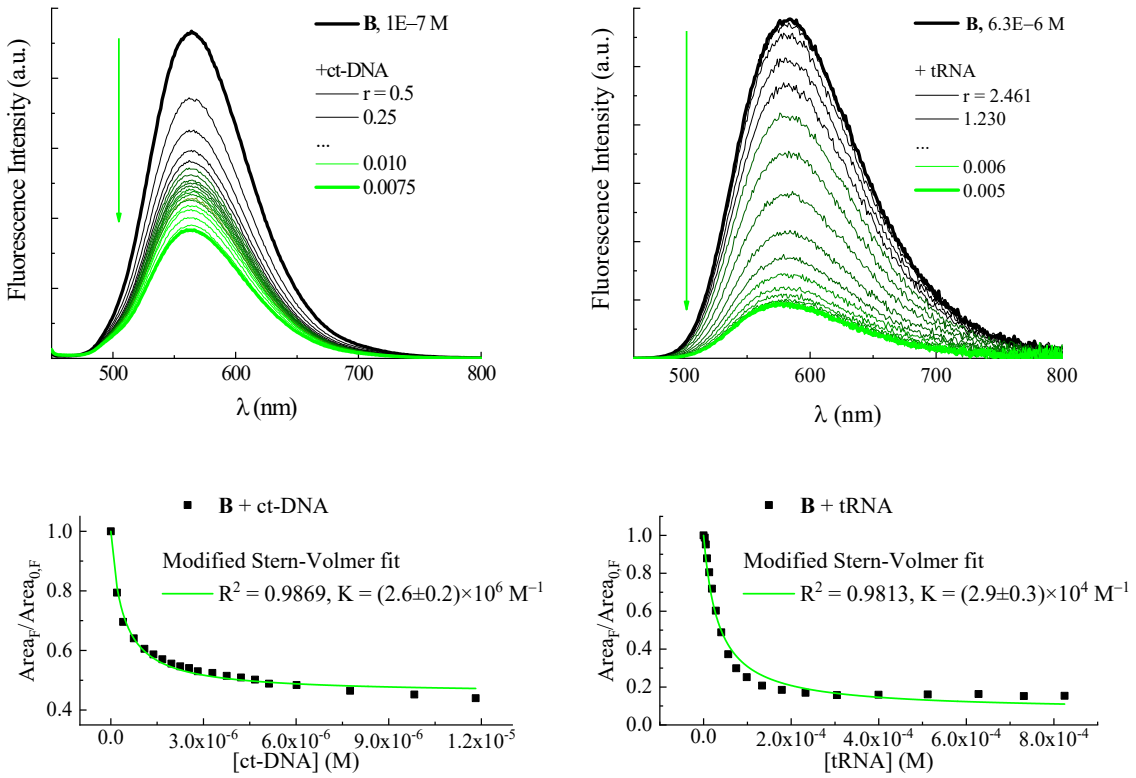

Figure S1. Upper panels: fluorimetric titrations of compound **B** with ct-DNA (left, taken from ref. 27) and t-RNA (right, taken from ref. 30). r is the ratio between drug and nucleic acid concentrations: r=[**B**]/[ct-DNA] or [tRNA]. Fluorescence intensity is corrected for the fraction of absorbed light. Green arrows show the fluorescence quenching with increasing [ct-DNA] or [tRNA]. Lower panels: fluorescence intensity of **B** as a function of ct-DNA and tRNA concentrations and its fitting according to a modified Stern-Volmer equation (eq. 1).

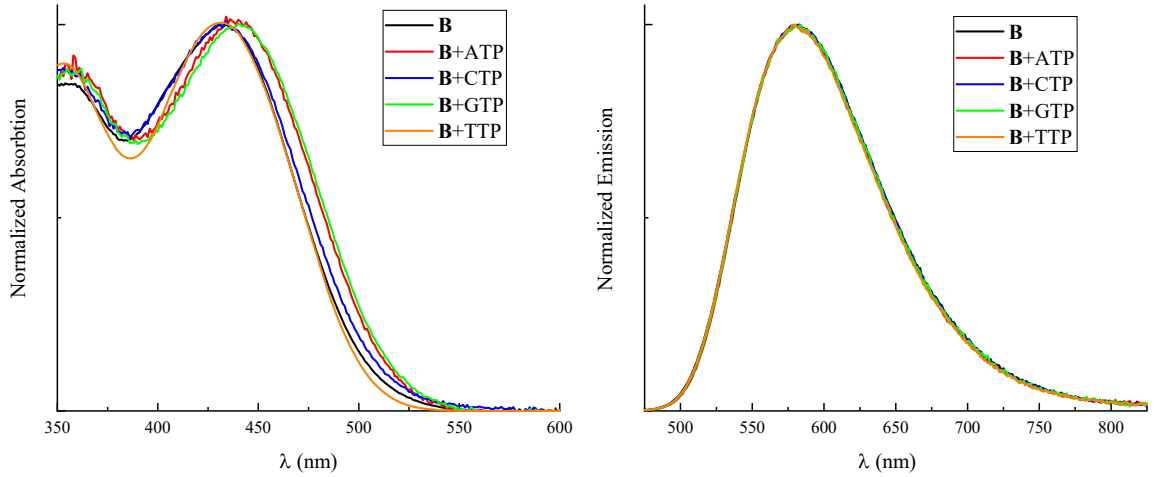

Figure S2. Normalized absorption and emission spectra for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM).

Table S1. Absorption and emission maxima and Stokes shifts for compounds **A** and **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM).

	λabs (nm)	λem (nm)	Δυ (cm^{-1})
A	450	604	5670
A+ATP	458	604	5280
A+CTP	453	604	5520
A+GTP	460	604	5180
A+TTP	450	604	5670
B	433	581	5880
B+ATP	439	581	5570
B+CTP	433	581	5880
B+GTP	441	581	5460
B+TTP	435	581	5780

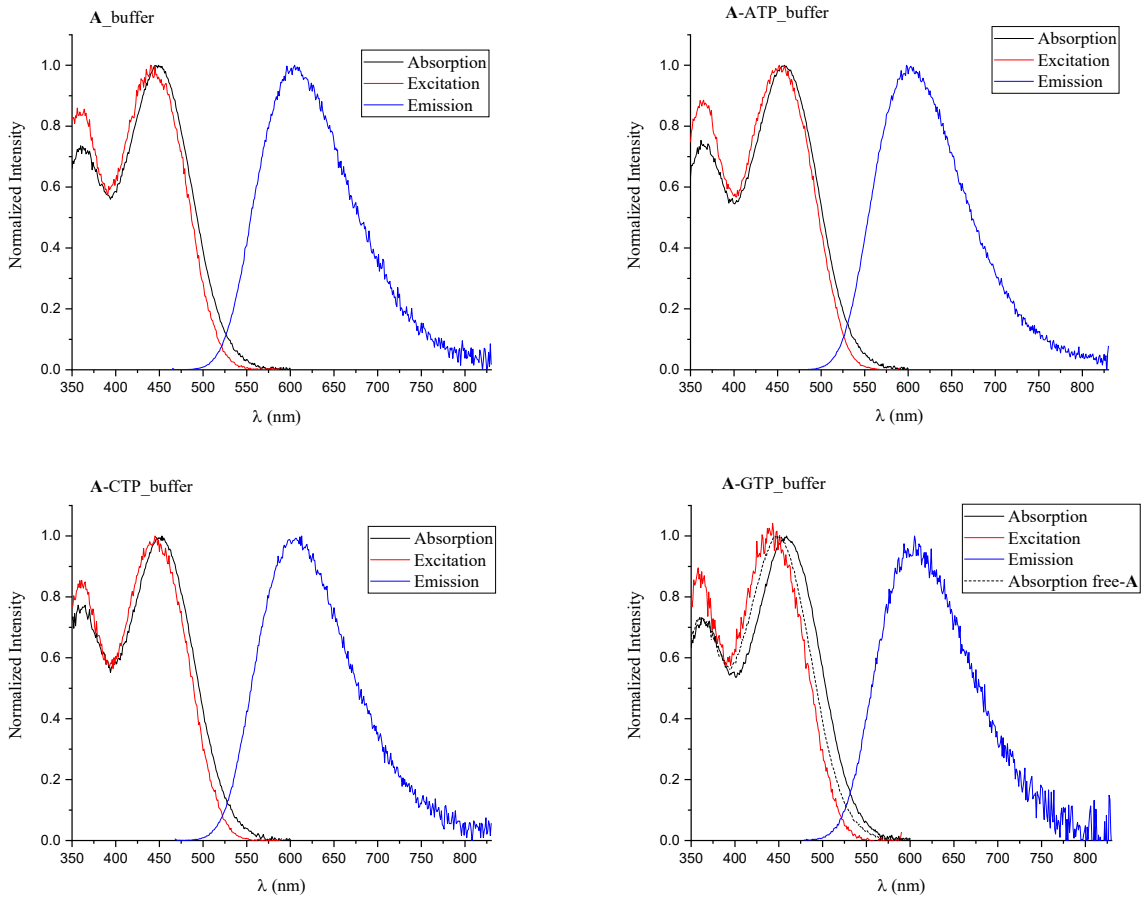

Figure S3. Normalized Absorption, Excitation and Emission spectra for compound **A**, alone and in the presence of nucleotides (ca. 5 mM).

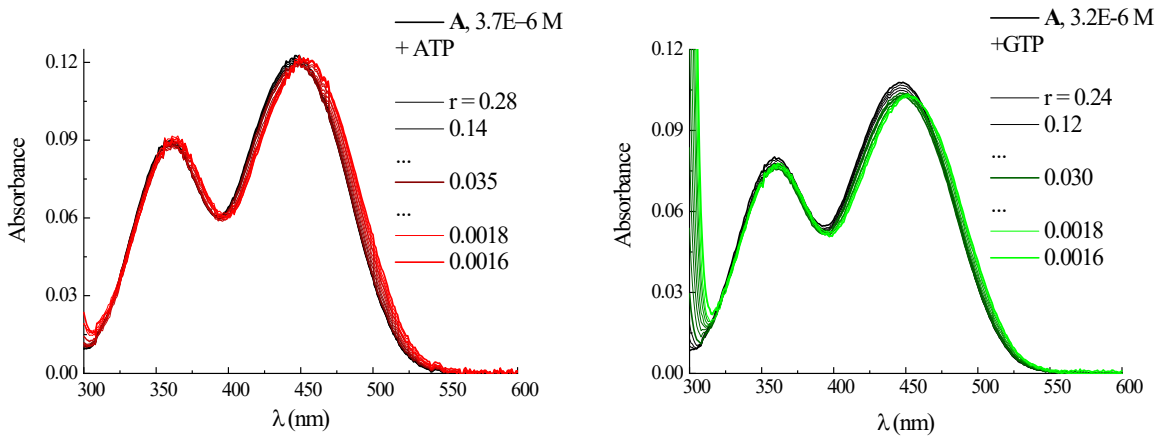

Figure S4. Spectrophotometric titrations of compound **A** with ATP (left) and GTP (right). r is the ratio between drug and nucleotide concentrations: r=[**A**]/[ATP] or [GTP]. Absorbance is corrected for dilution.

Table S2. Fluorescence quantum yields, lifetimes, and average lifetimes of compound **A** in buffer at pH 7 alone and in the presence of increasing concentrations of ATP as a function of r (r = [A]/[ATP]).

r = [A]/[ATP]	ϕ_F	τ_F (ns)	$\tau_{F,av}$ (ns)
	0.180	1.68	1.68
0.27578	0.180	1.68	1.68
0.13823	0.180	1.69	1.69
0.06946	0.182	1.68 (98.5%); 3.12 (1.5%)	1.70
0.03507	0.186	1.68 (94.3%); 3.12 (5.7%)	1.76
0.01788	0.194	1.68 (87%); 3.12 (13%)	1.87
0.01127	0.201	1.68 (81%); 3.12 (19%)	1.95
0.00757	0.211	1.68 (72%); 3.12 (28%)	2.08
0.00527	0.223	1.68 (65%); 3.12 (35%)	2.18
0.00374	0.236	1.68 (55%); 3.12 (45%)	2.33
0.00298	0.241	1.68 (50%); 3.12 (50%)	2.40
0.00241	0.250	1.68 (44%); 3.12 (56%)	2.49
0.00206	0.261	1.68 (40%); 3.12 (60%)	2.54
0.00183	0.269	1.68 (37%); 3.12 (63%)	2.59
0.00160	0.271	1.68 (34%); 3.12 (66%)	2.63

Table S3. Fluorescence quantum yields, lifetimes, and average lifetimes of compound **A** in buffer at pH 7 alone and in the presence of increasing concentrations of GTP as a function of r (r = [**A**]/[GTP]).

r = [A]/[GTP]	ϕ_F	τ_F (ns)	$\tau_{F,av}$ (ns)
	0.180	1.59	1.59
0.23851	0.181	1.59	1.59
0.11955	0.181	1.59	1.59
0.06007	0.180	1.58	1.58
0.03033	0.177	1.59	1.59
0.01546	0.169	1.58	1.58
0.00975	0.162	1.57	1.57
0.00654	0.155	1.0 (1.6%); 1.6 (98.4%)	1.59
0.00456	0.145	1.0 (3.3%); 1.6 (96.7%)	1.58
0.00324	0.134	1.0 (4.8%); 1.6 (95.2%)	1.57
0.00258	0.125	1.0 (5.6%); 1.6 (94.4%)	1.57
0.00208	0.118	1.0 (8.1%); 1.6 (91.9%)	1.57
0.00178	0.110	1.0 (9.6%); 1.6 (90.4%)	1.54
0.00159	0.108	1.0 (10.3%); 1.6 (89.7%)	1.54

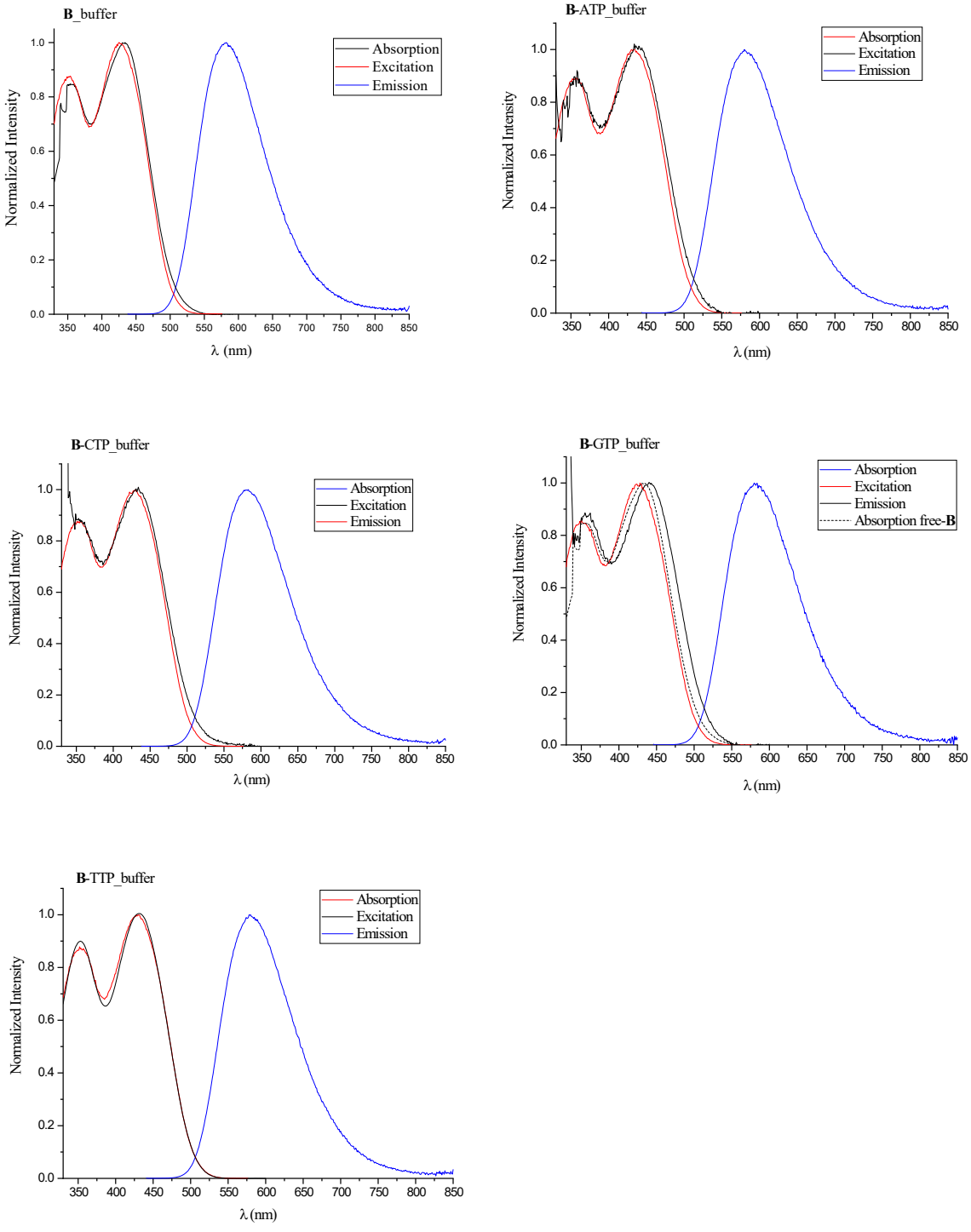

Figure S5. Normalized Absorption, Excitation and Emission spectra for compound **B**, alone and in the presence of nucleotides (ca. 5 mM).

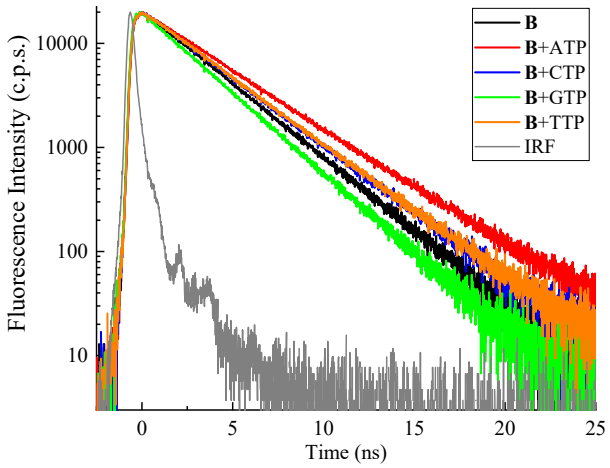

Figure S6. Fluorescence decay kinetics recorded by TC-SPC (λ_{exc} = 450 nm) for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5mM) together with the Instrumental Response Function (IRF).

Table S4. Fluorescence quantum yields and lifetimes for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5mM).

	ϕ_F	ϕ_F (%)	τ_F (ns)
B	0.43	43%	2.98
B+ATP	0.44	44%	3.71
B+CTP	0.41	41%	3.22
B+GTP	0.17	17%	0.45(3%) and 2.73(97%)
B+TTP	0.41	41%	3.26

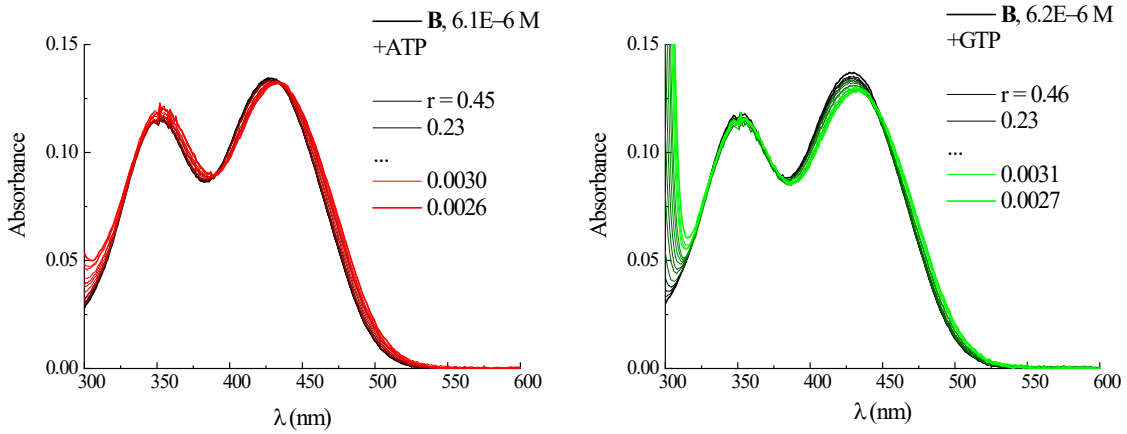

Figure S7. Spectrophotometric titrations of compound **B** with ATP (left) and GTP (right). r is the ratio between drug and nucleotide concentrations: r=[**B**]/[ATP] or [GTP]. Absorbance is corrected for dilution.

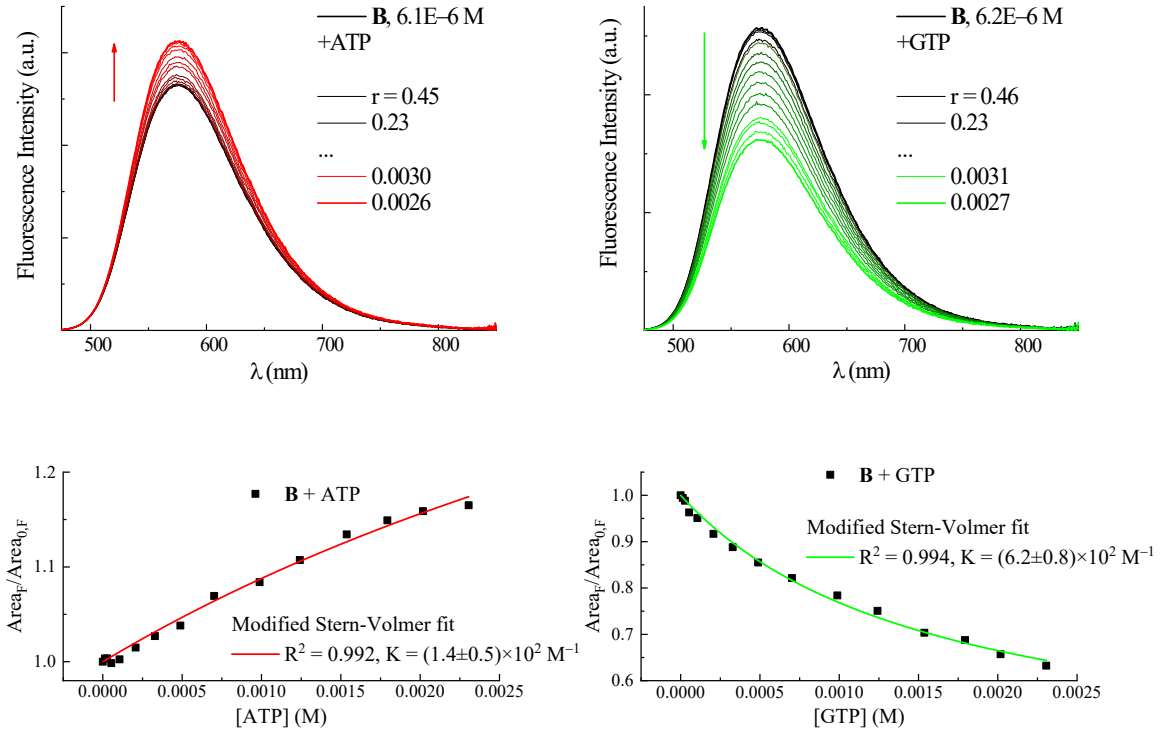

Figure S8. Upper panels: fluorimetric titrations of compound **B** with ATP (left) and GTP (right). r is the ratio between drug and nucleotide concentrations: r=[**B**]/[ATP] or [GTP]. Fluorescence intensity is corrected for the fraction of absorbed light. Arrows indicate the trend of the fluorescence intensity with decreasing r: the red arrow shows the fluorescence enhancement due to increasing [ATP]; the green arrow shows the fluorescence quenching with increasing [GTP]. Lower panels: fluorescence intensity of **B** as a function of ATP and GTP concentrations and its fitting according to a modified Stern-Volmer equation (eq. 1).

Table S5. Fluorescence quantum yields and lifetimes of compound **B** in buffer at pH 7 alone and in the presence of increasing concentrations of ATP as a function of r (r = [**B**]/[ATP]).

r = [B]/[ATP]	ϕ_F	τ_F (ns)
--	0.430	2.98
0.45467	0.431	2.99
0.22790	0.432	2.98
0.11452	0.429	3.00
0.05783	0.431	3.03
0.02948	0.436	3.09
0.01858	0.442	3.15
0.01247	0.446	3.22
0.00869	0.460	3.30
0.00617	0.466	3.40
0.00491	0.476	3.46
0.00397	0.488	3.53
0.00340	0.494	3.57
0.00302	0.498	3.60
0.00265	0.501	3.65

Table S6. Fluorescence quantum yields and lifetimes of compound **B** in buffer at pH 7 alone and in the presence of increasing concentrations of GTP as a function of r (r = [**B**]/[GTP]).

r = [B]/[GTP]	ϕ_F	τ_F (ns)
--	0.430	2.89
0.46212	0.428	2.88
0.23164	0.425	2.86
0.11639	0.414	2.85
0.05877	0.409	2.85
0.02996	0.394	2.86
0.01888	0.382	2.83
0.01268	0.368	2.82
0.00884	0.353	2.80
0.00627	0.337	2.78
0.00499	0.323	2.76
0.00403	0.303	2.74
0.00346	0.296	2.72
0.00307	0.283	2.71
0.00269	0.272	2.70

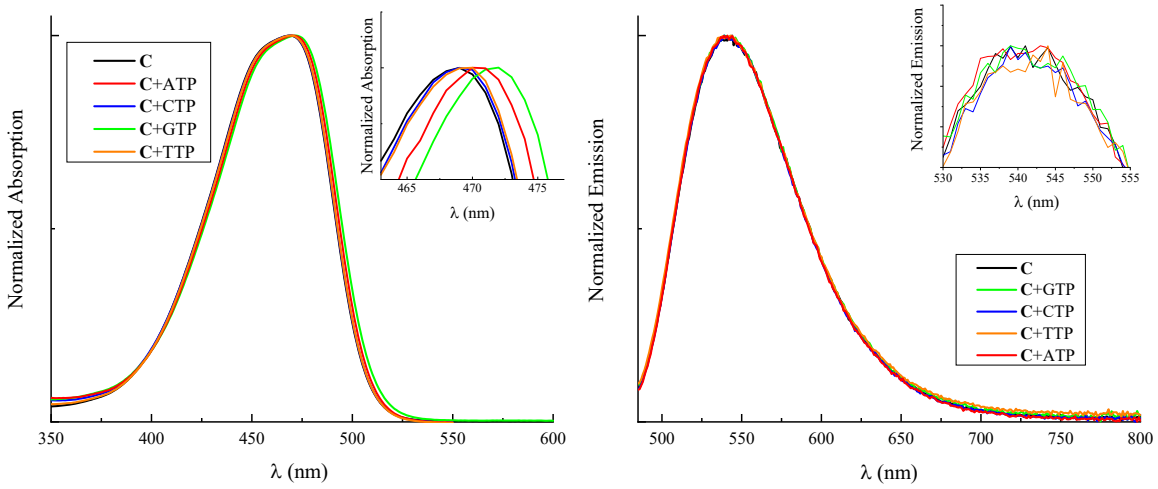

Figure S9. Normalized absorption and emission spectra for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM).

Table S7. Absorption and emission maxima and Stokes shifts for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM).

	λabs (nm)	λem (nm)	Δυ (cm^{-1})
C	469	542	2872
C+ATP	470	541	2792
C+CTP	469	541	2838
C+GTP	472	541	2702
C+TTP	469	542	2872

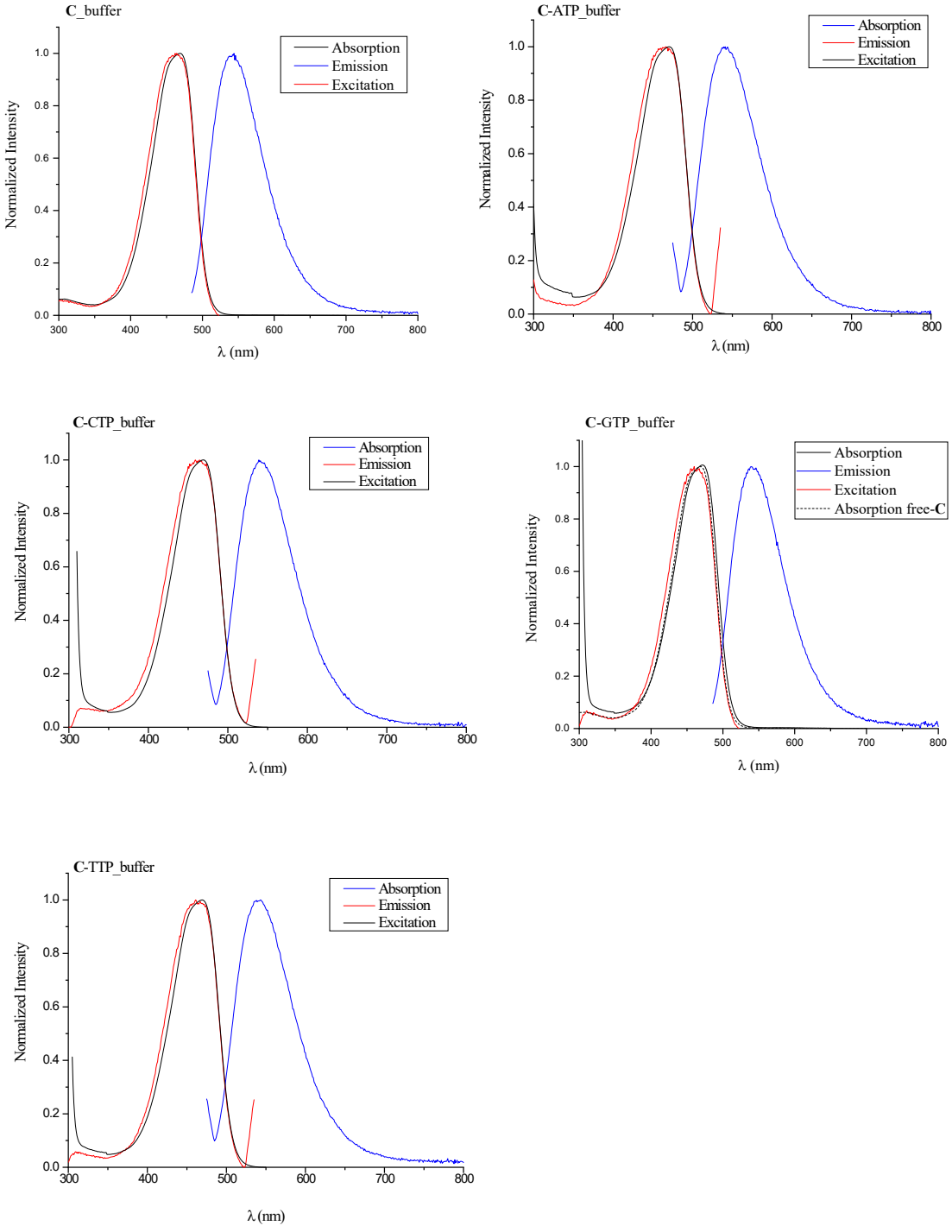

Figure S10. Normalized Absorption, Excitation and Emission spectra for compound **C**, alone and in the presence of nucleotides (ca. 5 mM).

Table S8. Fluorescence quantum yields and lifetimes for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM). Lifetimes were obtained from Fluorescence Up Conversion measurements.

	ϕ_F	τ_F (ps)
C	0.0065	24
C+ATP	0.0072	28
C+CTP	0.0068	22
C+GTP	0.0046	3.4(28%) and 25(72%)
C+TTP	0.0072	21

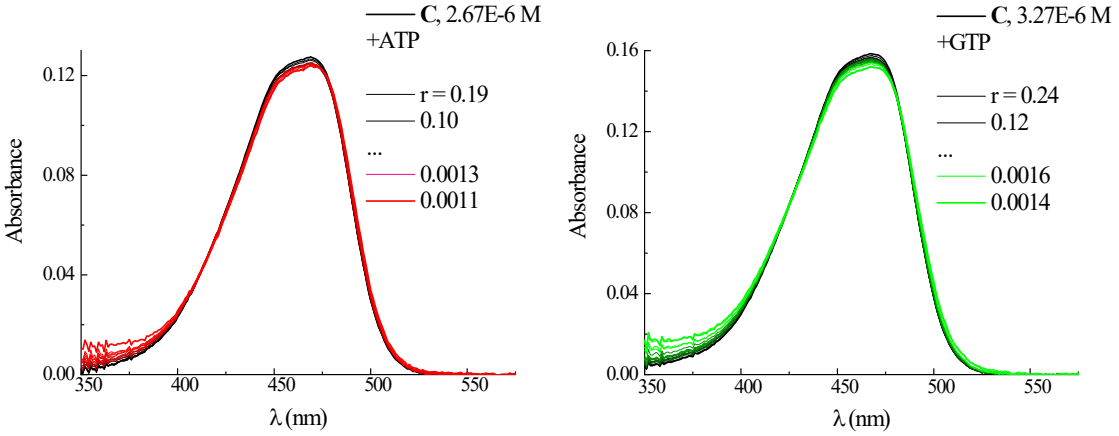

Figure S11. Spectrophotometric titrations of compound **C** with ATP (left) and GTP (right). r is the ratio between drug and nucleotide concentrations: r=[**C**]/[ATP] or [GTP]. Absorbance is corrected for dilution.

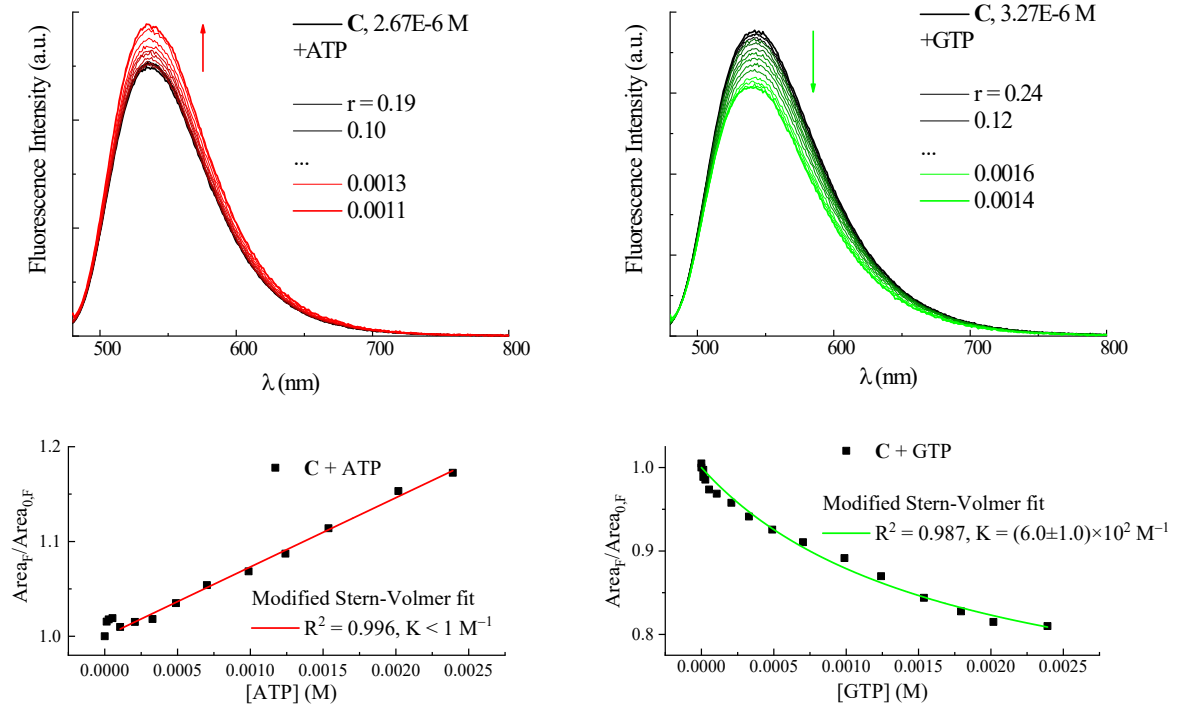

Figure S12. Upper panels: fluorimetric titrations of compound **C** with ATP (left) and GTP (right). r is the ratio between drug and nucleotide concentrations: r=[**C**]/[ATP] or [GTP]. Fluorescence intensity is corrected for the fraction of absorbed light. Arrows indicate the trend of the fluorescence intensity with decreasing r: the red arrow shows the fluorescence enhancement due to increasing [ATP]; the green arrow shows the fluorescence quenching with increasing [GTP]. Lower panels: fluorescence intensity of **C** as a function of ATP and GTP concentrations and its fitting according to a modified Stern-Volmer equation (eq. 1).

Table S9. Fluorescence quantum yields of compound **C** in buffer at pH 7 alone and in the presence of increasing concentrations of ATP (left) or GTP (right) as a function of r (r = [**C**]/[ATP] or [GTP]).

r = [C]/[ATP]	ϕ_F
--	0.0065
0.19901	0.0066
0.09975	0.00662
0.05012	0.00662
0.02531	0.00656
0.0129	0.0066
0.00813	0.00662
0.00546	0.00673
0.0038	0.00685
0.0027	0.00695
0.00215	0.00707
0.00174	0.00724
0.00132	0.0075
0.00112	0.00762

r = [C]/[GTP]	ϕ_F
--	0.0065
0.24373	0.00648
0.12217	0.00641
0.06139	0.00633
0.031	0.0063
0.0158	0.00623
0.00996	0.00612
0.00669	0.00602
0.00466	0.00592
0.00331	0.00579
0.00263	0.00565
0.00213	0.00549
0.00182	0.00538
0.00162	0.0053
0.00137	0.00526

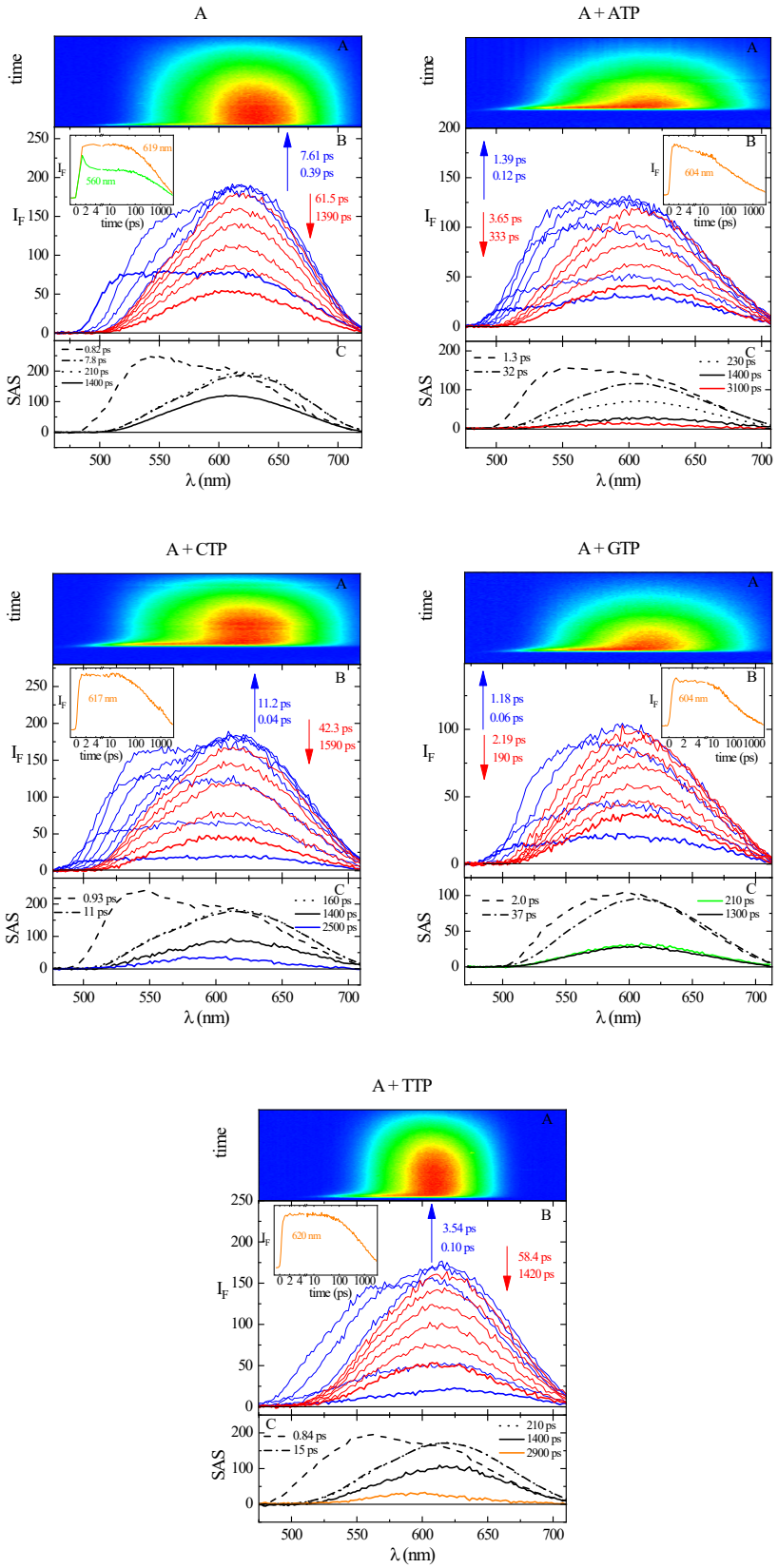

Figure S13. Femtosecond fluorescence up conversion measurements for compound **A** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

Table S10. Results of Target Analysis of the femtosecond fluorescence up conversion data for compound **A** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm.

Compound	Nucleotide	τ_{FUC} (ps)	λ_F^{max}(nm)
A	-	0.82	547, 611[sp]
		7.8	621
		210	621
		1400	611
	ATP	1.3	555, 605[sp]
		32	607
		230	610
		1400	607
		3100	600
	CTP	0.93	545, 600[sp]
		11	615
		160	615
		1400	607
		2500	602
	GTP	2.0	598
		37	608
		210	608
		1300	606
	TTP	0.84	562, 602[sp]
		15	620
		210	620
		1400	613
		2900	600

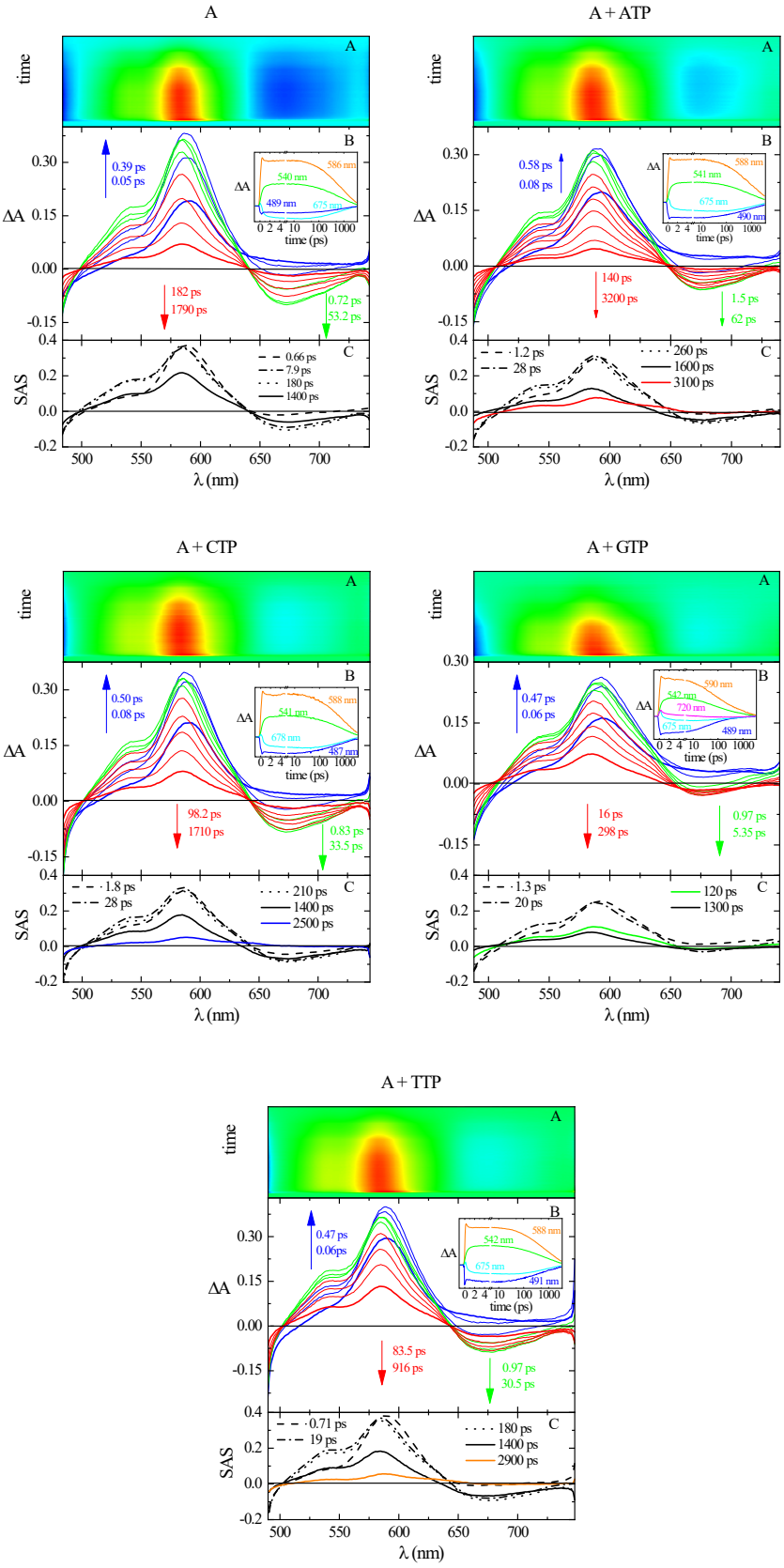

Figure S14. Femtosecond transient absorption measurements for compound **A** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

Table S11. Results of Target Analysis of the femtosecond fluorescence up conversion and transient absorption data for compound **A** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm and relative assignments.

Compound	Nucleotide	τ_{FUC} (ps)	τ_{TA} (ps)	Assignment
A	-	0.82	0.66	Solvation/$S_{1,LE}$
		7.8	7.9	Vibrational Cooling
		210	180	Structural Relaxation
		1400	1400	$S_{1,ICT}$
	ATP	1.3	1.2	Solvation/$S_{1,LE}$
		32	28	Vibrational Cooling
		230	260	Structural Relaxation
		1400	1600	$S_{1,ICT}$
		3100	3100	S_1 complex
	CTP	0.93	1.8	Solvation/$S_{1,LE}$
		11	28	Vibrational Cooling
		160	210	Structural Relaxation
		1400	1400	$S_{1,ICT}$
		2500	2500	S_1 complex
	GTP	2.0	1.3	Solvation/$S_{1,LE}$
		37	20	Vibrational Cooling
		210	120	S_1 complex
		1300	1300	$S_{1,ICT}$
	TTP	0.84	0.71	Solvation/$S_{1,LE}$
		15	19	Vibrational Cooling
		210	280	Structural Relaxation
		1400	1400	$S_{1,ICT}$
		2900	2900	S_1 complex

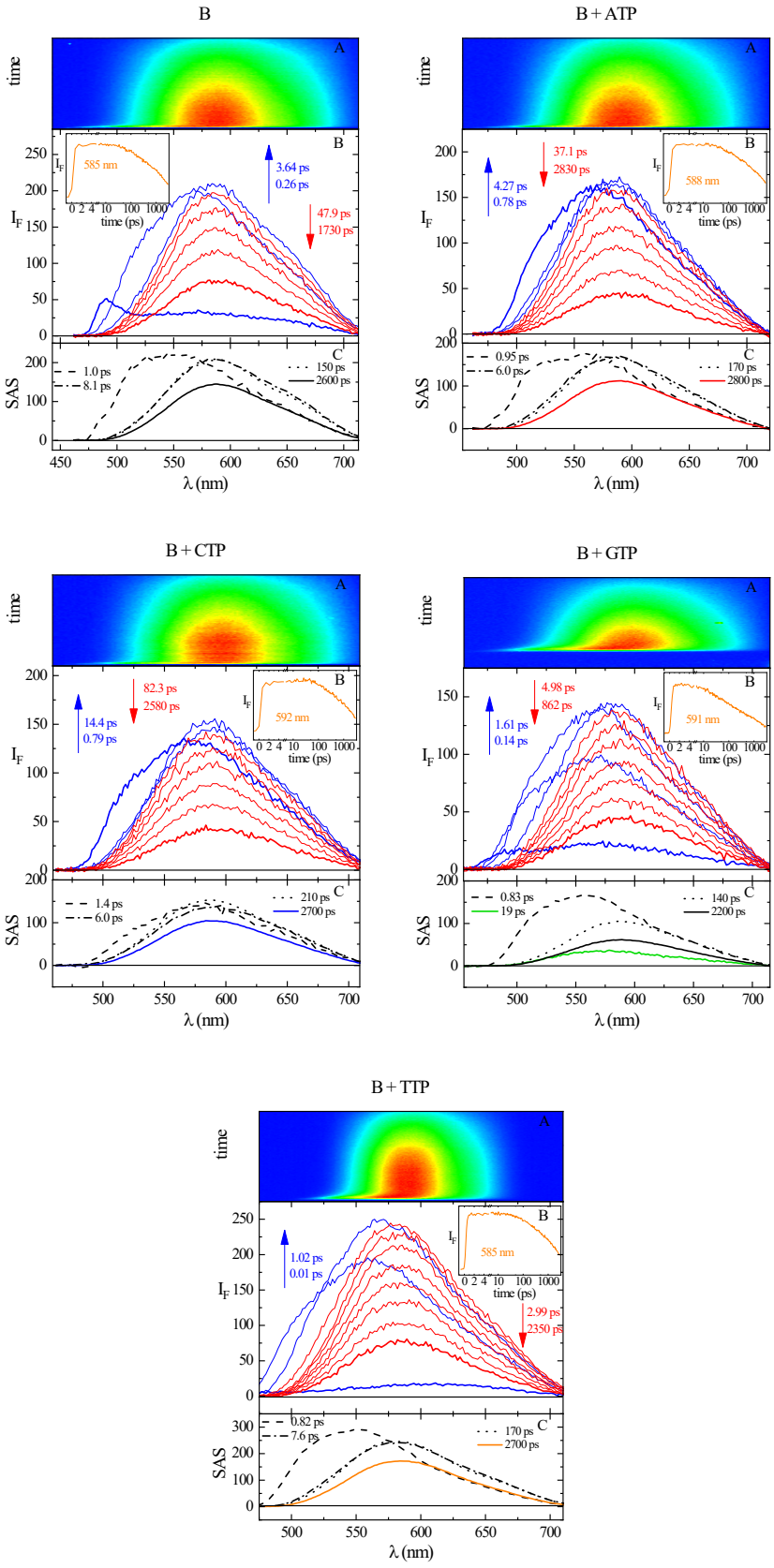

Figure S15. Femtosecond fluorescence up conversion measurements for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

Table S12. Results of Target Analysis of the femtosecond fluorescence up conversion data for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm.

Compound	Nucleotide	τ_{FUC} (ps)	λ_F^{max} (nm)
B	-	1.0	545
		8.1	587, 632^{sp}
		150	587, 643^{sp}
		2600	589
	ATP	0.95	555
		6.0	586
		170	586, 646^{sp}
		2800	591
	CTP	1.4	584
		6.0	591
		210	587, 636^{sp}
		2700	591
	GTP	0.83	557
		19	587
		140	587
		2200	591
	TTP	0.82	547
		7.6	582
		170	582, 643^{sp}
		2700	587

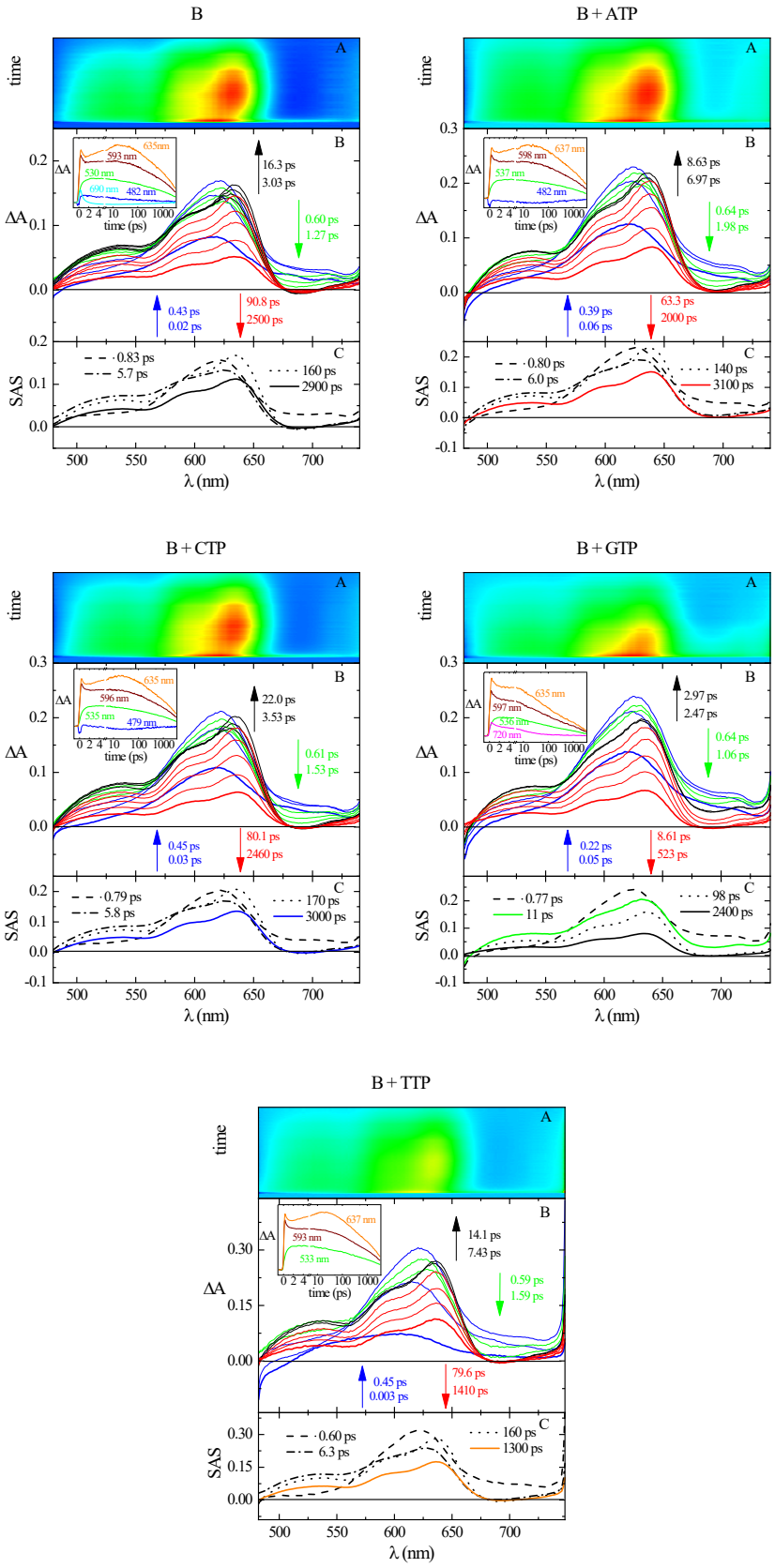

Figure S16. Femtosecond transient absorption measurements for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

Table S13. Results of Target Analysis of the femtosecond fluorescence up conversion and transient absorption data for compound **B** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm and relative assignments.

Compound	Nucleotide	τ_{FUC} (ps)	τ_{TA} (ps)	Assignment
B	-	1.0	0.83	Solvation/$S_{1,LE}$
		8.1	5.7	Vibrational Cooling
		150	160	Structural Relaxation
		2600	2900	$S_{1,ICT}$
	ATP	0.95	0.80	Solvation/$S_{1,LE}$
		6.0	6.0	Vibrational Cooling
		170	140	Structural Relaxation
		2800	3100	$S_{1,ICT}$/complex
	CTP	1.4	0.79	Solvation/$S_{1,LE}$
		6.0	5.8	Vibrational Cooling
		210	170	Structural Relaxation
		2700	3000	$S_{1,ICT}$/complex
	GTP	0.83	0.77	Solvation/$S_{1,LE}$
		19	11	S_1 complex
		140	98	Structural Relaxation
		2200	2400	$S_{1,ICT}$
	TTP	0.82	0.60	Solvation/$S_{1,LE}$
		7.6	6.3	Vibrational Cooling
		170	160	Structural Relaxation
		2700	3000	$S_{1,ICT}$/complex

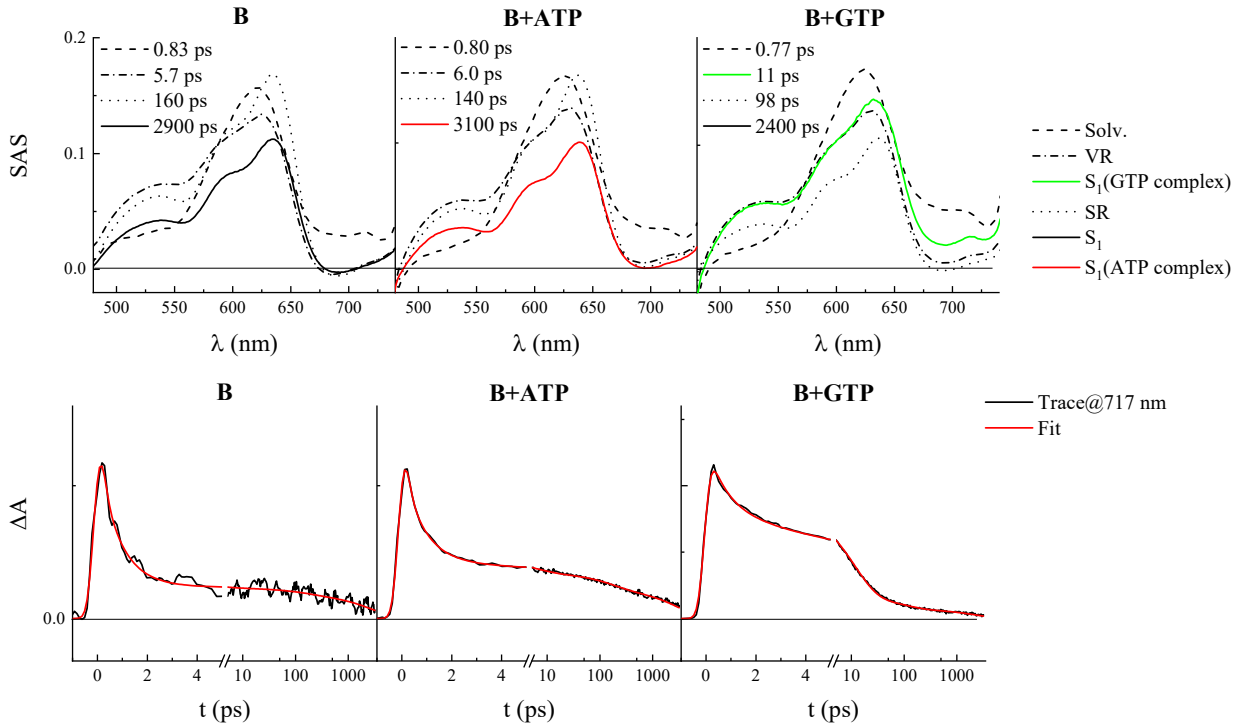

Figure S17. Species Associated Spectra (SAS) obtained by Target Analysis of the femtosecond transient absorption data (upper graphs) and associated kinetics recorded at 717 nm (lower graphs) for compound **B** in buffer at pH 7 alone (left), and in the presence of ca. 5 mM ATP (central) or GTP (right).

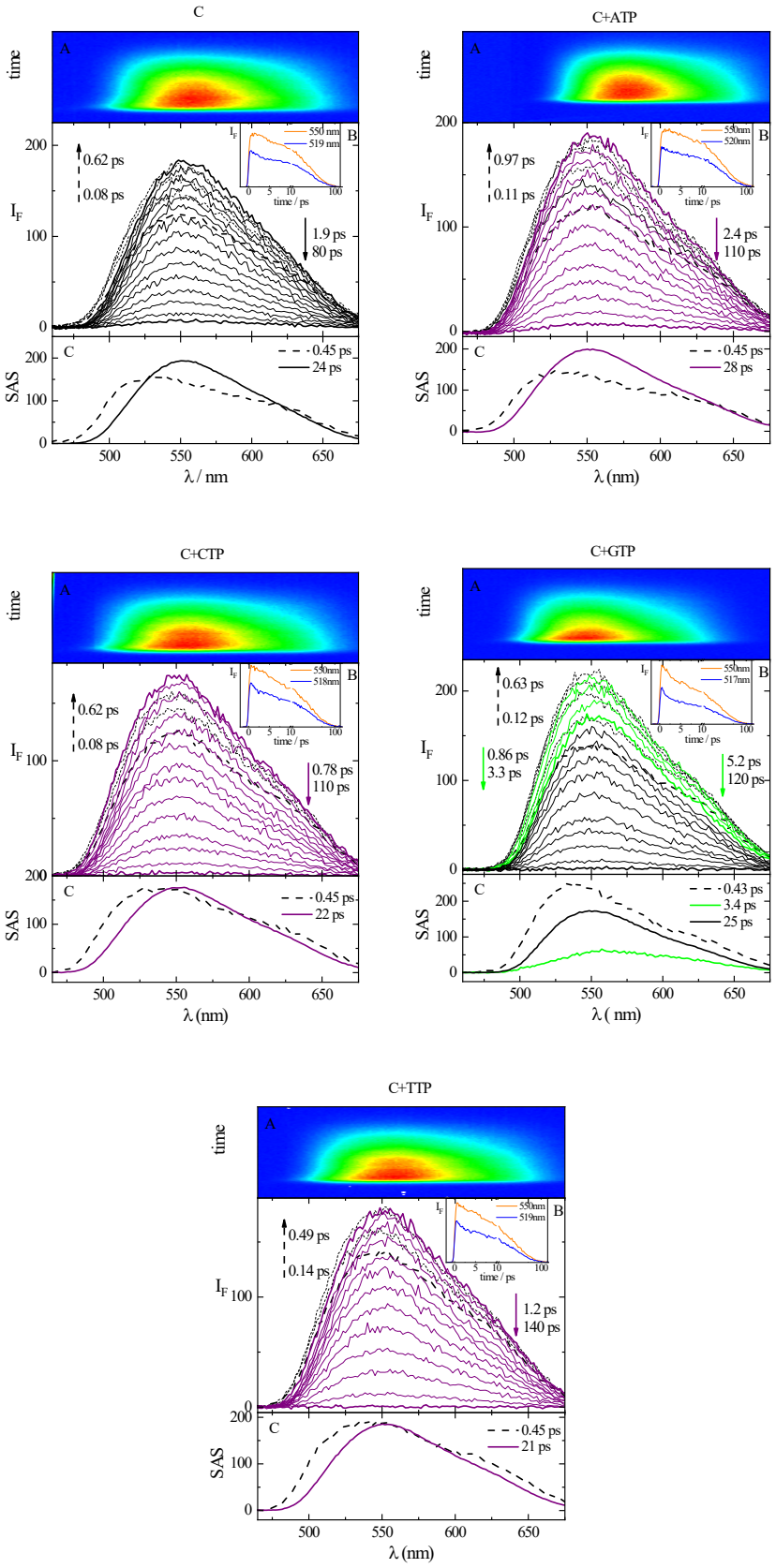

Figure S18. Femtosecond fluorescence up conversion measurements for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

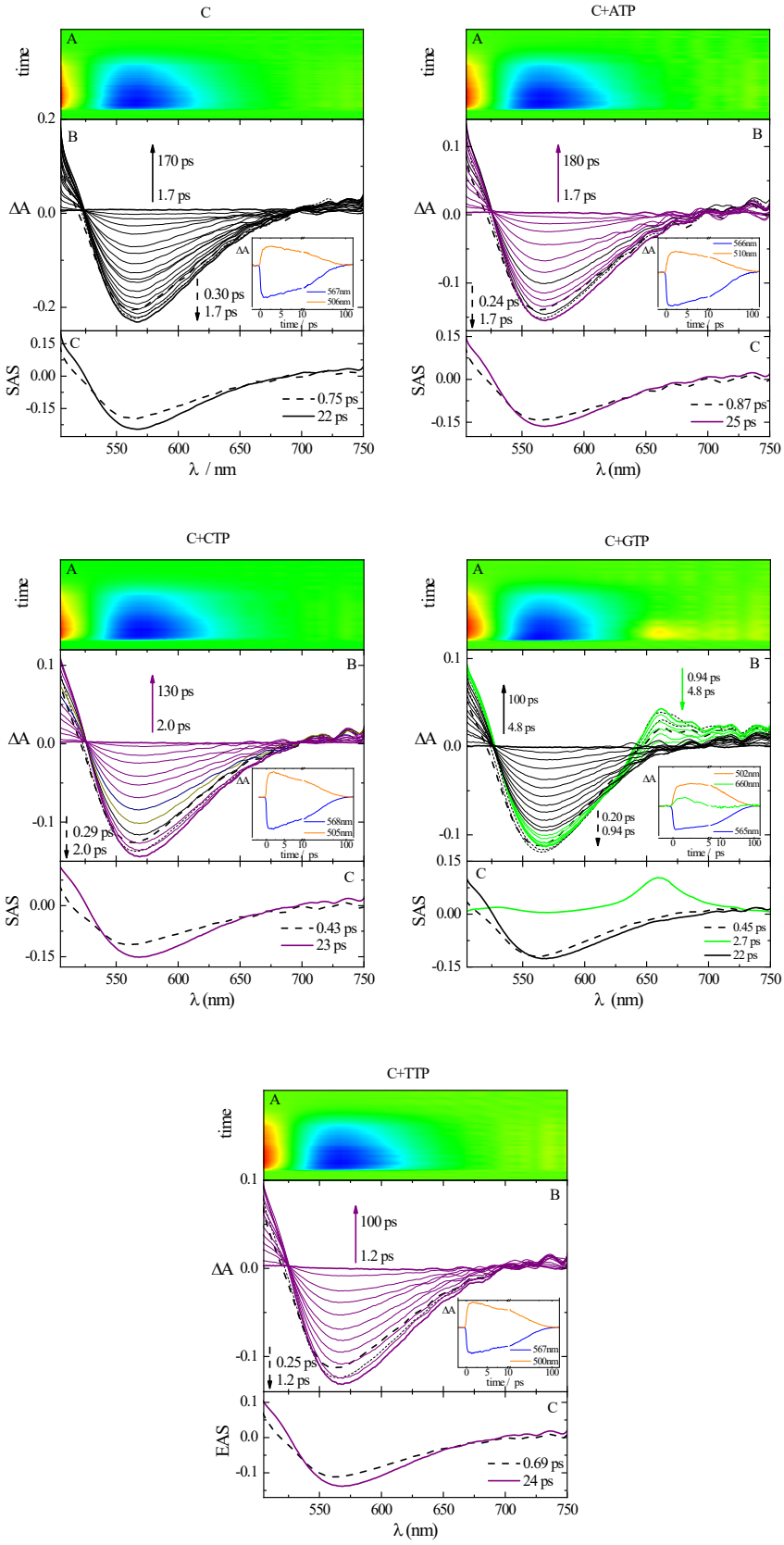

Figure S19. Femtosecond transient absorption measurements for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm. Panel A: experimental 3D matrix; Panel B: representative spectra at different delay times and representative kinetics (inset) at different wavelengths; Panel C: Species Associated Spectra (SAS) obtained by Target Analysis.

Table S14. Results of Target Analysis of the femtosecond fluorescence up conversion and transient absorption data for compound **C** in buffer at pH 7 alone and in the presence of nucleotides (ca. 5 mM) with λ_{pump} = 400 nm and relative assignments.

Compound	Nucleotide	τ_{FUC} (ps)	τ_{TA} (ps)	Assignment
C	-	0.45	0.75	Solvation
		24	22	S1
	ATP	0.45	0.86	Solvation
		28	25	S1 free/complex
	CTP	0.45	0.43	Solvation
		22	23	S1 free/complex
	GTP	0.43	0.45	Solvation
		3.4	2.7	S1 complex
		25	22	S1 free
	TTP	0.45	0.69	Solvation
		21	24	S1 free/complex

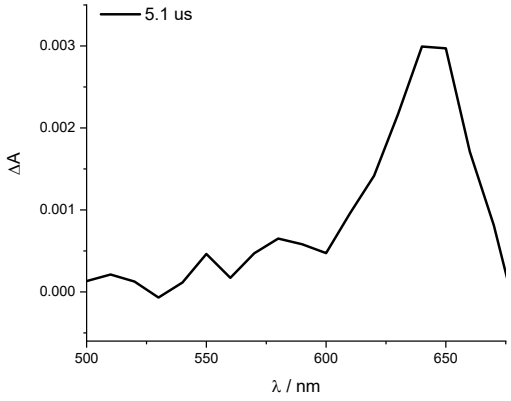

Figure S20. Nanosecond transient absorption spectrum for compound **C** (5×10^{-5} M) in acetonitrile in the presence of N,N-diethylaniline (DEA, 0.1 M) obtained by laser flash photolysis with λ_{pump} = 355 nm. No signal was detected in the control experiment with the same concentration of just compound **C** in acetonitrile.

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