
Supporting Information

**β -Diketone derivatives: influence of the chelating
group on the photophysical and
mechanofluorochromic properties**

Marine Louis,^[a] Régis Guillot,^[b] Rémi Métivier*^[a] and Clémence Allain*^[a]

[a] PPSM, ENS Cachan, CNRS, Université Paris-Saclay, 94235 Cachan (France)

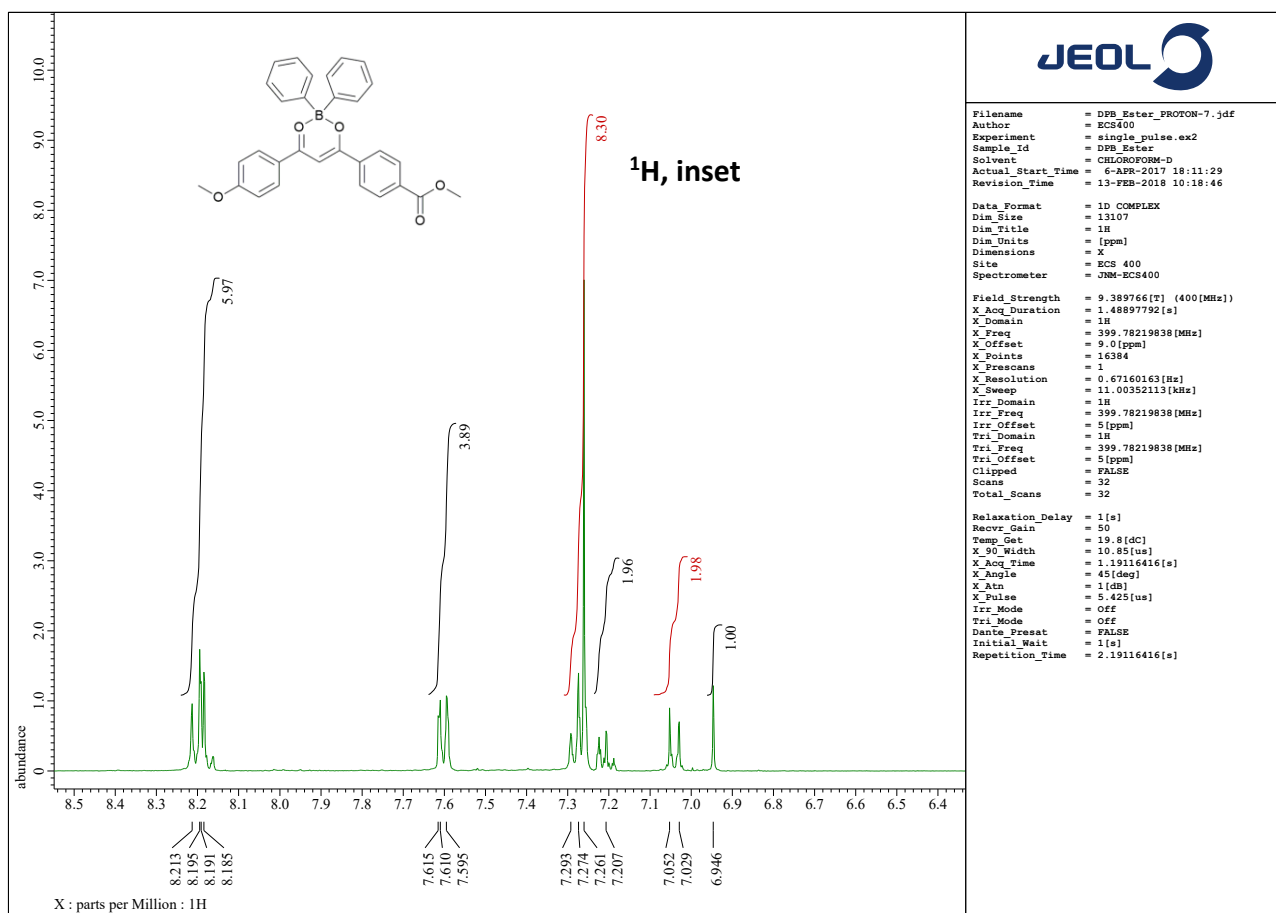
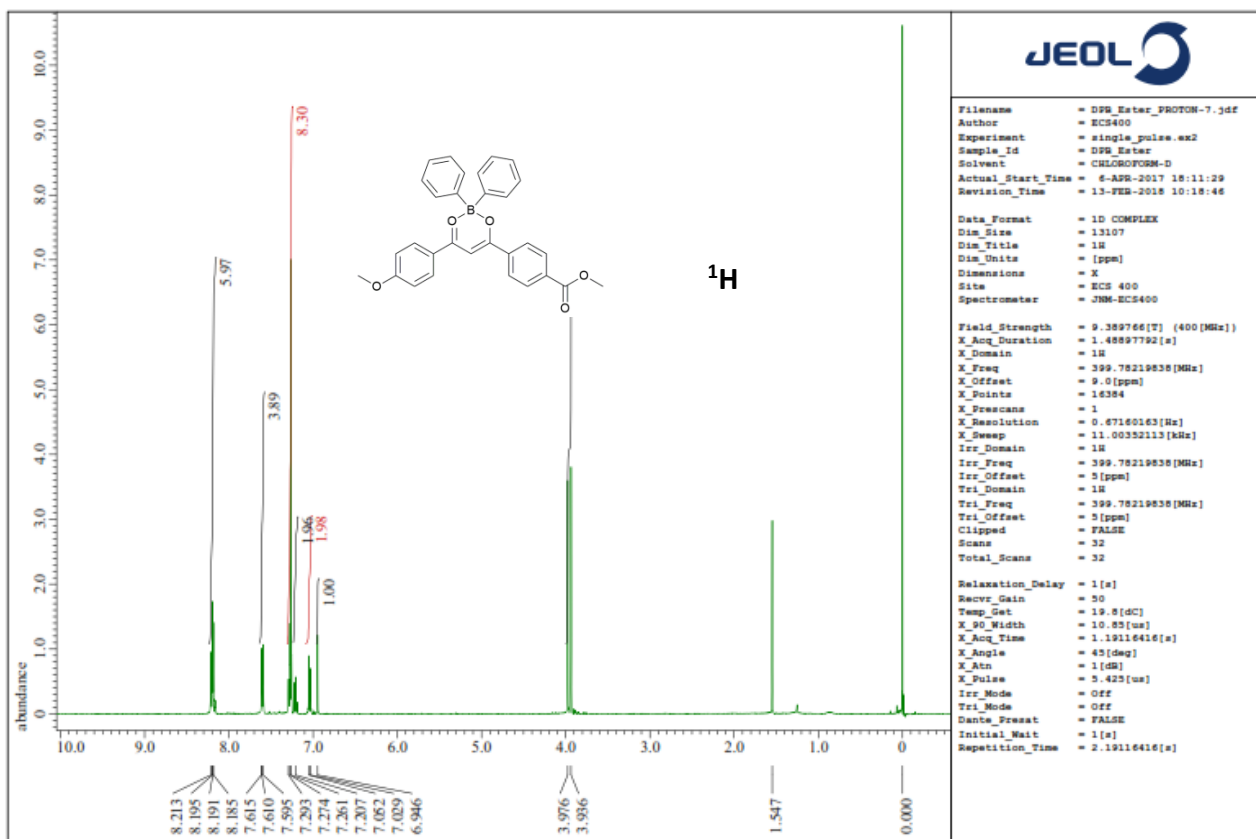
[b] ICMMO, Univ Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay (France)

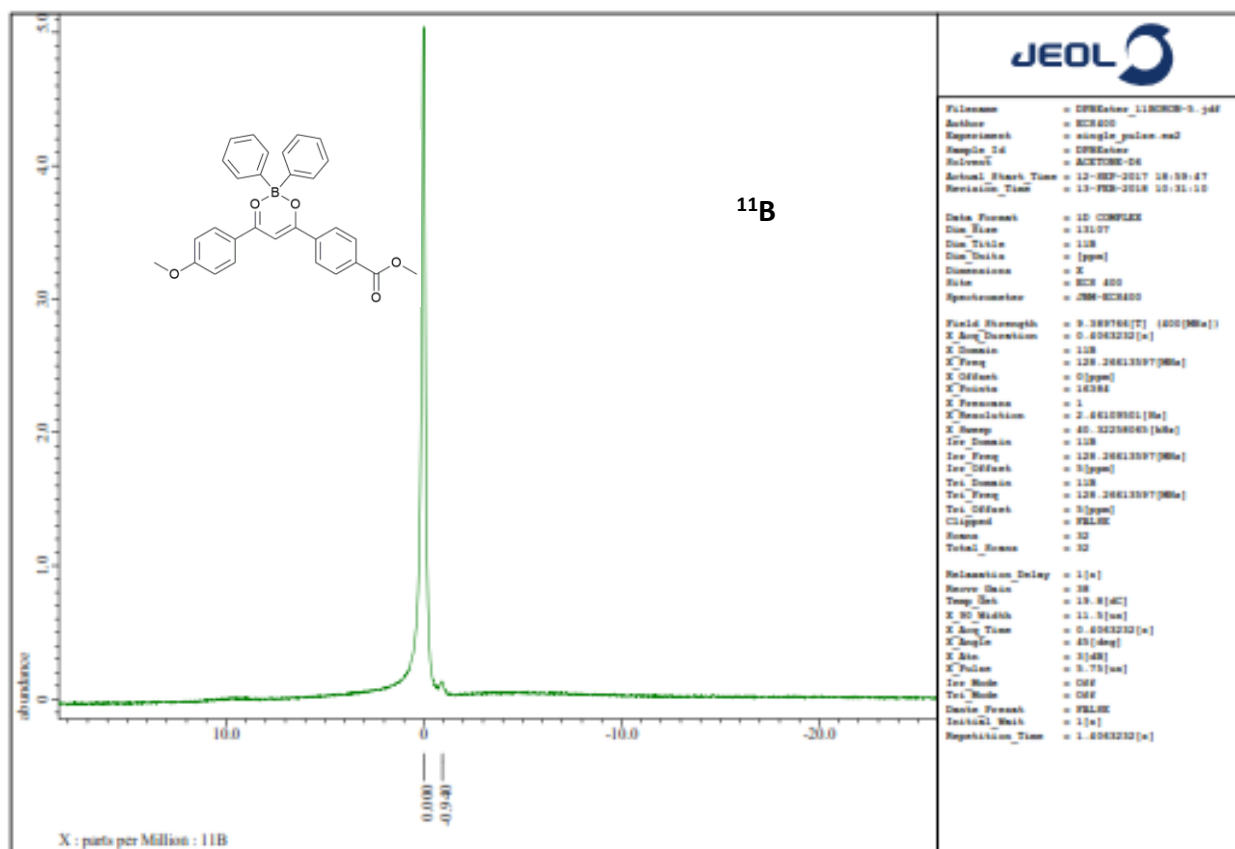
* Corresponding authors: metivier@ppsm.ens-cachan.fr, clemence.allain@ens-cachan.fr

Table S1. Crystallographic data and structure refinement details.

Compounds	P-Ester
Empirical Formula	C ₁₈ H ₁₅ O ₅
<i>M_r</i>	312.31
Crystal size, mm ³	0.12 x 0.11 x 0.03
Crystal system	monoclinic
Space group	<i>C c</i>
a, Å	34.531(3)
b, Å	7.3710(7)
c, Å	11.7082(9)
α, °	90
β, °	100.238(9)
γ, °	90
Cell volume, Å ³	2932.6(5)
Z ; Z'	8 ; 2
T, K	100(1)
Radiation type ; wavelength Å	MoKα ; 0.71073
F ₀₀₀	1304
μ, mm ⁻¹	0.104
θ range, °	2.397 - 23.392
Reflection collected	41 501
Reflections unique	4 252
R _{int}	0.0721
GOF	1.071
Refl. obs. (<i>I</i> >2σ(<i>I</i>))	3 592
Parameters	421
wR ₂ (all data)	0.1523
R value (<i>I</i> >2σ(<i>I</i>))	0.0619
Largest diff. peak and hole (e ⁻ .Å ⁻³)	0.443 ; -0.368

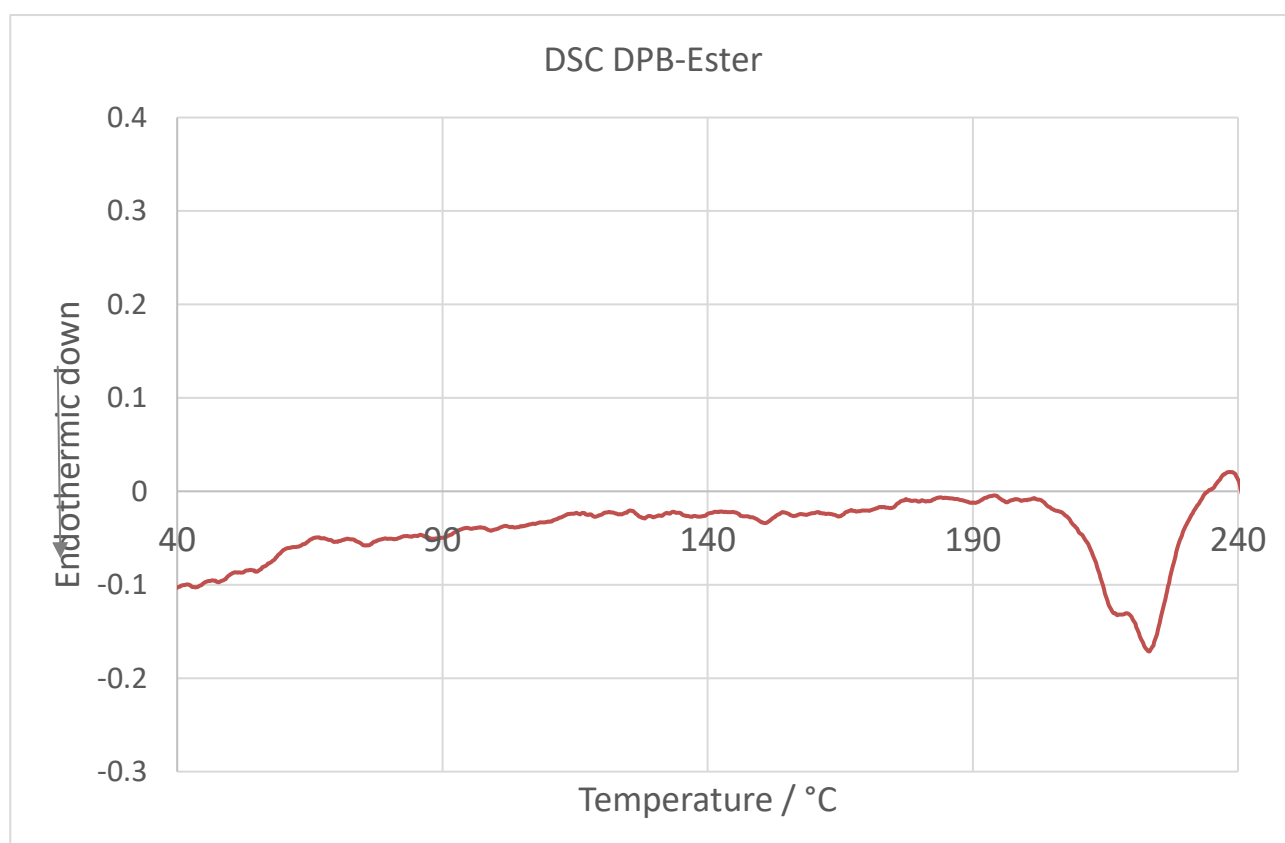
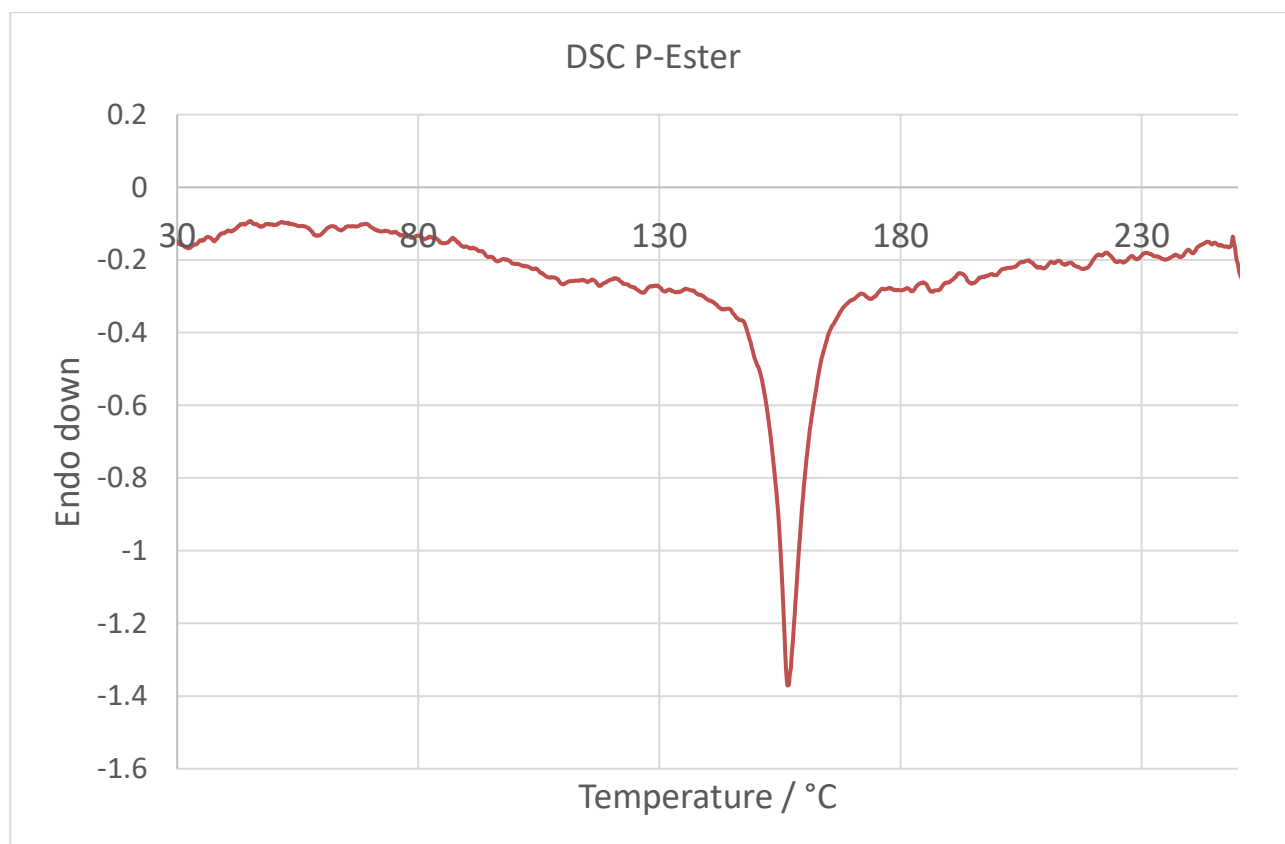
NMR spectra

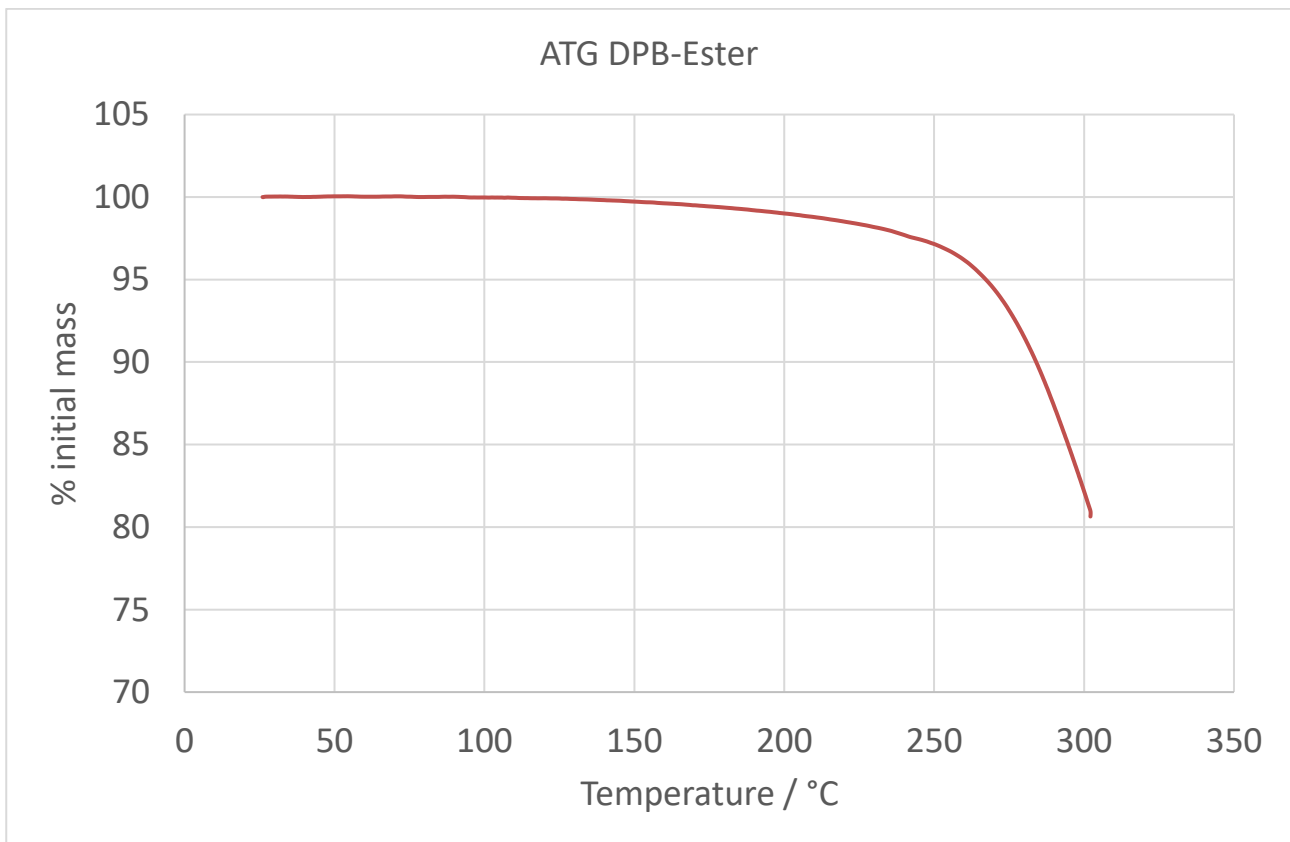
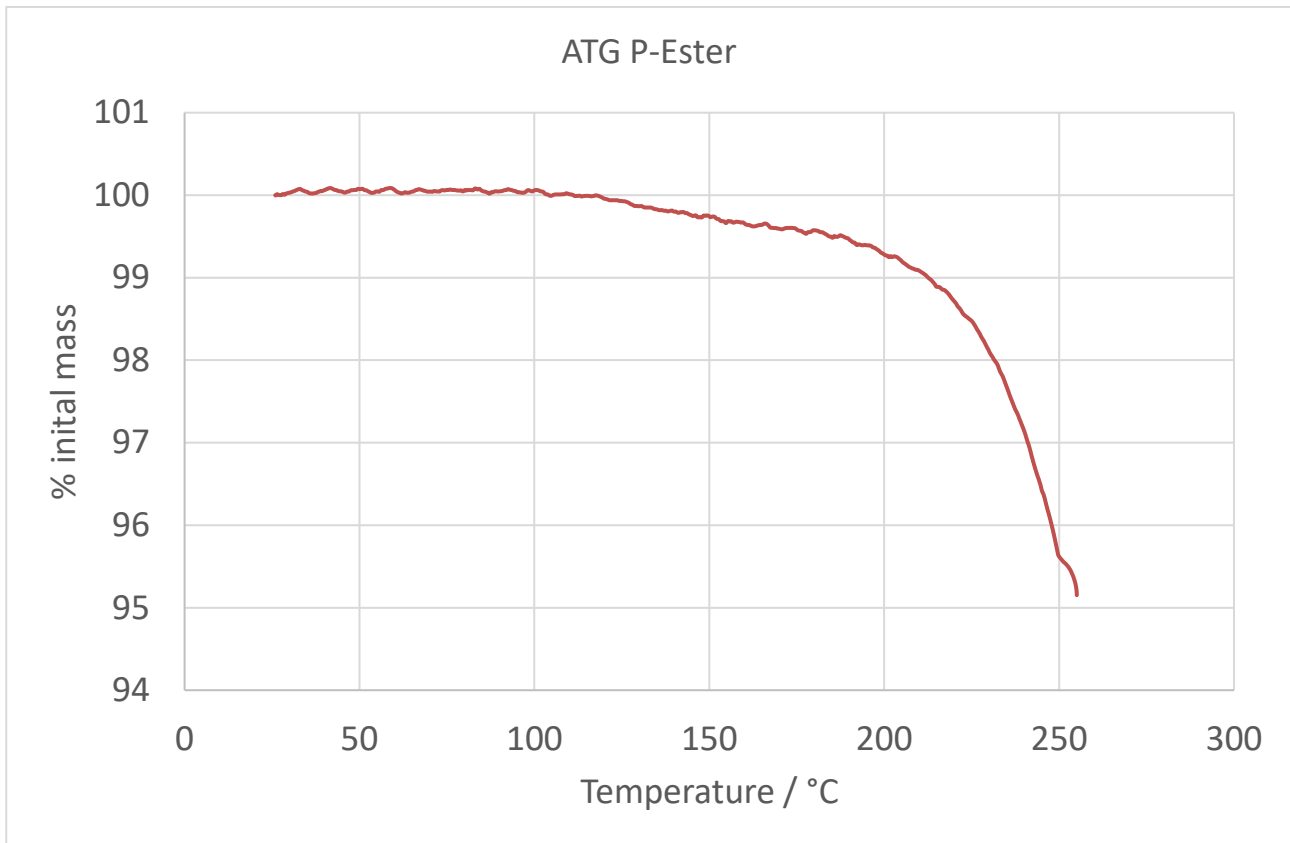




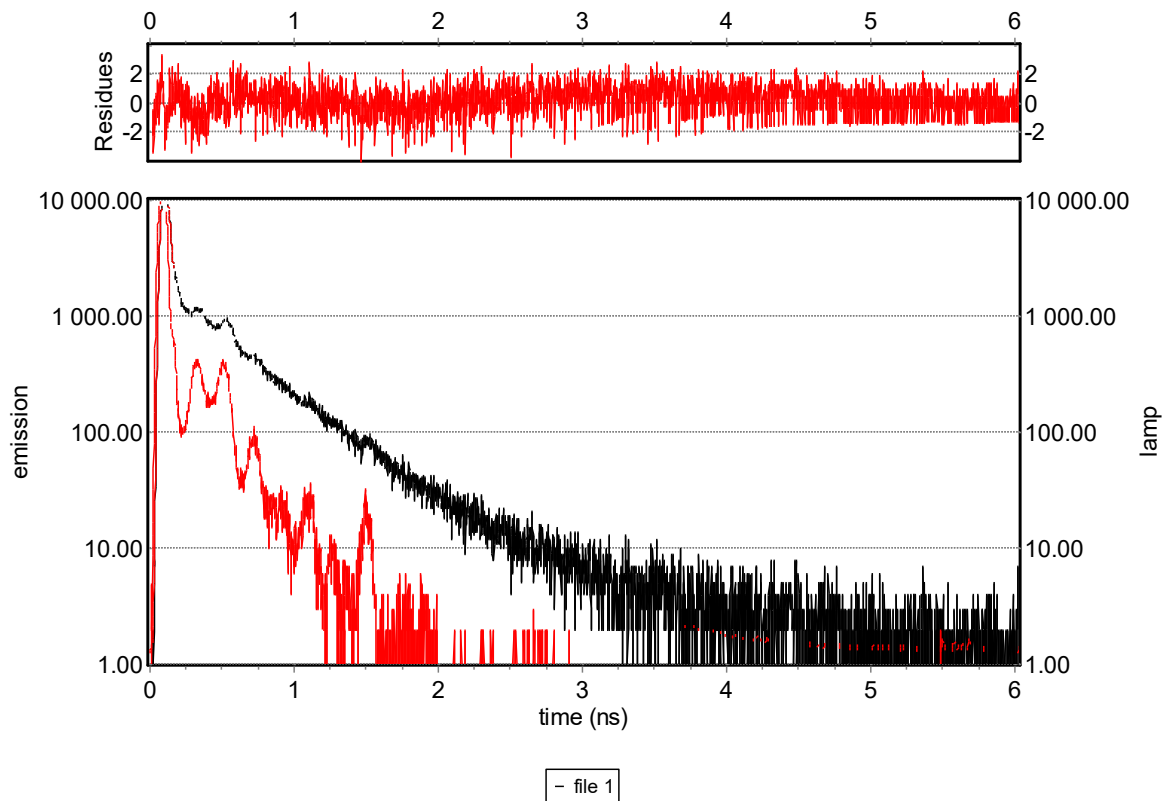
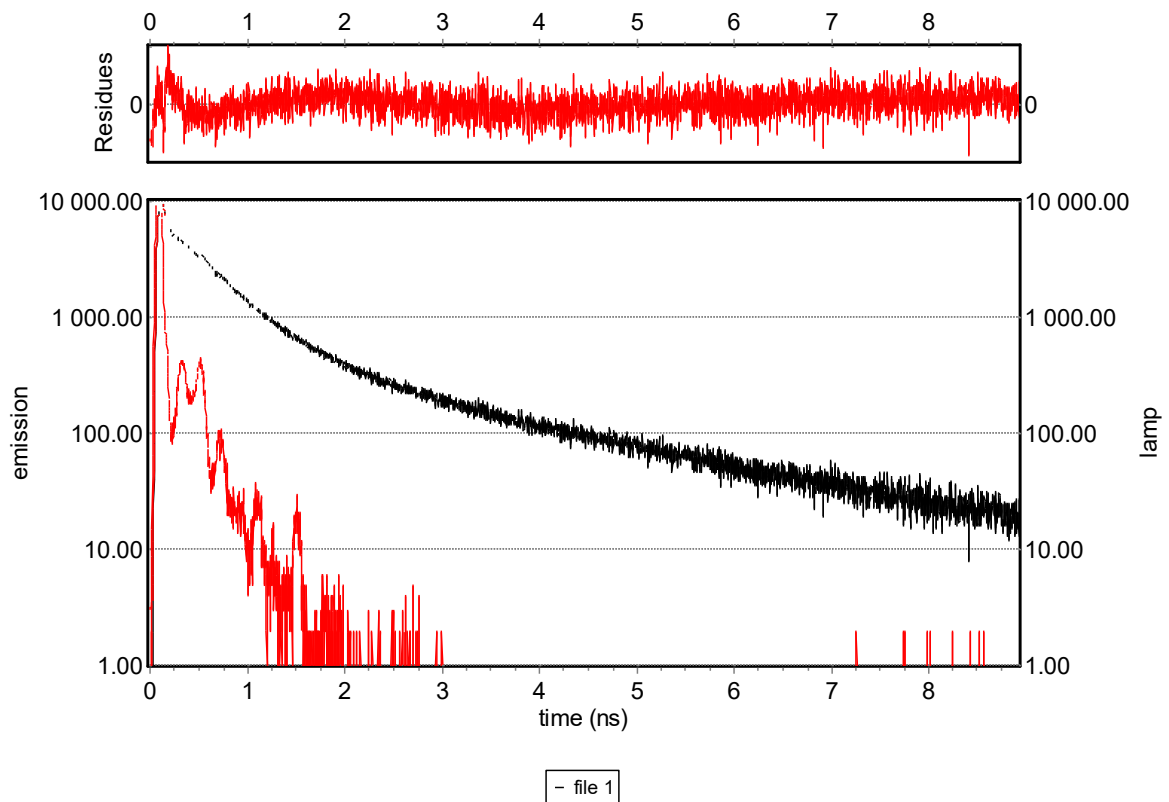
Differential Scanning Calorimetry and Thermogravimetric Analysis

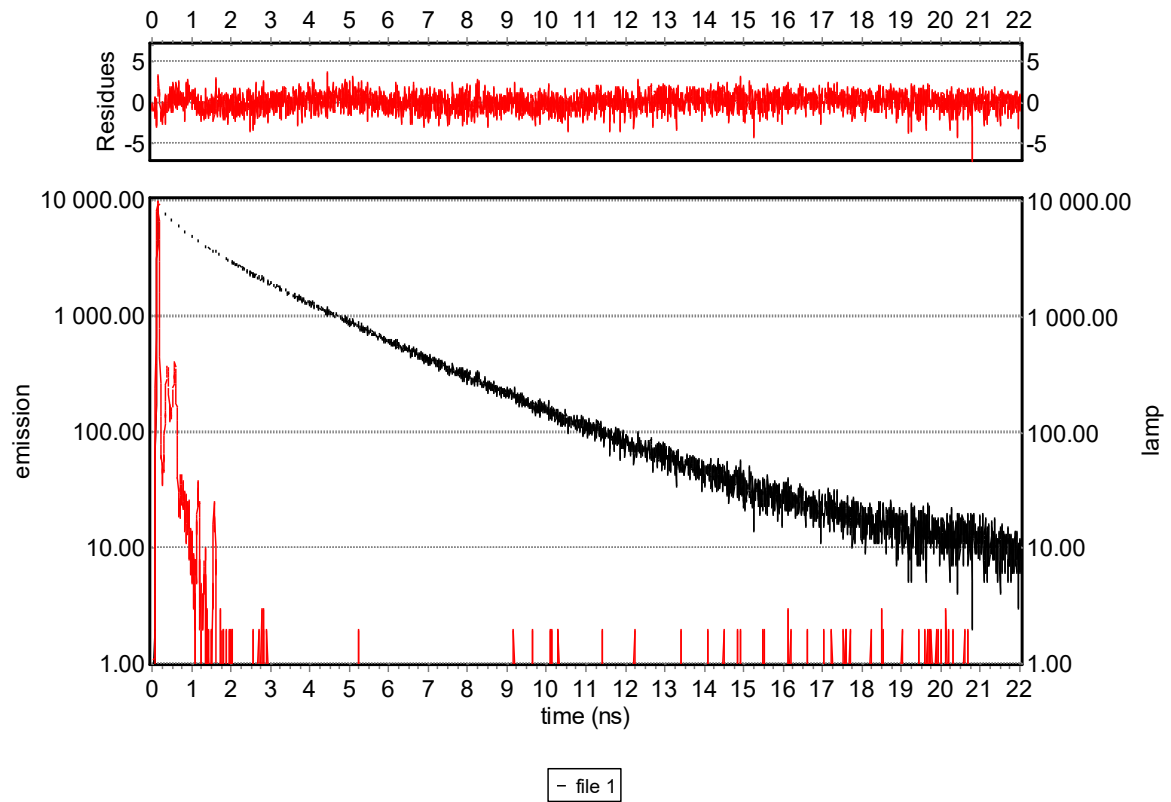
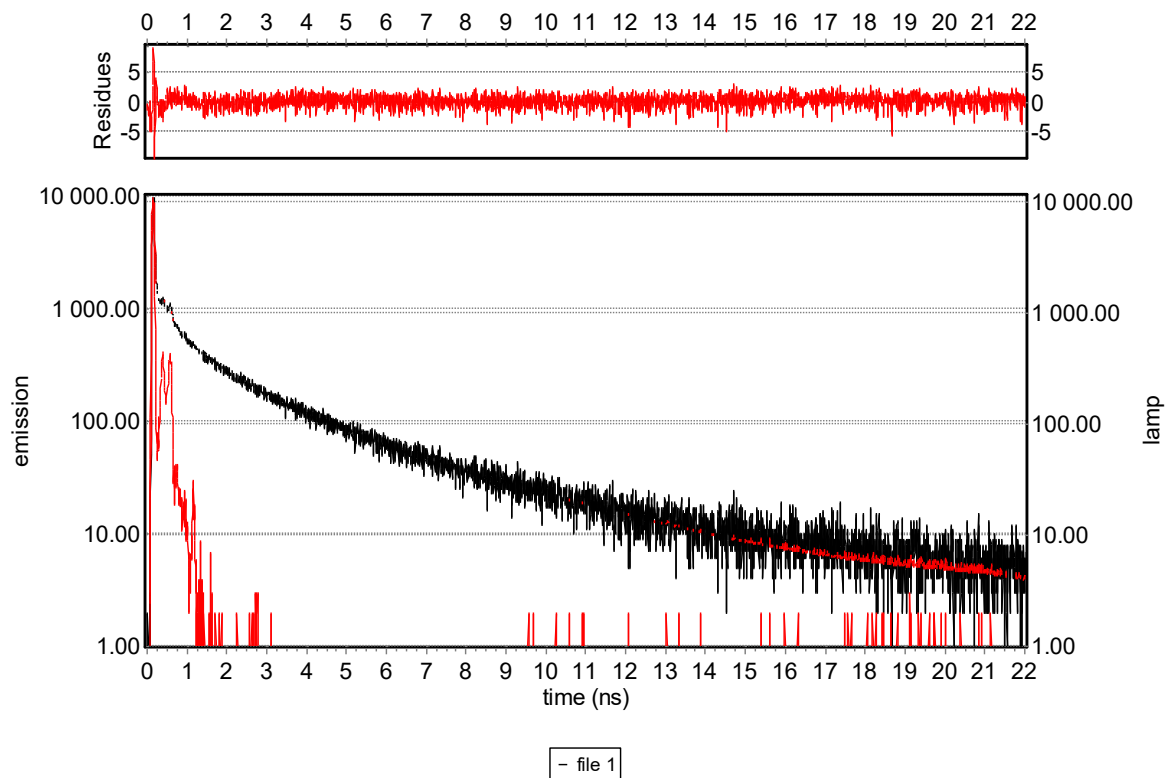
Differential scanning calorimetry and thermogravimetric analyses were performed on a Mettler Toledo TGA/DSC Star System, under air at 5 to 10°C / min.





Fluorescence decays

P-Ester in THF solution $\langle\tau\rangle = 0.19$ ns at 430 nmDPB-Ester in THF solution $\langle\tau\rangle = 0.92$ ns at 440 nm

P-Ester in the powder state $\langle\tau\rangle = 2.41$ ns at 450 nm**DPB-Ester in the powder state $\langle\tau\rangle = 2.32$ ns at 550 nm**

Fluorescence excitation spectra

