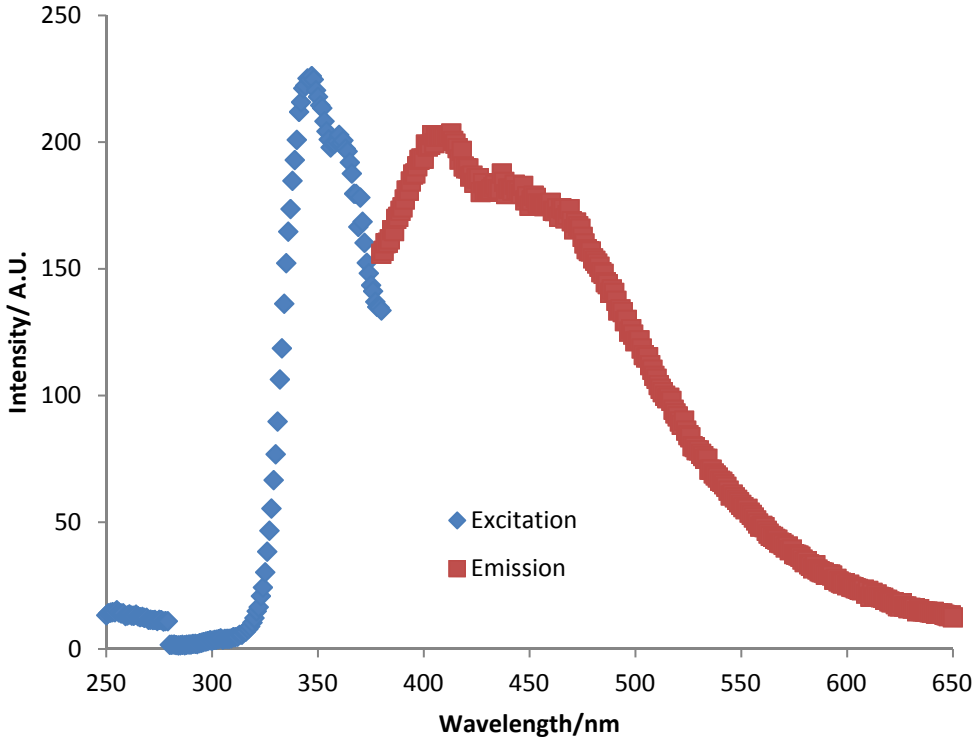
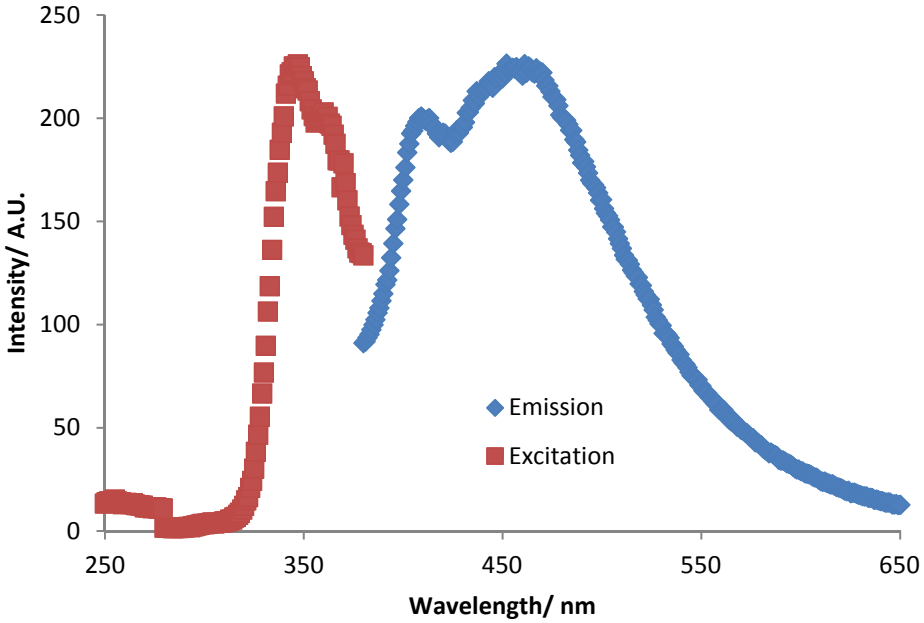
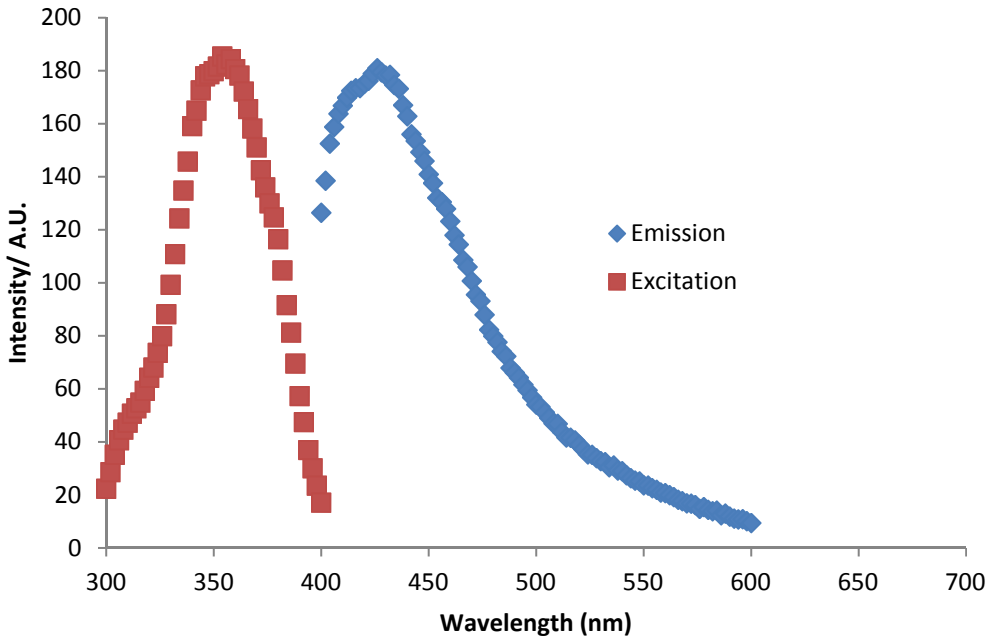
Ligand excitation and emission spectra



Excitation and Emission spectra of ligand *tris*(4-[4'-methyl-2,2'-bipyridyl]methyl)cyclotriguaiacylene L1 in dimethylsulfoxide

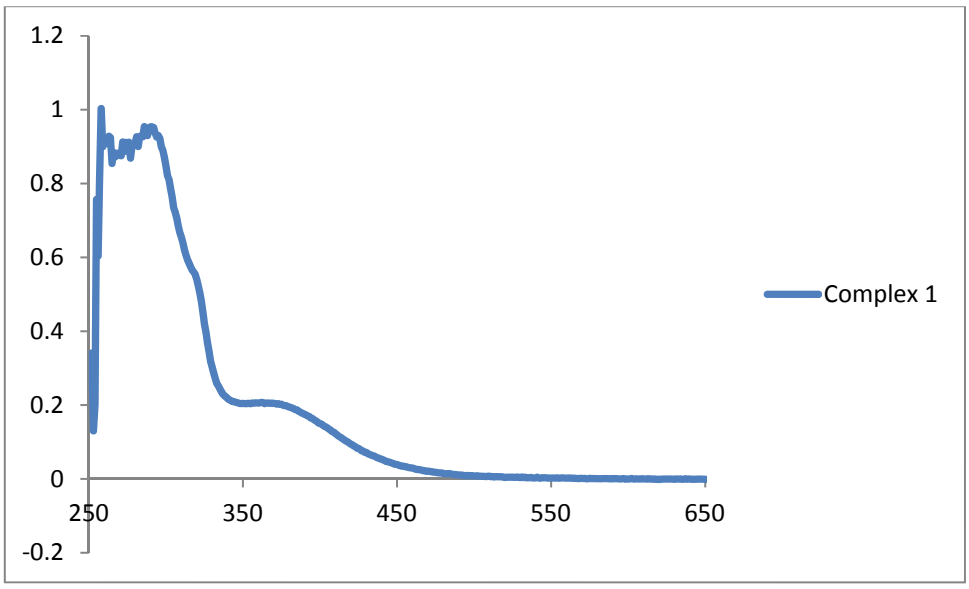


Excitation and Emission spectra of ligand tris(4-[4-methyl-2,2'-bipyridoyl])cyclotriguaiacylene L2 in dimethylsulfoxide

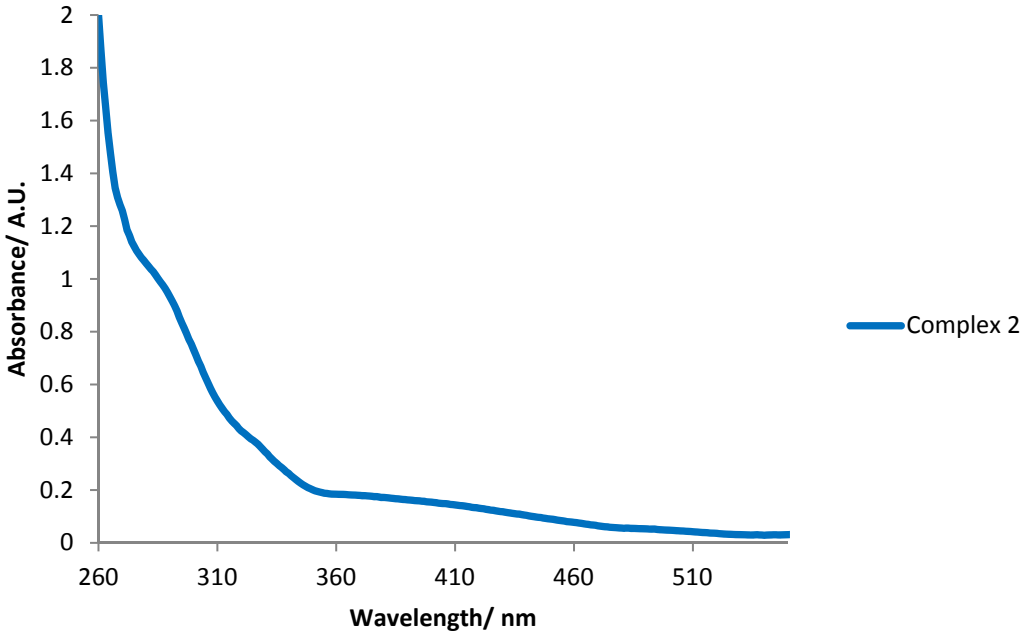


Excitation and Emission spectra of ligand tris-(4-[2,2',6',2"-terpyridyl]benzyl)cyclotriguaiacylene L3 in dimethylsulfoxide

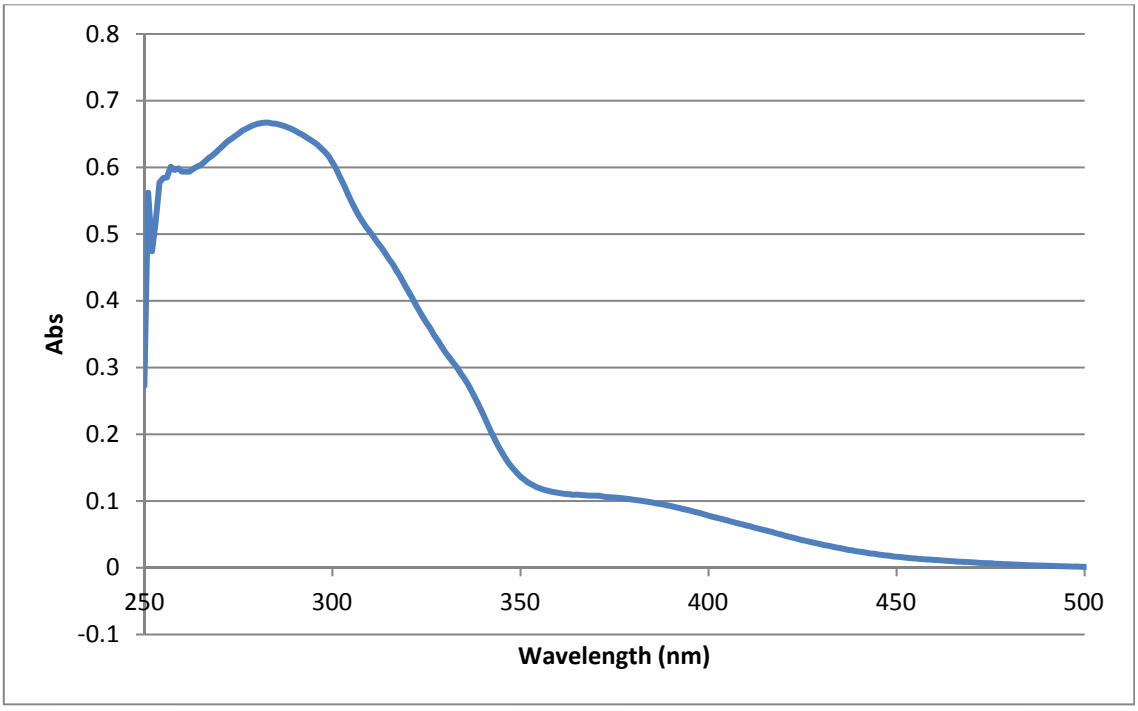
UV-visible spectra of complexes



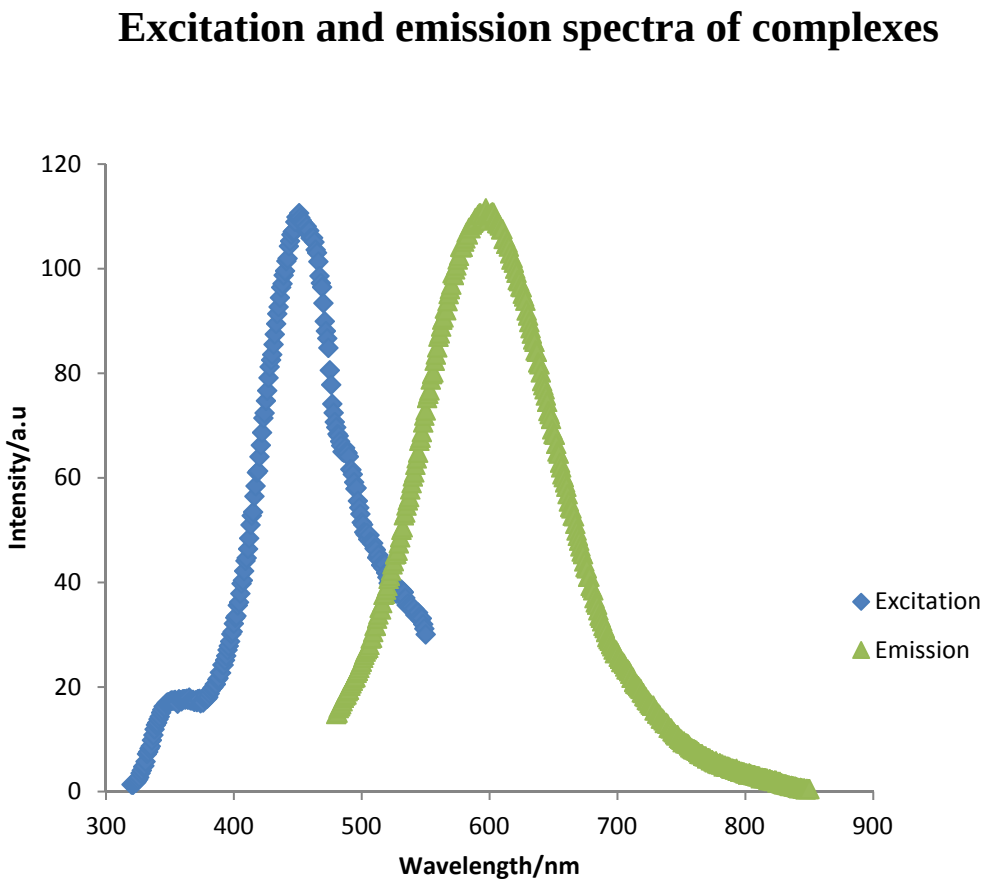
UV-visible spectrum of complex 1 in dimethylsulfoxide.



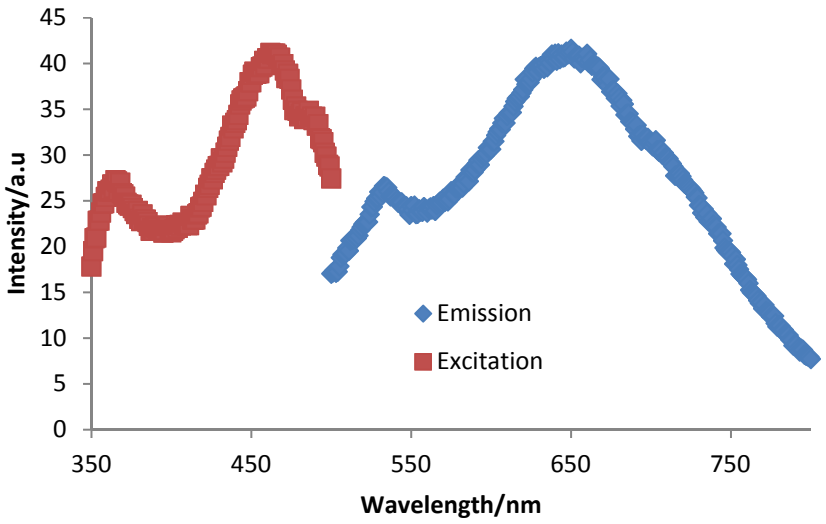
UV-visible spectrum of complex 2 in dimethylsulfoxide.



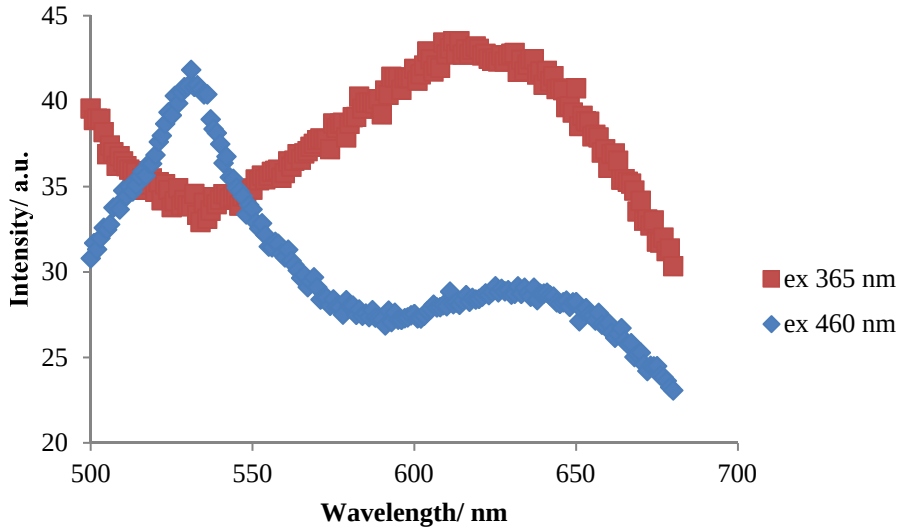
UV-visible spectrum of complex 3 in dimethylsulfoxide



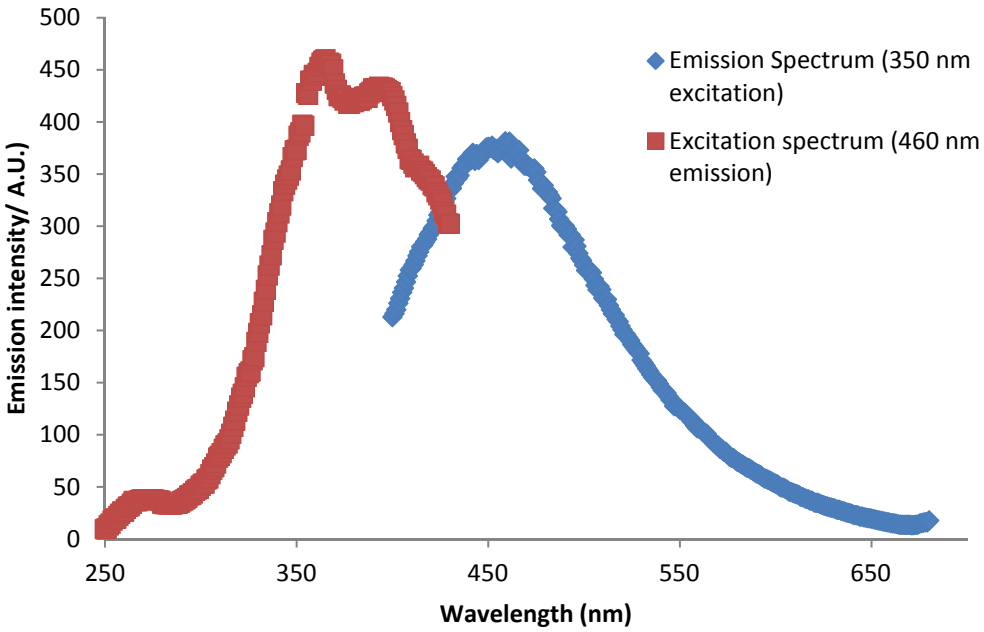
Excitation and Emission spectra of complex 1 in dimethylsulfoxide, emission spectrum excited at 450 nm, excitation spectrum recorded with emission monochromated at 600 nm



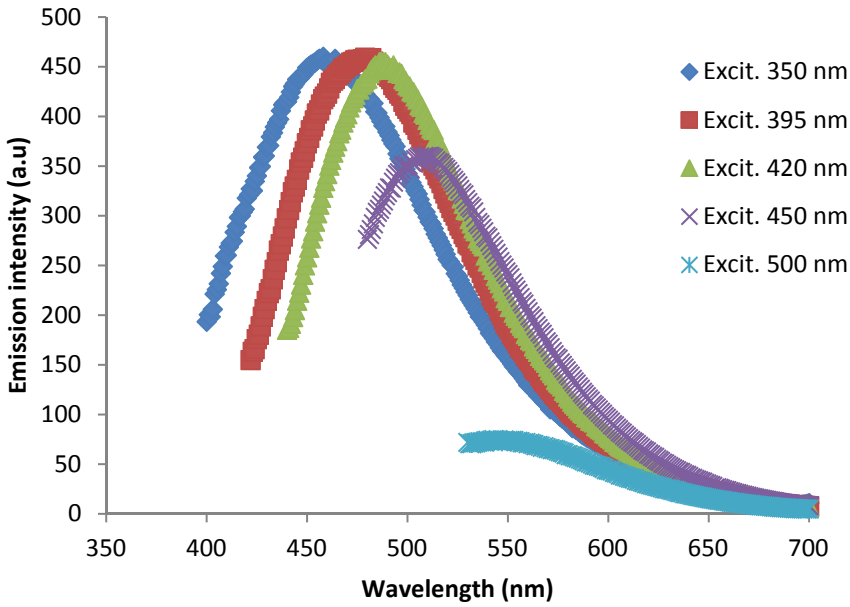
Excitation and Emission spectra of complex 2 in dimethylsulfoxide



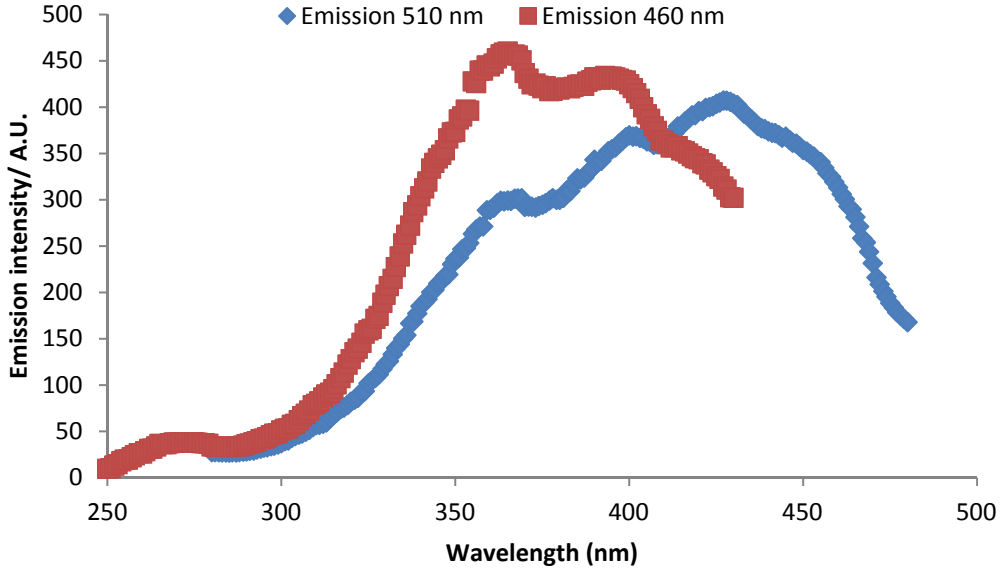
Emission spectra of complex 2 in dimethylsulfoxide at different excitation wavelengths



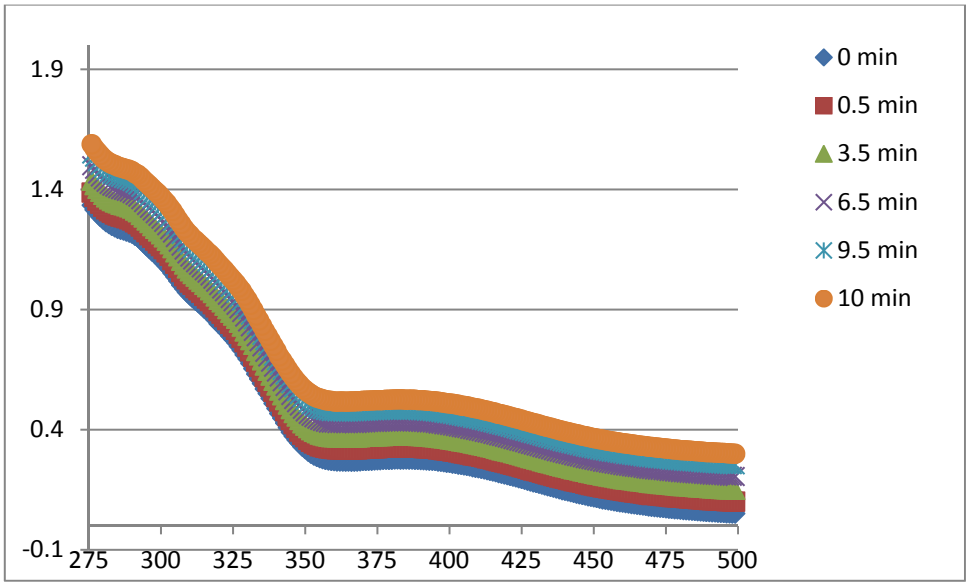
Excitation and Emission spectra of complex 3 in dimethylsulfoxide



Varying excitation wavelength for emission of complex 3

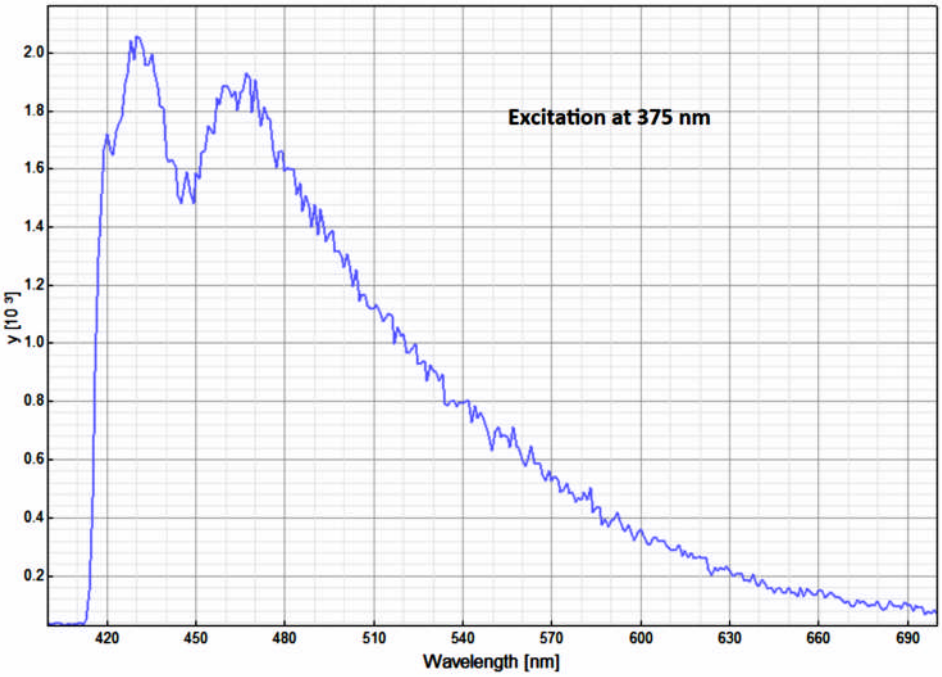


Emission monochromated at 460 and 510 nm for excitation spectra of complex 3.

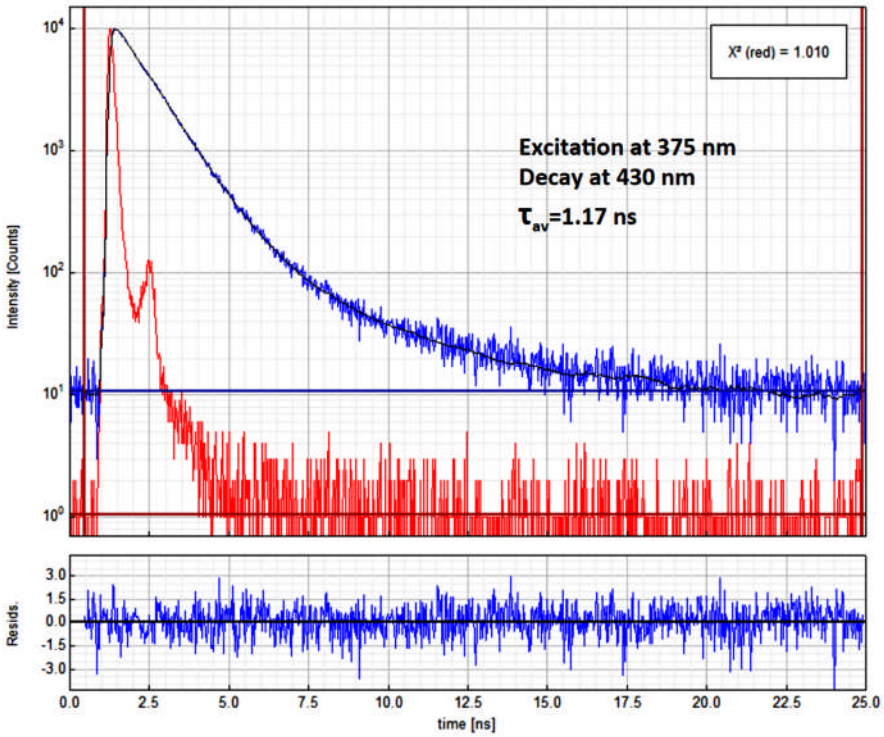


Electronic absorption spectra of complex 2 following irradiation. Sequential spectra offset vertical axis by 0.05 absorption with 0 min at native value.

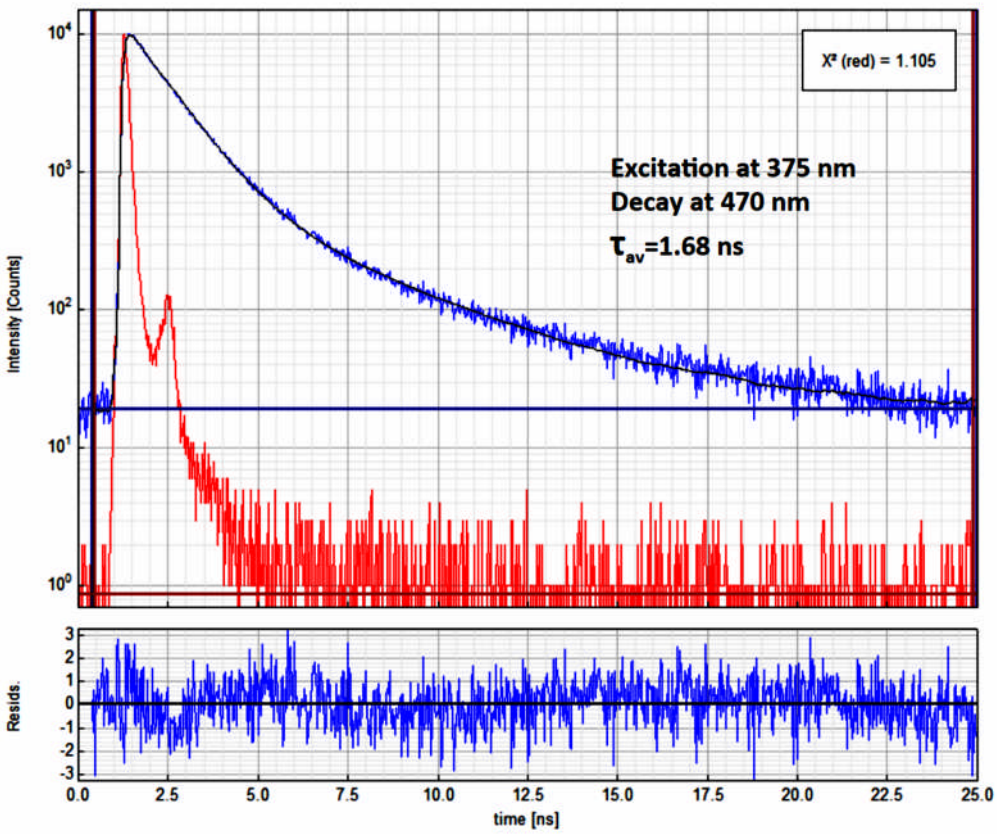
Lifetime data



(a)



(b)



(c)

TRES Lifetime data for ligand L3 showing excitation spectrum at 375 nm (a) and two components contributing to the observed lifetime corresponding to τ = 1.17 ns (b) and τ = 1.68 ns (c).

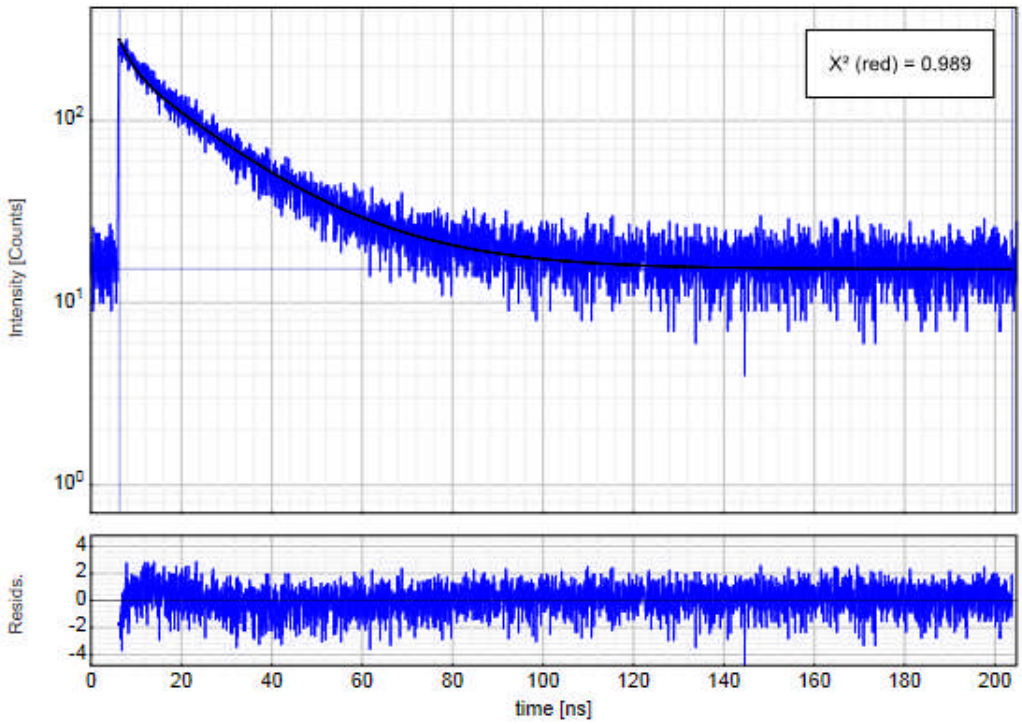
PicoQuant FluoFit 6/12/2014

Re | Dimethyl sulfoxide

Re in DMSO

Model: Exp. [Tailfit] (Exponential)
Plotted Data Set #60 Decay: "\..\TRES+IRF_20140612_1712.etf" (61)
X²(reduced): 1.2764 ; Fitted Data Points: 240889

Main Plot



$$I(t) = \sum_{i=1}^{n} A_i \, e^{-\frac{t}{\tau_i}}$$

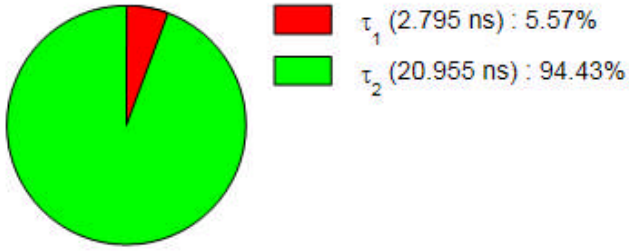
Parameter	Value	Conf. Lower	Conf. Upper	Conf. Estimation
A_1 [Cnts]	81	-251	+251	Fitting
τ_1 [ns]	2.795	-0.152	+0.152	Fitting
A_2 [Cnts]	183.0	-68.0	+68.0	Fitting
τ_2 [ns]	20.955	-0.565	+0.565	Fitting
Bkgr. Dec [Cnts]	15.29	-6.76	+6.76	Fitting

Average Lifetime:

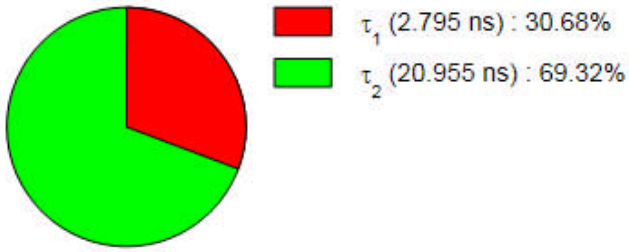
$\tau_{Av.1}$=19.943 ns (intensity weighted)

$\tau_{Av.2}$=15.383 ns (amplitude weighted)

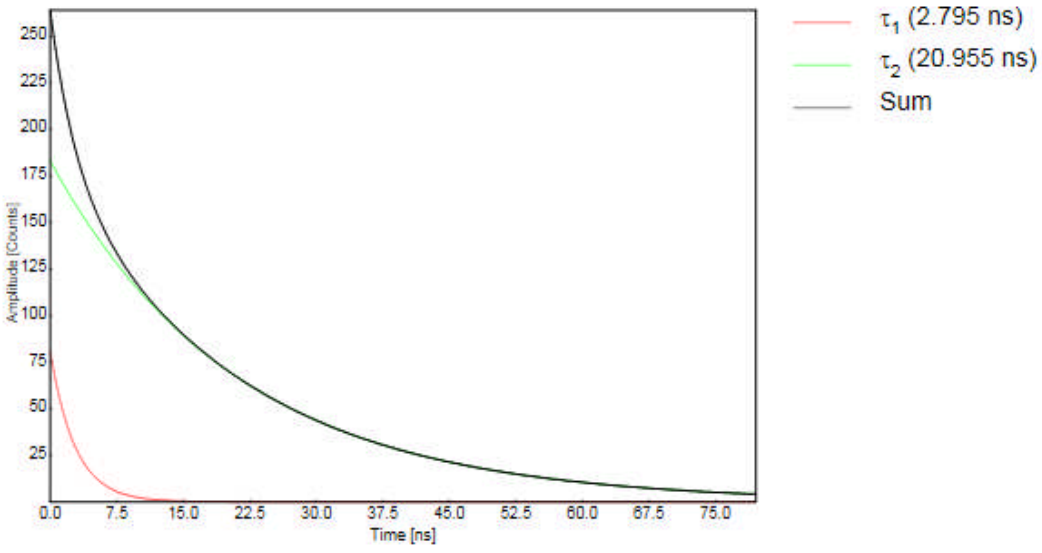
Fractional Intensities of the Positive Decay Components:



Fractional Amplitudes of the Positive Decay Components:

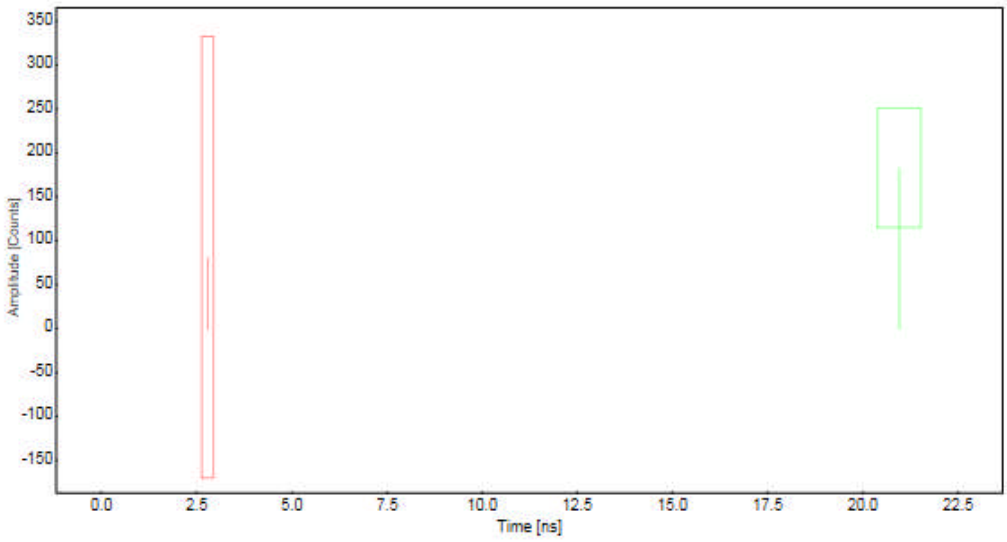


Fitted Decay and Exponential Components:

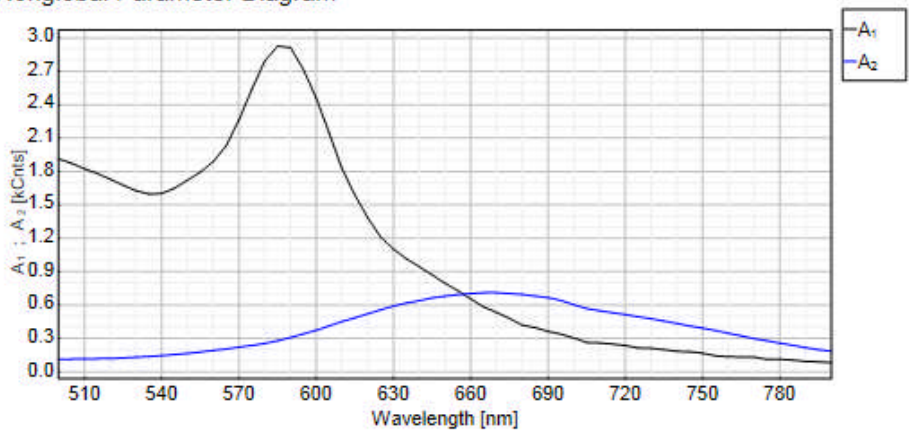


PicoQuant FluoFit 6/12/2014

Confidence Intervals:



Nonglobal Parameter Diagram



TRES Lifetime data for complex 2 **showing two different components contributing to the observed lifetime corresponding to τ = 20.96 ns and τ = 2.80 ns.**

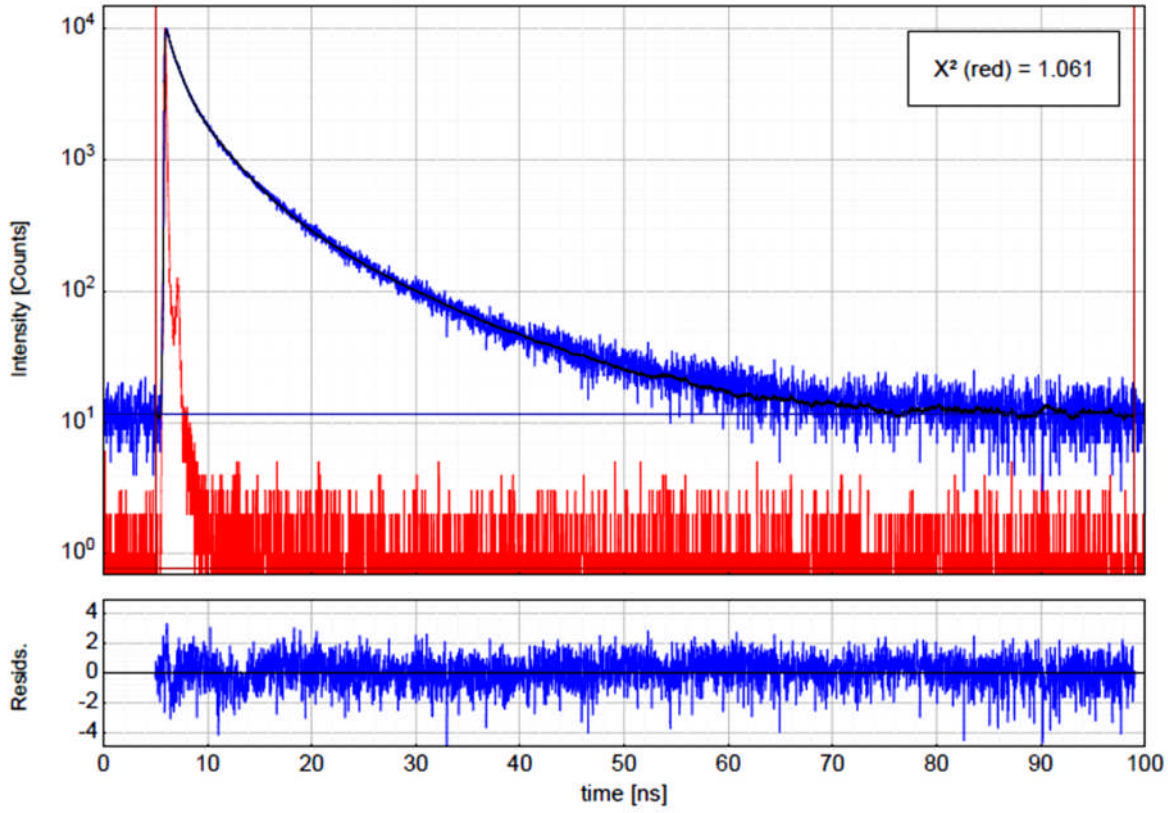
PicoQuant FluoFit 11/2/2015

FTE | Dimethyl sulfoxide

emission 470 nm
405nm filter

Model: Exp. [Reconv.] (Exponential)
Plotted Data Set #0 Decay: "\..\Custom_20151016_2012 (2).etf" (0)
Plotted Data Set #0 IRF: "\..\irf-10mhz.dat" (1)
X²(reduced): 1.0614 ; Fitted Data Points: 3763

Main Plot



$$I(t) = \int_{-\infty}^{t} IRF(t') \sum_{i=1}^{n} A_i \, e^{-\frac{t-t'}{\tau_i}} \, dt'$$

PicoQuant FluoFit 11/2/2015

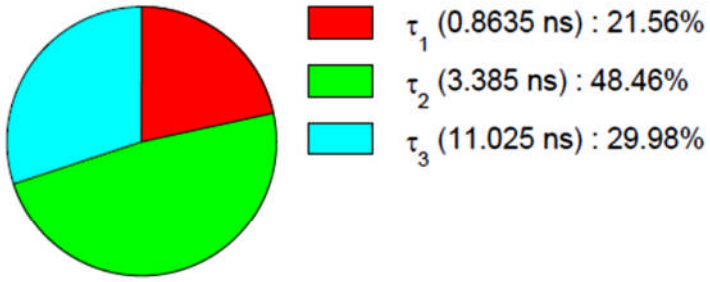
Parameter	Value	Conf. Lower	Conf. Upper	Conf. Estimation
A_1 [Cnts]	1027.0	-33.9	+33.9	Fitting
τ_1 [ns]	0.8635	-0.0702	+0.0972	Bootstrap
A_2 [Cnts]	588.9	-10.9	+10.9	Fitting
τ_2 [ns]	3.385	-0.206	+0.303	Bootstrap
A_3 [Cnts]	111.85	-2.83	+2.83	Fitting
τ_3 [ns]	11.025	-0.464	+0.581	Bootstrap
Bkgr. $_{Dec}$ [Cnts]	11.678	-0.827	+0.827	Fitting
Bkgr. $_{IRF}$ [Cnts]	0.7746	-0.0622	+0.0622	Fitting
Shift $_{IRF}$ [ns]	0.00413	-0.00397	+0.00397	Fitting
A $_{Scat}$ [Cnts]	29740	-2970	+2970	Fitting
Period $_{Rep}$ [ns]	0.00396	-0.00209	+0.00209	Fitting

Average Lifetime:

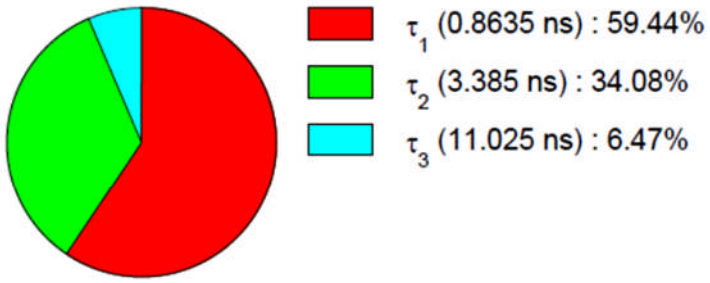
$\tau_{Av.1}$=5.1318 ns (intensity weighted)

$\tau_{Av.2}$=2.3808 ns (amplitude weighted)

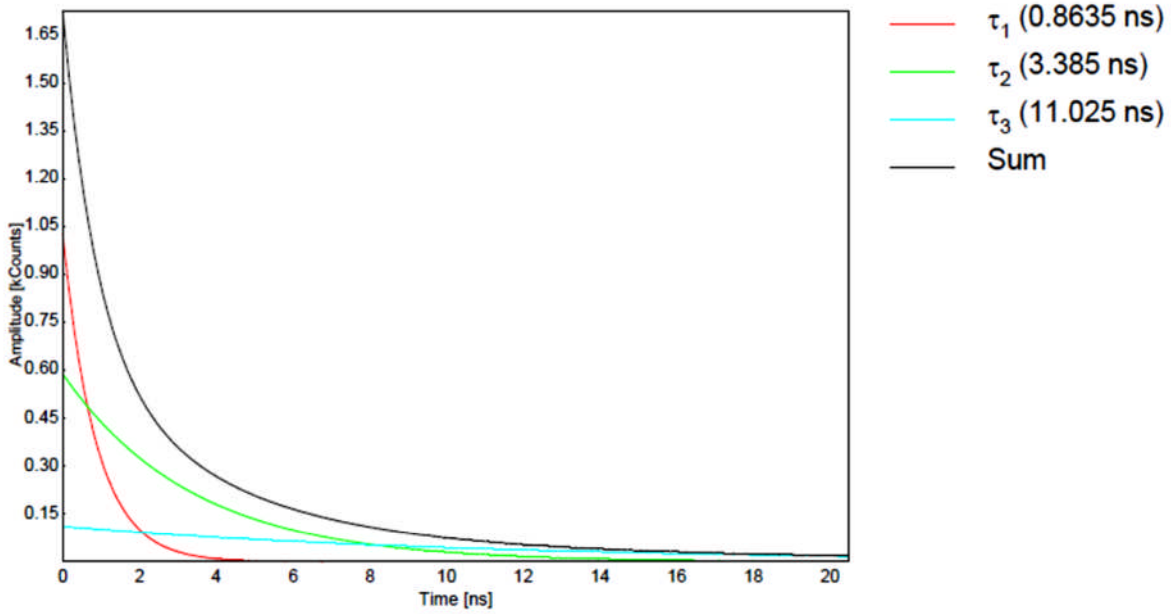
Fractional Intensities of the Positive Decay Components:



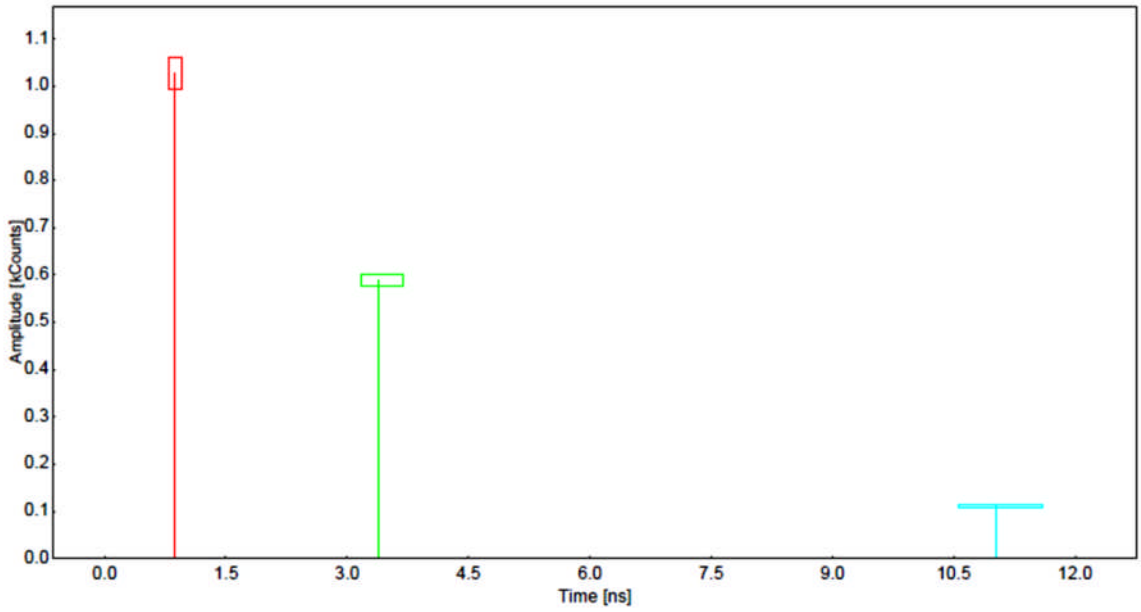
Fractional Amplitudes of the Positive Decay Components:



Fitted Decay and Exponential Components:

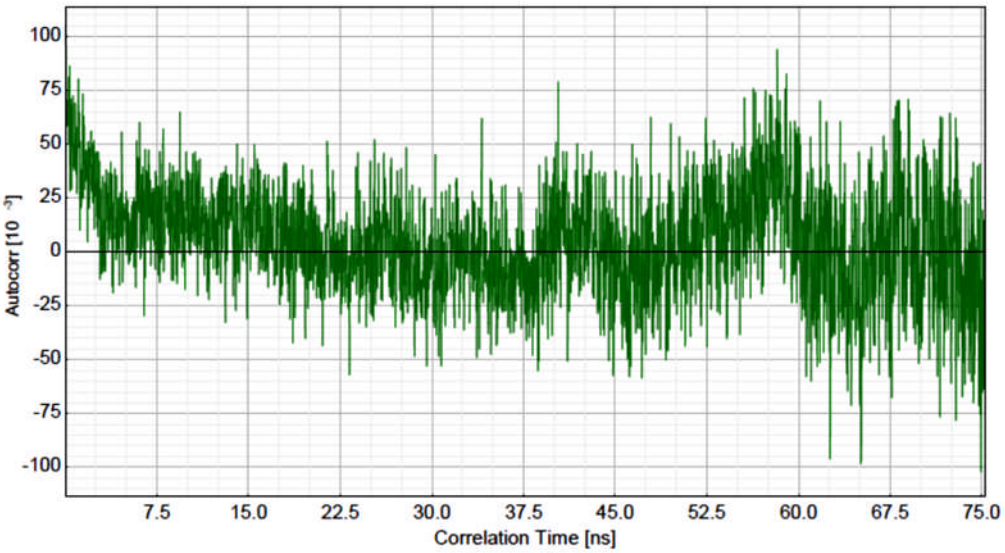


Confidence Intervals:

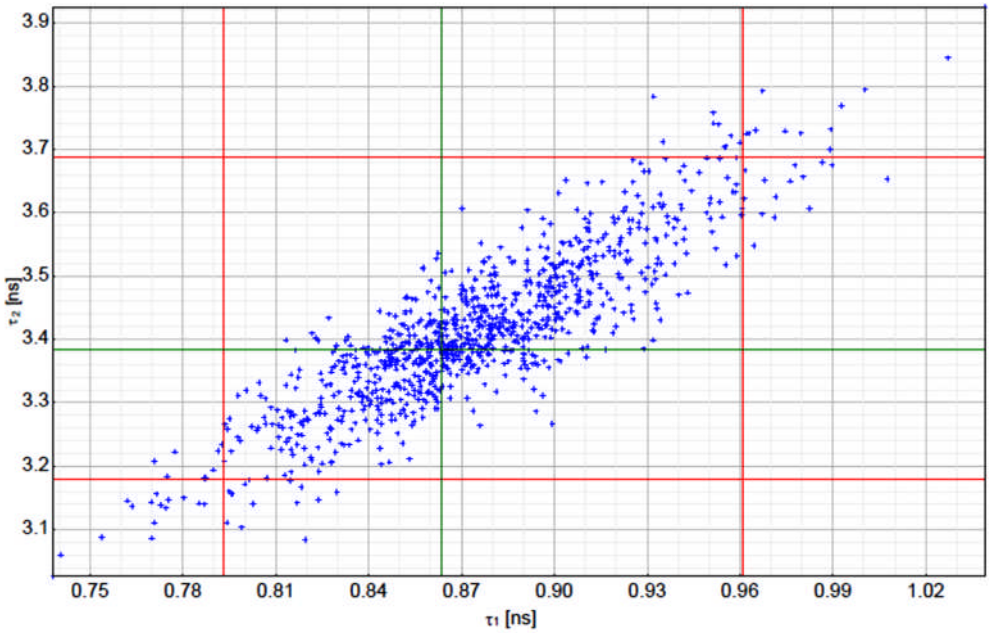


PicoQuant FluoFit 11/2/2015

Autocorrelation Function



Bootstrap Analysis



TRES lifetime data for complex 3 in DMSO showing three different components contributing to the observed lifetime corresponding to τ_1 = 11.03, τ_2 = 3.39 and τ_3 = 0.86 ns.