Supporting Information for

Tailoring Fluorescent Strigolactones for *in vivo* Investigations: a computational and experimental study

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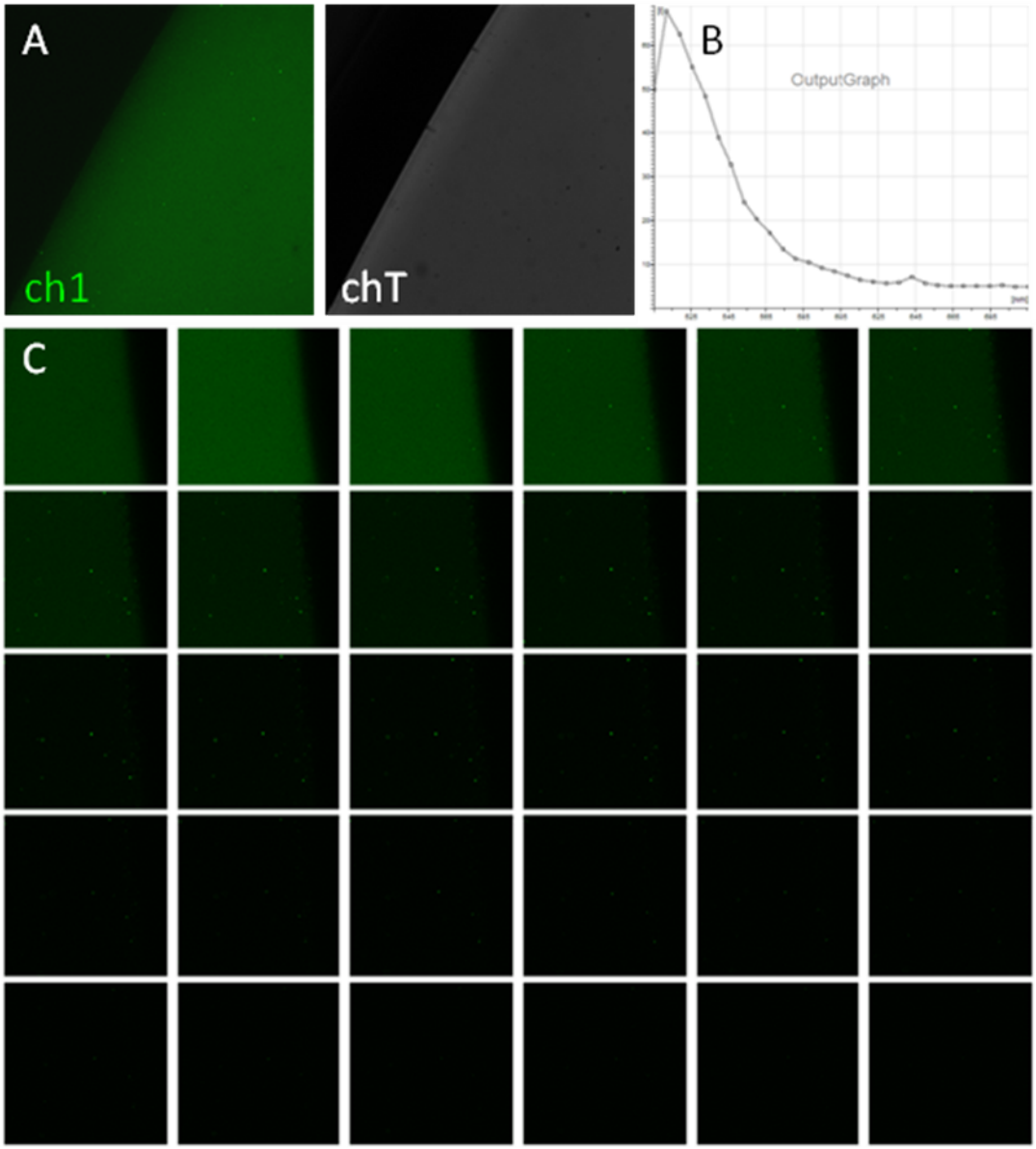
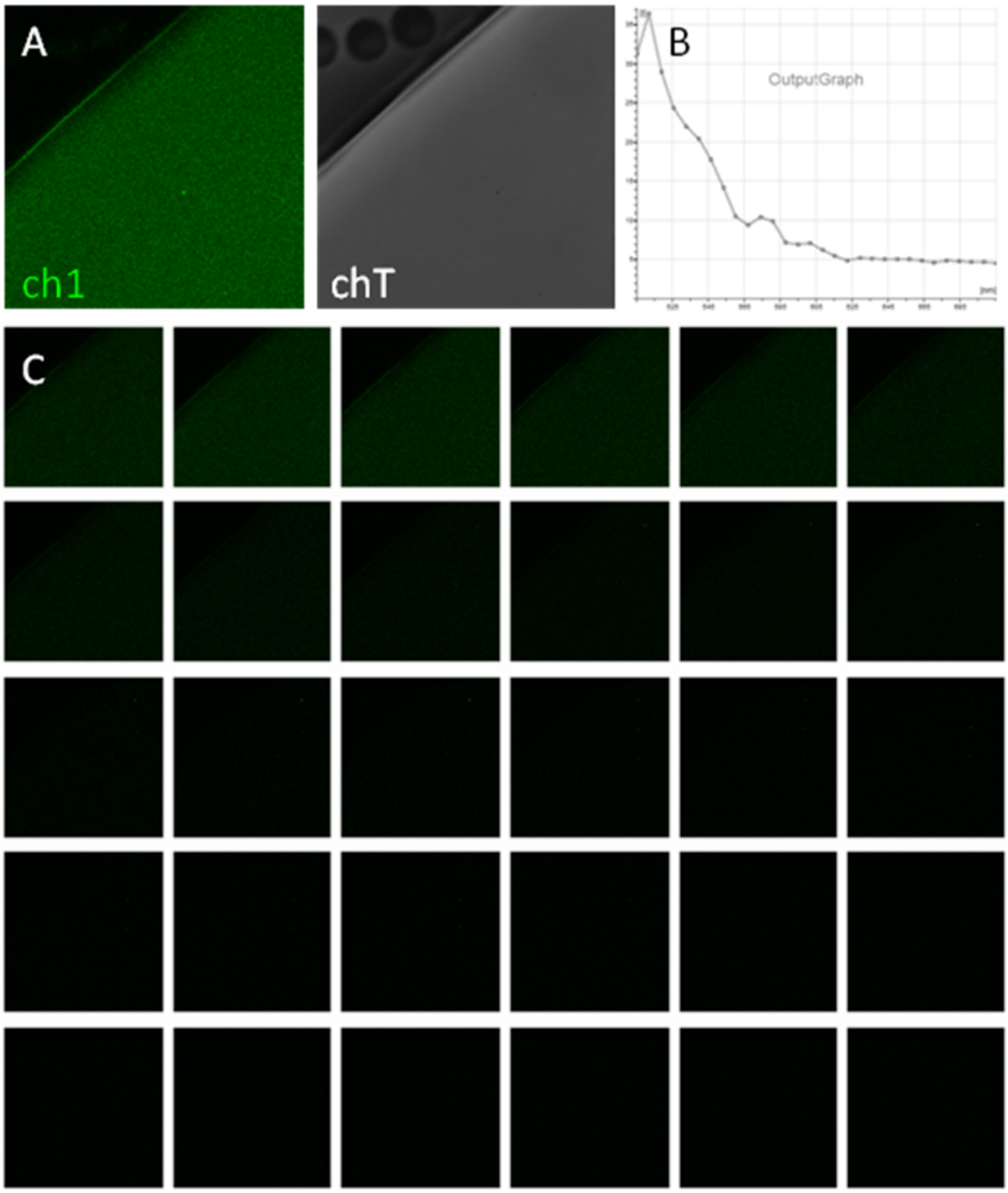
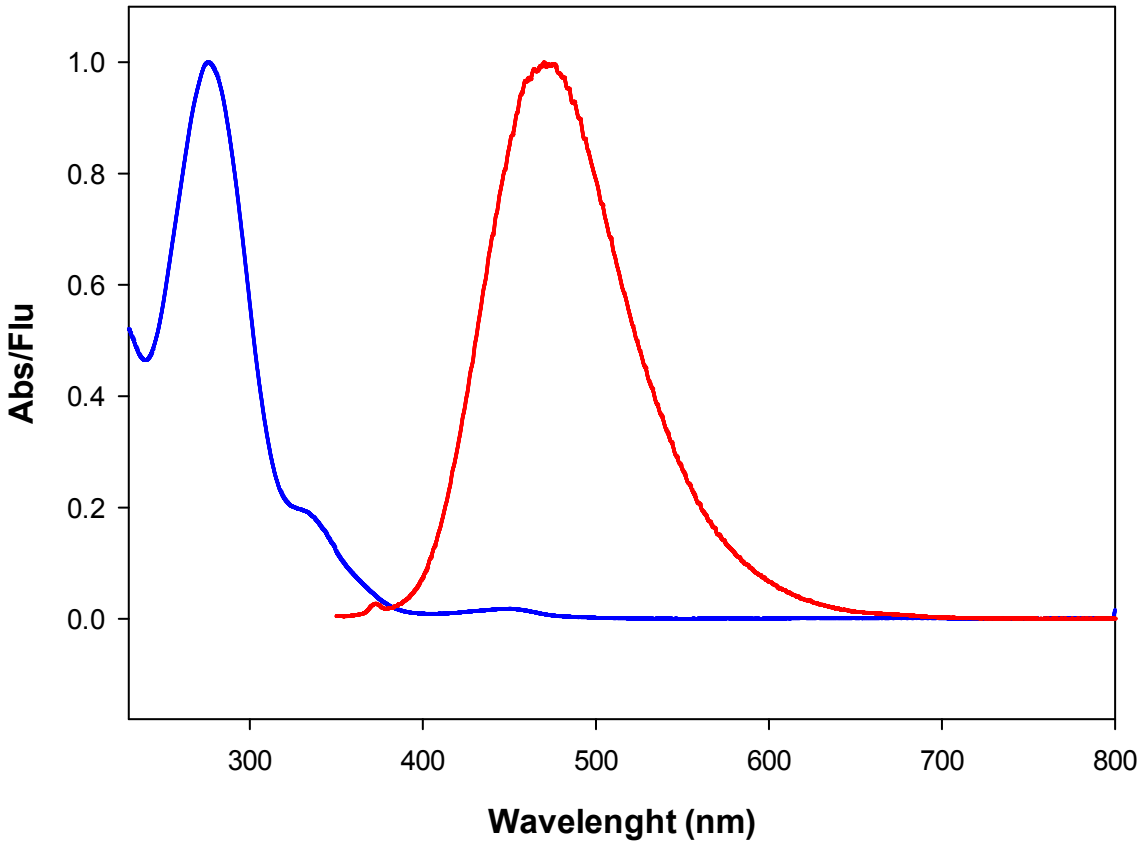


A. Fluorescence (left) and transmitted light (right) confocal images from a drop of HR 10^{-4} M solution in water. **B**. Fluorescence emission spectrum obtained from Lambda scan in C. **C**. Lambda scan of HR fluorescence in the same solution. Each image shows the fluorescence emission recorded between 505 nm and 705 nm with a 10 nm emission window and step size = 6.66 nm. Maximum emission was recorded at 515-525 nm. The fluorochrome was excited at 476 nm (Ar/Kr laser).

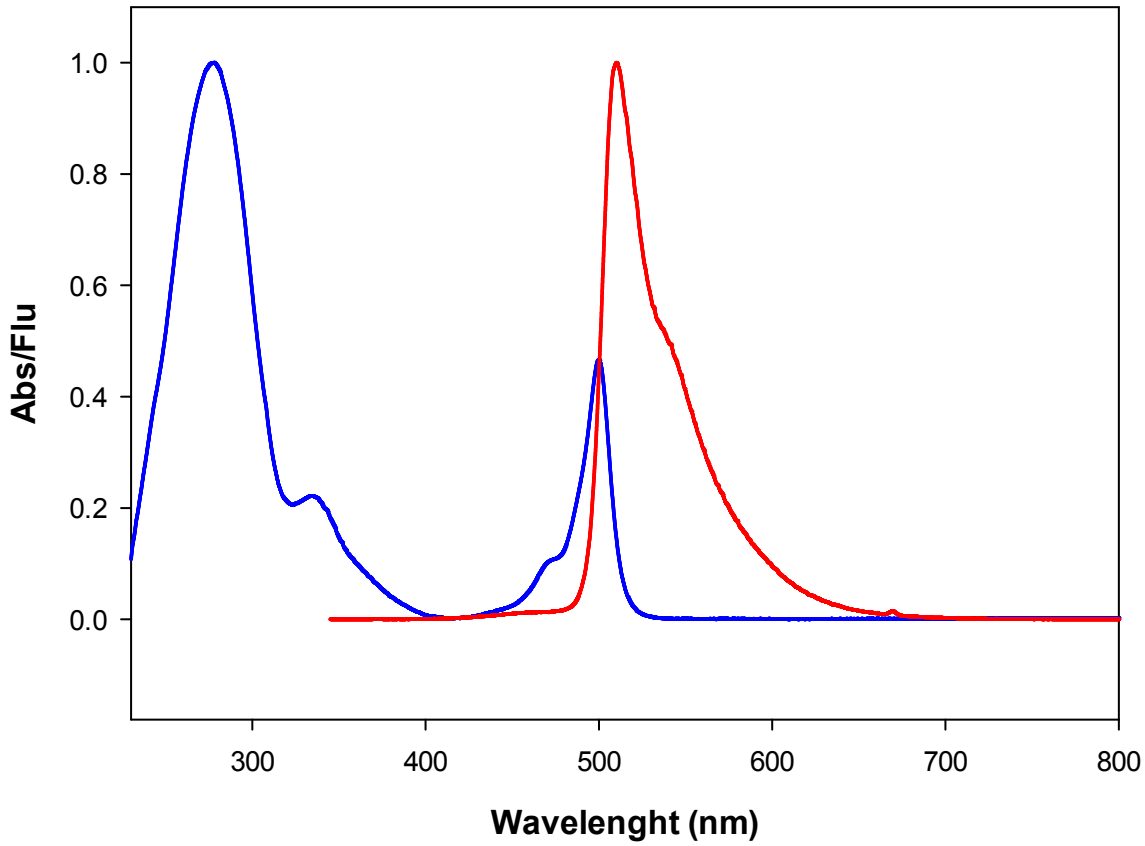


A. Fluorescence (left) and transmitted light (right) confocal images from a drop of EG 10^{-4} M solution in water. **B**. Fluorescence emission spectrum obtained from Lambda scan in C. **C**. Lambda scan of EG fluorescence in the same solution. Each image shows the fluorescence emission recorded between 505 nm and 705 nm with a 10 nm emission window and step size = 6.66 nm. Maximum emission was recorded at 515 nm. The fluorochrome was excited at 476 nm (Ar/Kr laser).

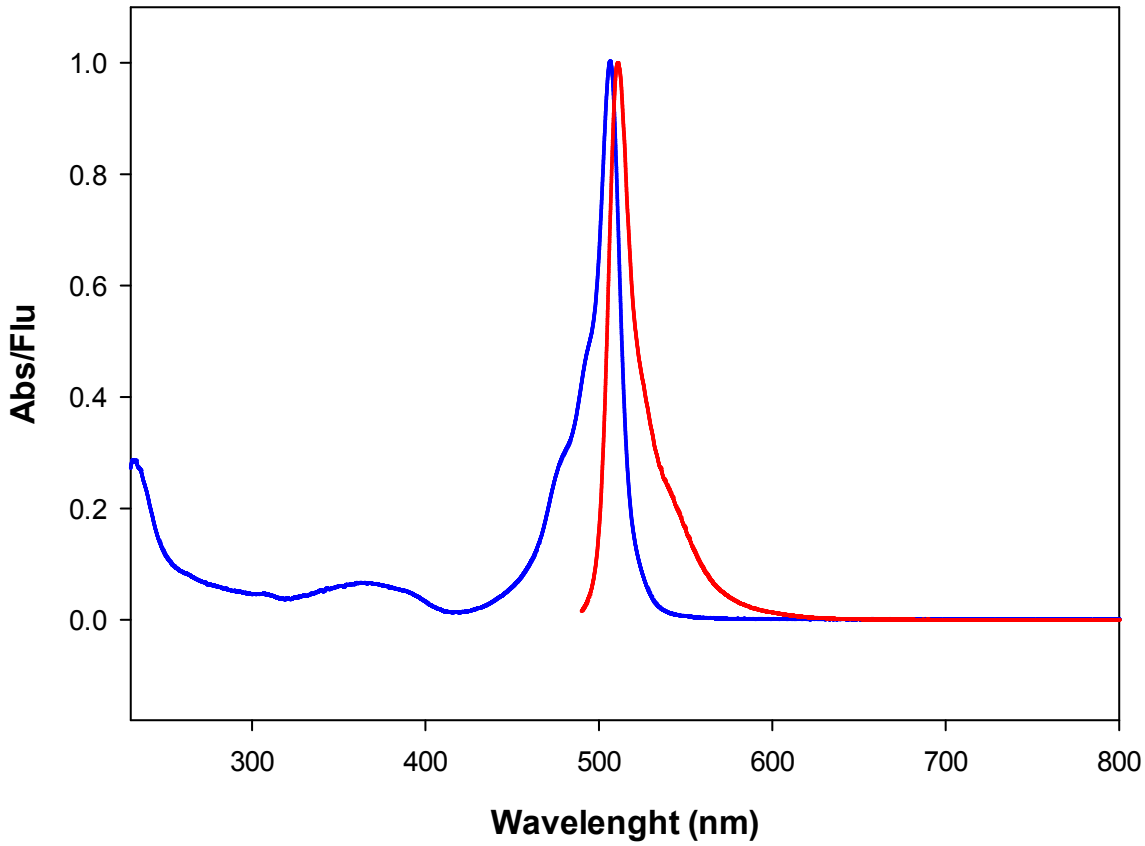
Normalized absorption (blue line) and emission (red line) spectra of **BL** (1×10^{-5} M) in DCM.

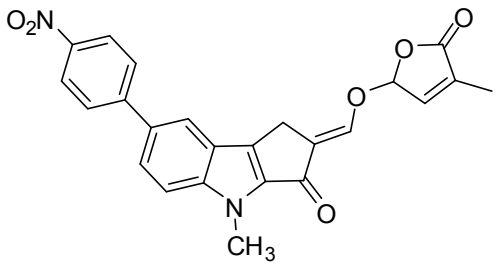


Normalized absorption (blue line) and emission (red line) spectra of **HR** (5×10^{-6} M) in DCM.

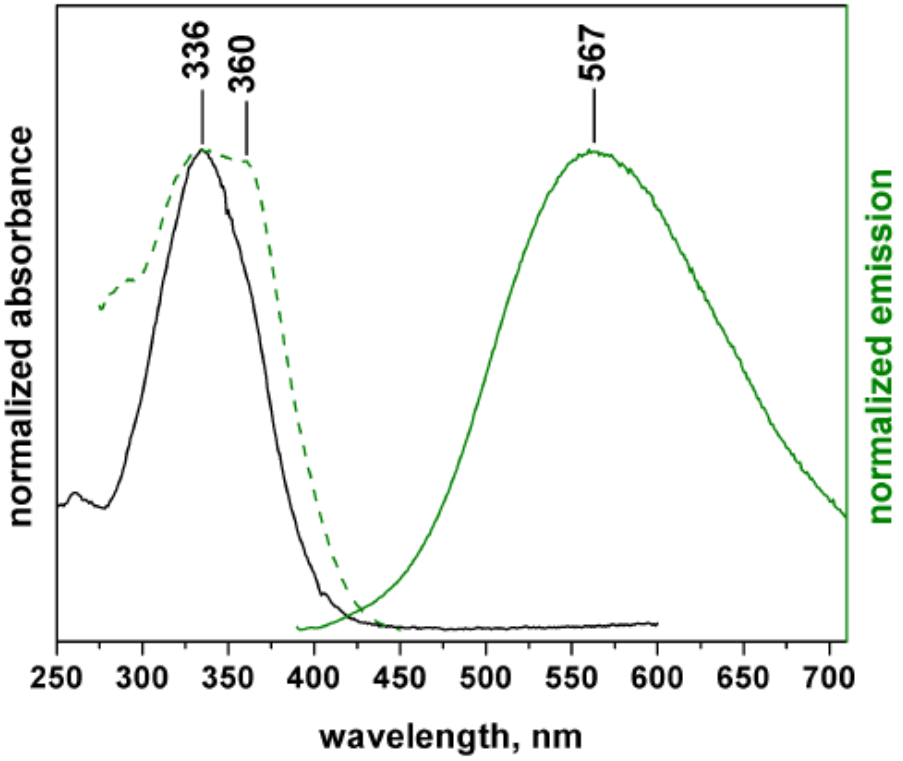


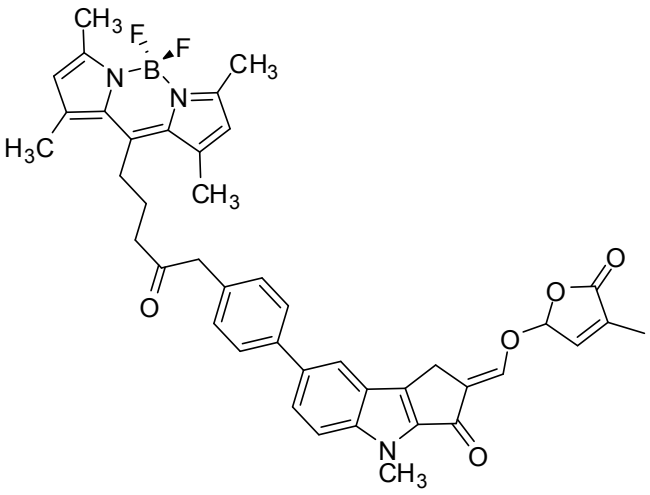
Normalized absorption (blue line) and emission (red line) spectra of **EG** (1×10^{-5} M) in DCM.



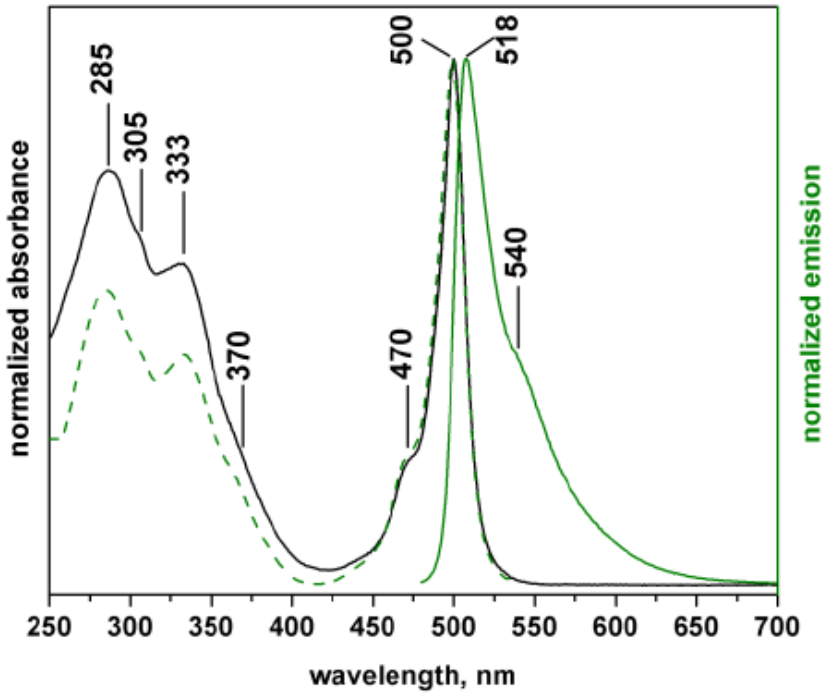

O2N
O
O
O
N
CH3
O

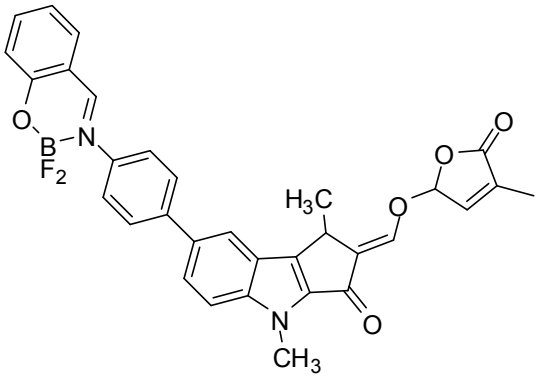
EGO9a


336
360
567
normalized absorbance
normalized emission
250
300
350
400
450
500
550
600
650
700
wavelength, nm

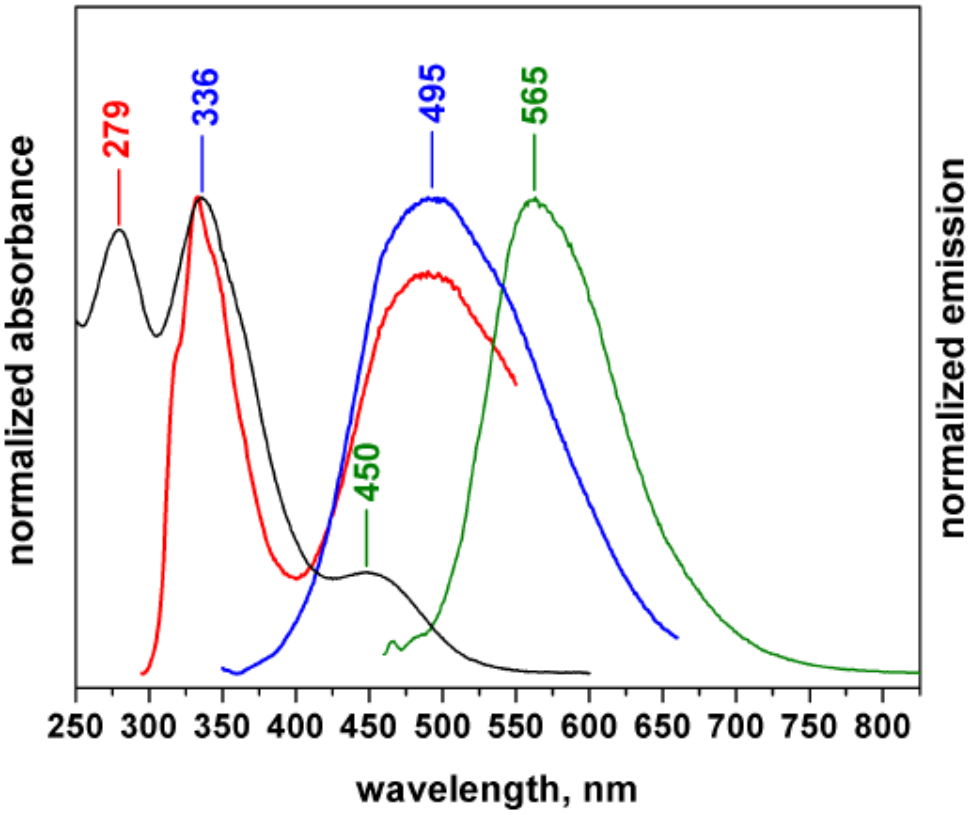

CH3
F
F
B
N
N
CH3
H3C
CH3
O
O
O
O
N
CH3

BODIPYEGO

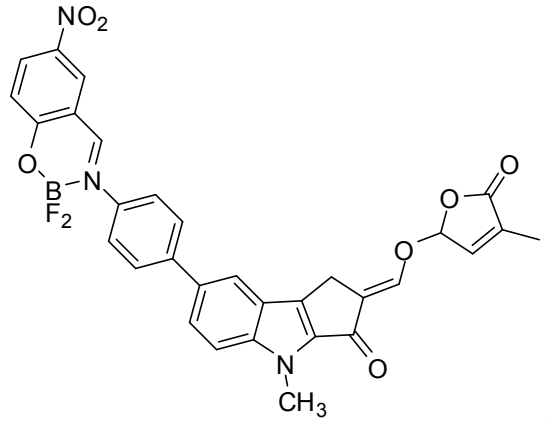

285
305
333
370
470
500
518
540
normalized absorbance
normalized emission
250
300
350
400
450
500
550
600
650
700
wavelength, nm



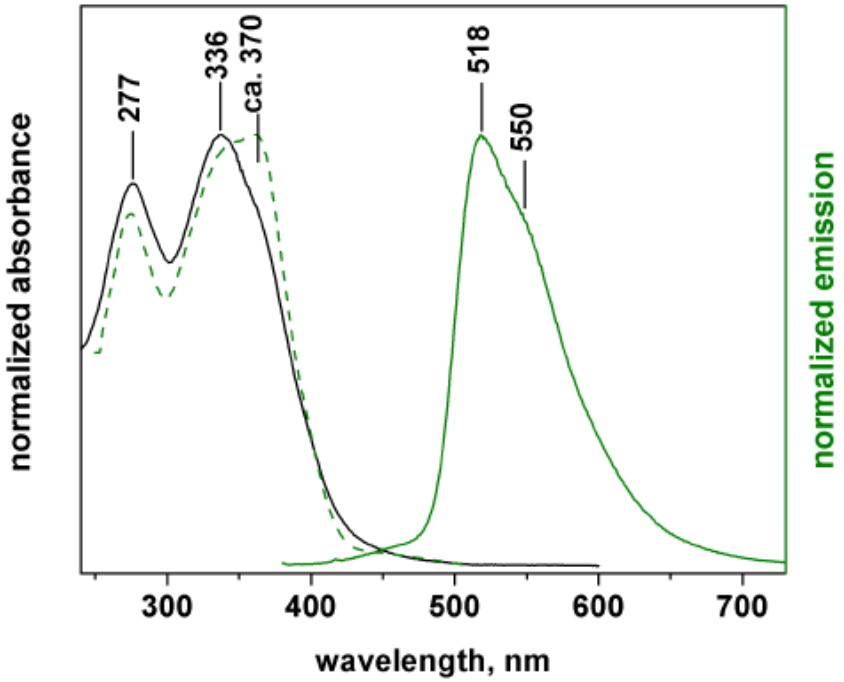
BorPhST



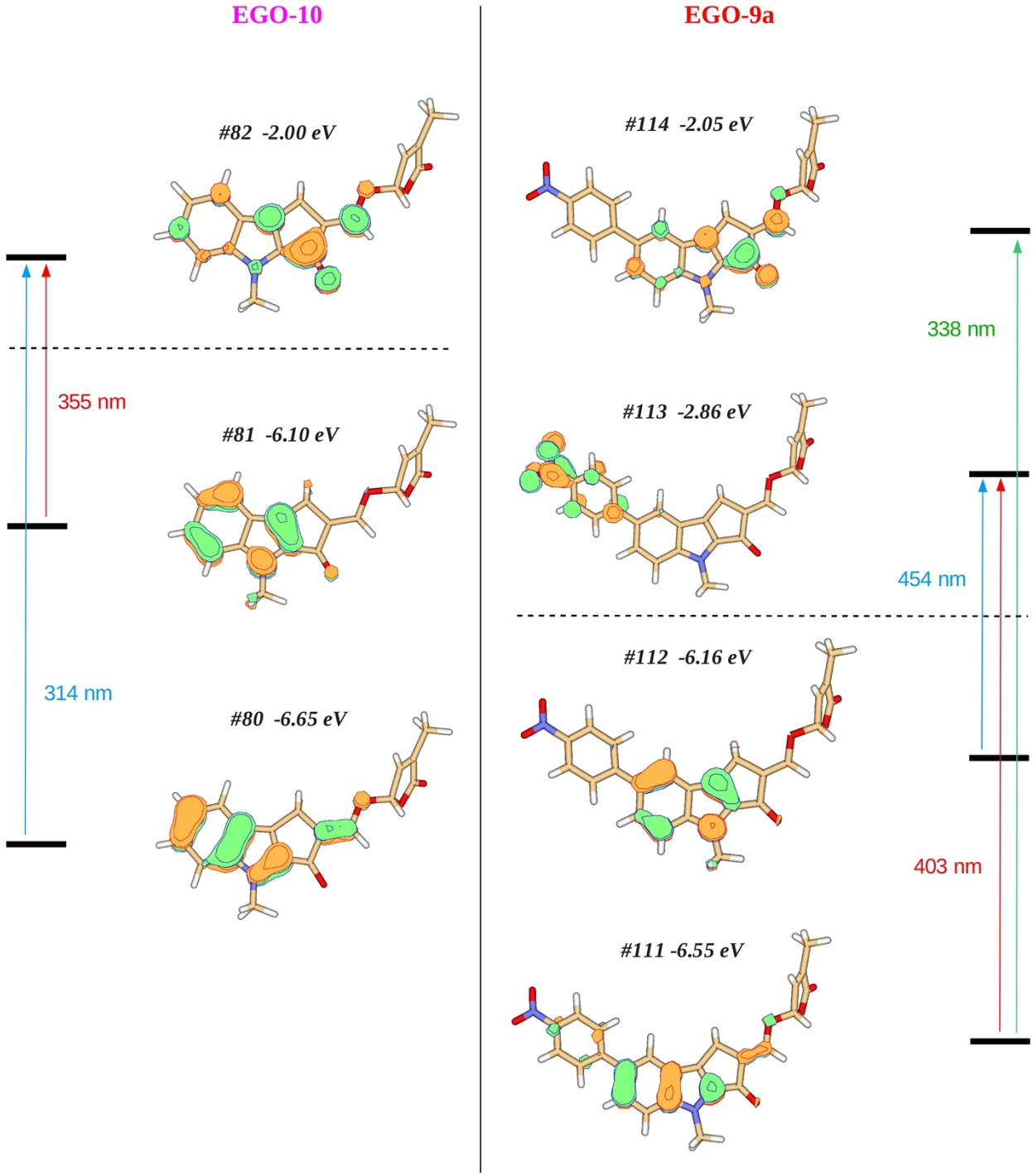
λ_{exc}(nm)	λ_{em}(nm)	τ_1^f (ns)	τ_2^f(ns)
297	495	3.26 (35%)	7.36 (65%)
455	565	0.48 (75%)	3.15 (35%)


NO2
O
B
F2
N
O
O
O
N
CH3
O

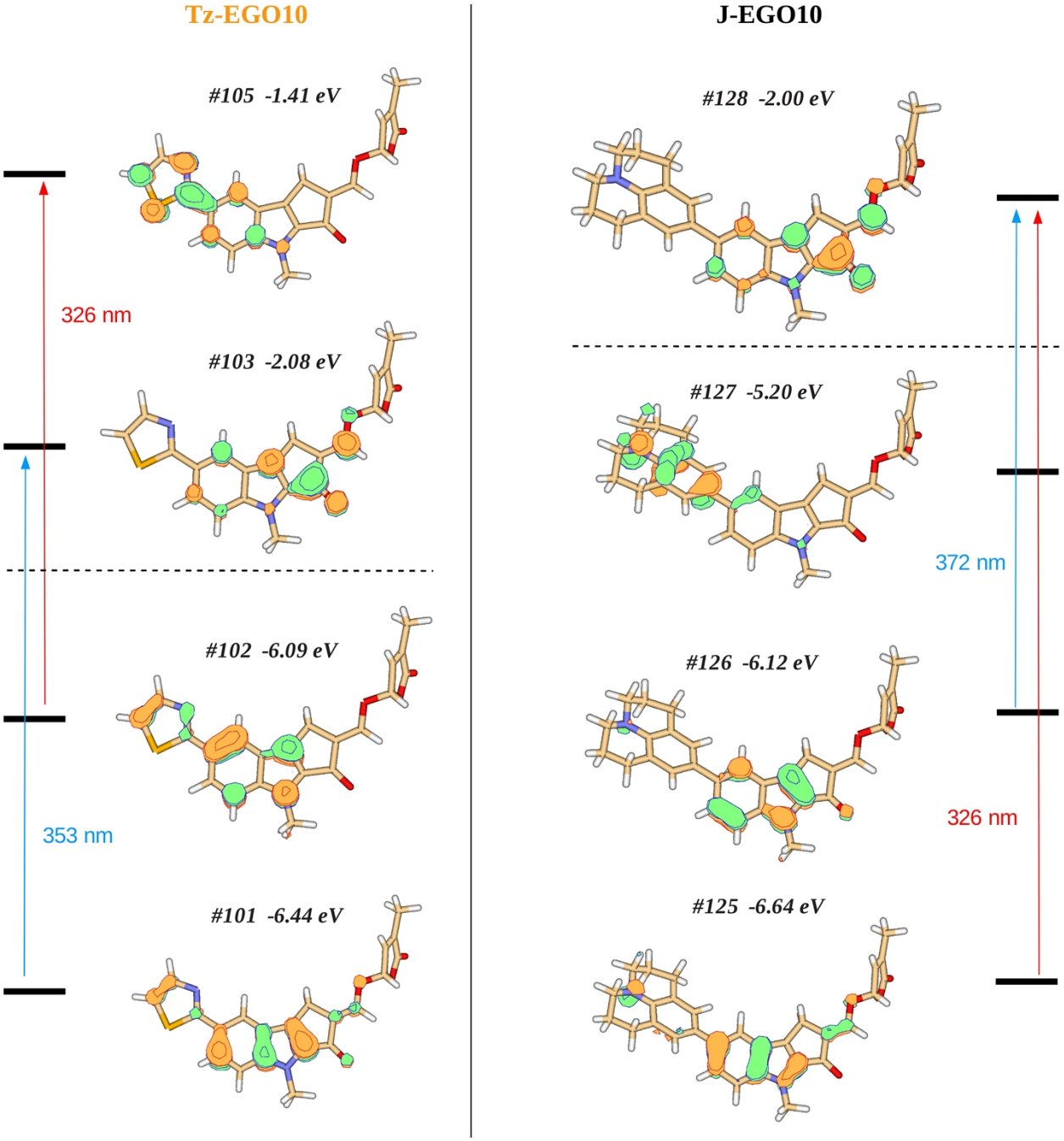
2a


277
336
ca. 370
518
550
normalized absorbance
normalized emission
300
400
500
600
700
wavelength, nm

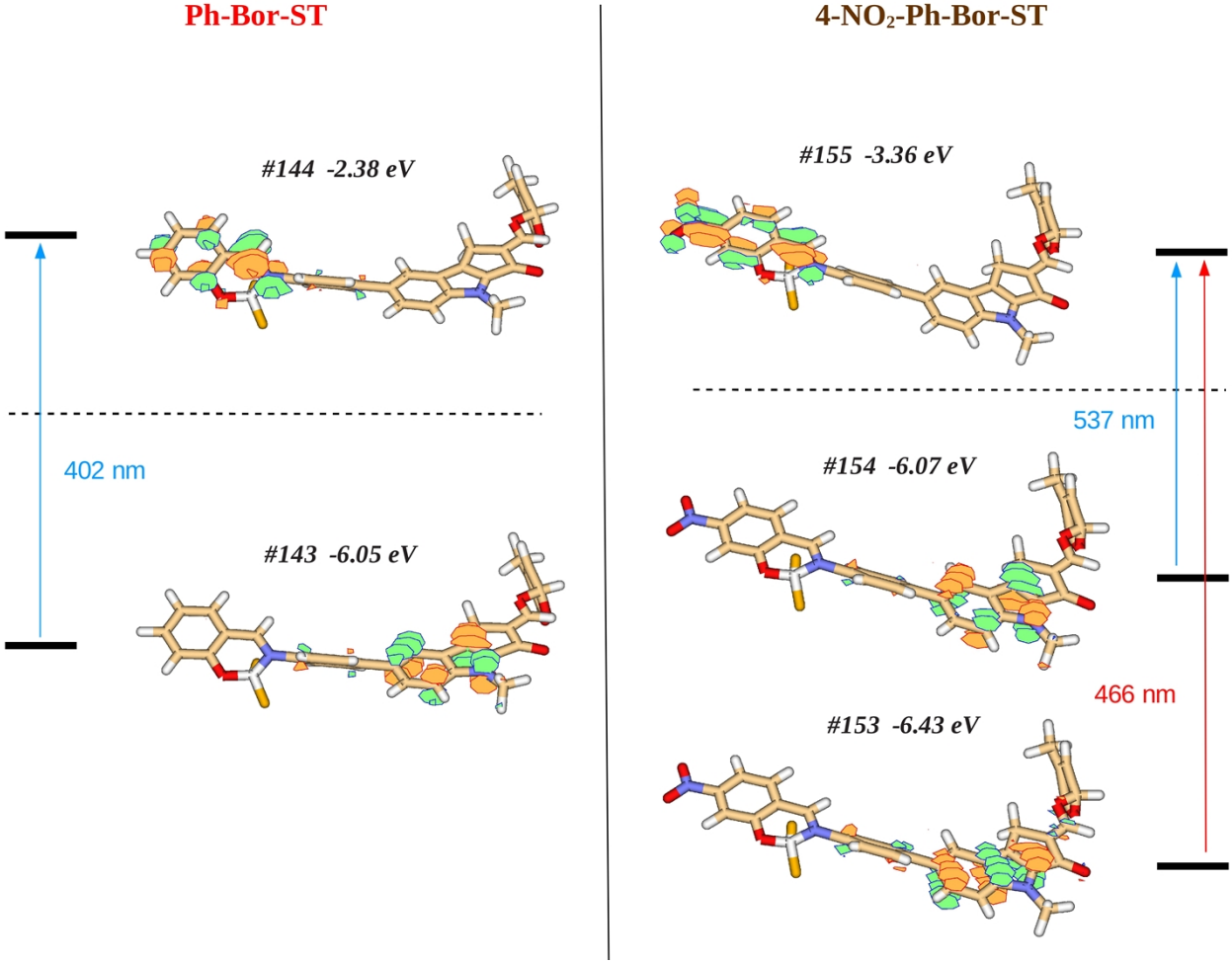
A-1. Molecular orbitals and electronic transitions in **EGO-10** and **EGO-9a**



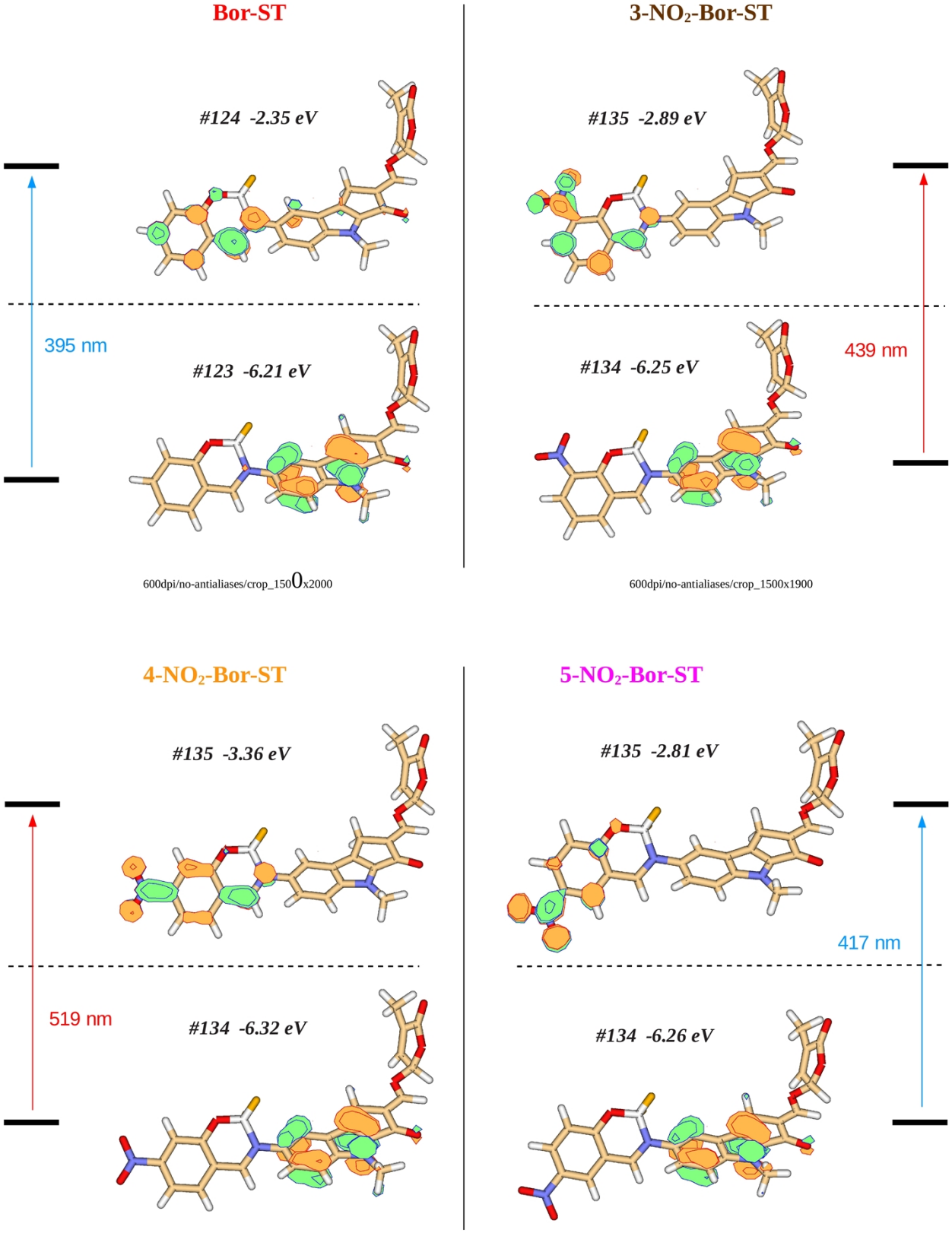
A-2. Molecular orbitals and electronic transitions in **Tz-EGO10** and **J-EGO10**



B-1. Molecular orbitals and electronic transitions in **Ph-Bor-ST** and **4-NO_2-Ph-Bor-ST**



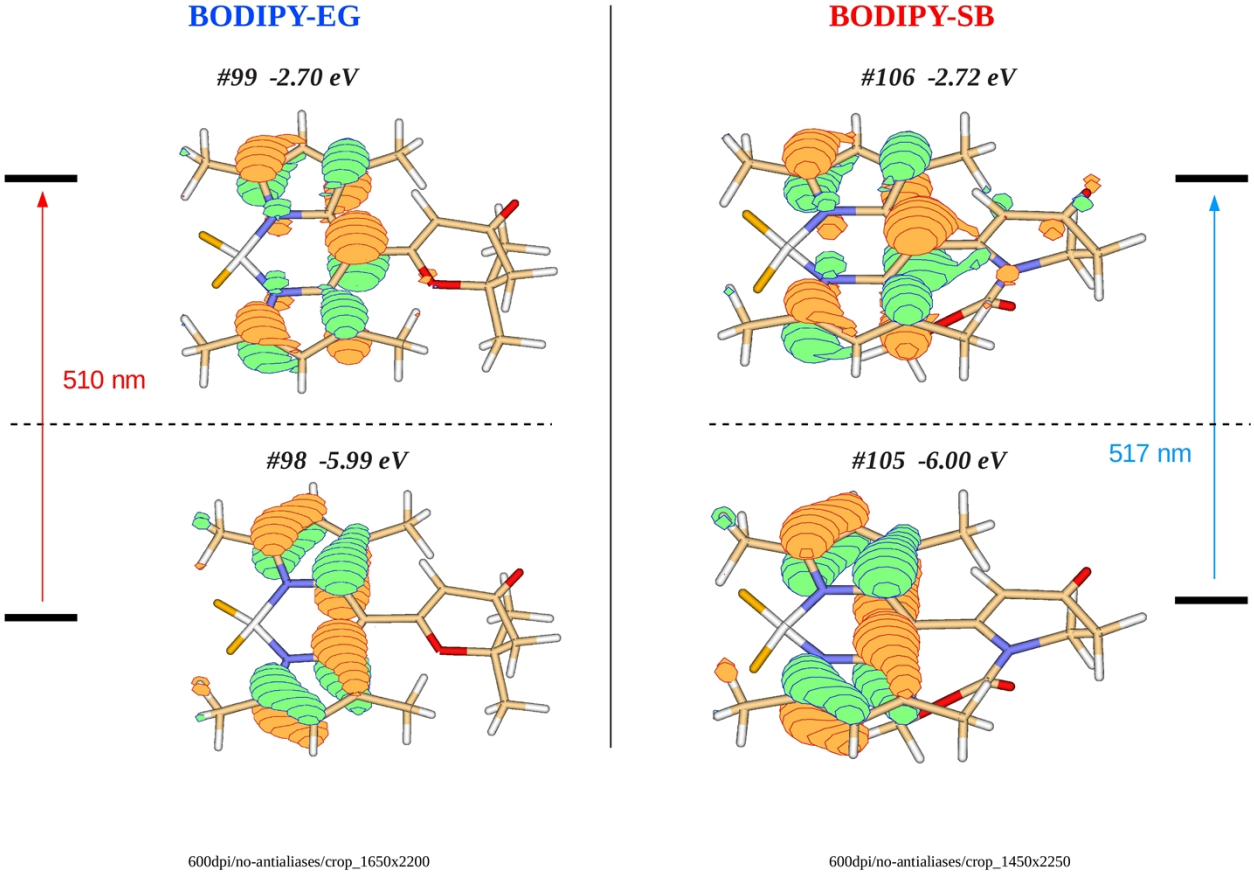
B-2. Molecular orbitals and electronic transitions in **Bor-ST**, **3-NO_2-Bor-ST**, **4-NO_2-Bor-ST**, and **5-NO_2-Bor-ST**

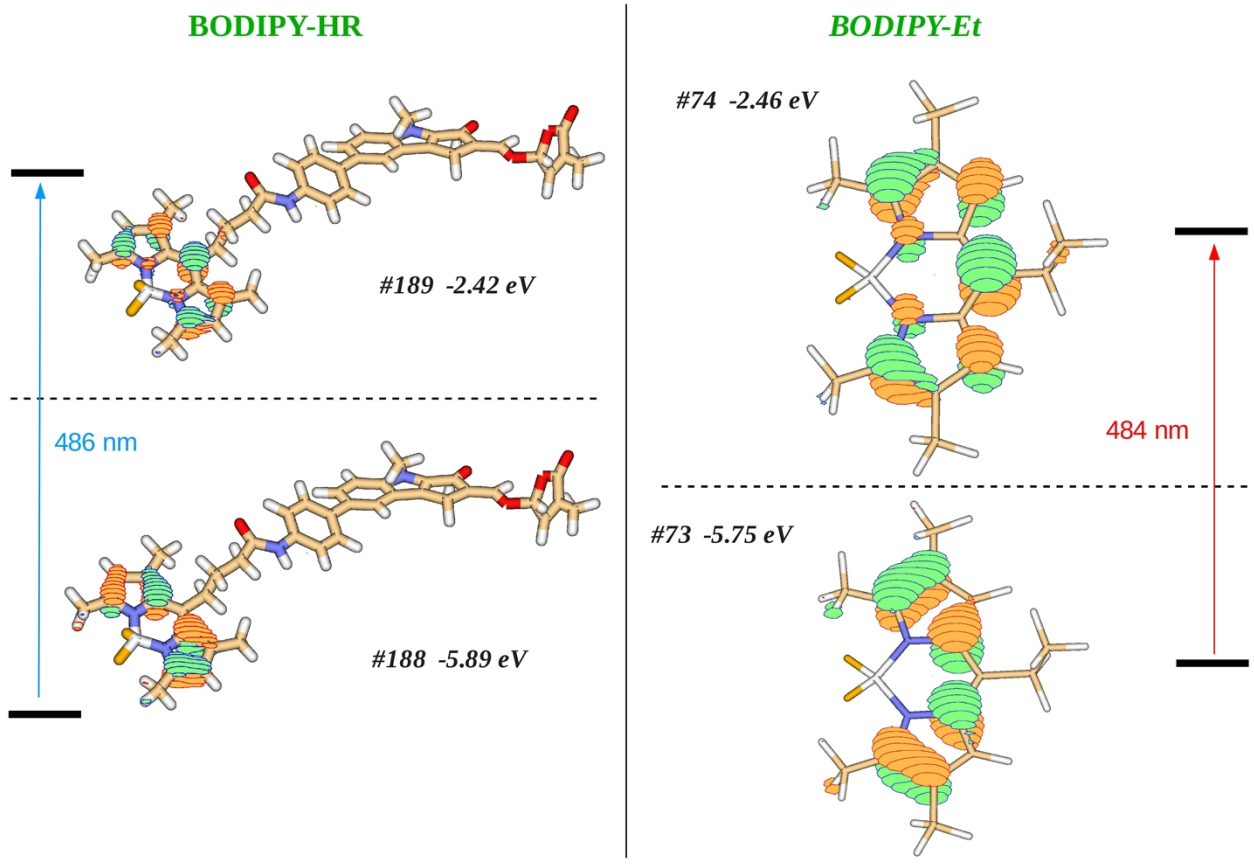


600dpi/no-antialiases/crop_1500x2000

600dpi/no-antialiases/crop_1500x1900

C-1. Molecular orbitals and electronic transitions in **BODIPY-EG**, **BODIPY-SB**, **BODIPY-HR**, and **BODIPY-Et**





T-1. Calculated vs. experimental electronic transitions for benchmark systems

All calculation with 6-31+G(d) basis set.

	exp.	CAM-B3LYP	PBE0	mPWPW91	M06-2X	M06-HF	M06
EGO-9c	320	313	334	343	304	284	350
in CH_2Cl_2	305	283	300	306	277	276	317
EurJOC.**2011**.3781		*-7*	*14*	*23*	*-17*	*-36*	*30*
		-22	*-5*	*1*	*-28*	*-29*	*12*
	3.87	3.96	**3.71**	3.61	4.09	4.37	3.54
	4.06	4.38	**4.13**	4.05	4.48	4.49	3.91
ε^2 =		**0.007**	**0.026**	**0.069**	**0.044**	**0.245**	**0.111**
ε^2 =		**0.098**	**0.005**	**0.000**	**0.172**	**0.184**	**0.024**
		0.053	**0.015**	**0.035**	**0.108**	**0.215**	**0.068**
BODIPY 6c	532	513	502	502	515	536	520
in ACN		*-19*	*-30*	*-30*	*-17*	*4*	*-12*
JOC.**2011**.*76*.8168	2.33	**2.42**	2.47	2.47	**2.41**	**2.32**	**2.39**
ε^2 =		**0.008**	**0.019**	**0.020**	**0.006**	**0.000**	**0.003**
BODIPY 4a	502	468	462	462	472	498	474
in CH_2Cl_2		***-34***	***-40***	***-40***	***-30***	***-4***	***-28***
EurJOC.**2011**.5460	2.47	2.65	2.69	2.69	2.63	**2.49**	***2.62***
ε^2 =		**0.032**	**0.047**	**0.047**	**0.025**	**0.000**	**0.021**
Boranil 5	372	333	374	373	334	291	378
in Toluene		*-39*	*2*	*1*	*-38*	*-81*	*6*
OrgLett.**2011**.*13*.3414	3.33	3.73	**3.31**	**3.32**	3.71	4.26	***3.28***
ε^2 =		**0.155**	**0.000**	**0.000**	**0.144**	**0.861**	**0.003**
Boranil 10	427	366	426	427	373	347	424
in Toluene		*-61*	*-1*	*0*	*-54*	*-80*	*-3*
OrgLett.**2011**.*13*.3414	2.90	3.39	**2.91**	**2.91**	3.32	3.57	**2.92**
ε^2 =		**0.236**	**0.000**	**0.000**	**0.176**	**0.447**	**0.000**
$\Sigma\ \varepsilon^2$ =		***0.536***	***0.097***	***0.136***	***0.567***	***1.738***	***0.163***
(($\Sigma\ \varepsilon^2$)/6)^{½}=		**0.30**	**0.13**	**0.15**	**0.31**	**0.54**	**0.16**
Boranil & EGO ONLY =		**0.35**	**0.09**	**0.13**	**0.37**	**0.66**	**0.19**
Boranil & BODIPY ONLY =		**0.33**	**0.13**	**0.13**	**0.30**	**0.57**	**0.08**

Conclusion:
For **Boranyl** use **PBE0** or **M06**
For **EGO** use **PBE0**
For **BODIPY** use **M06**