Electronic Supplementary Information

BODIPY-loaded polymer nanoparticles: chemical structure of cargo defines leakage from nanocarrier in living cells

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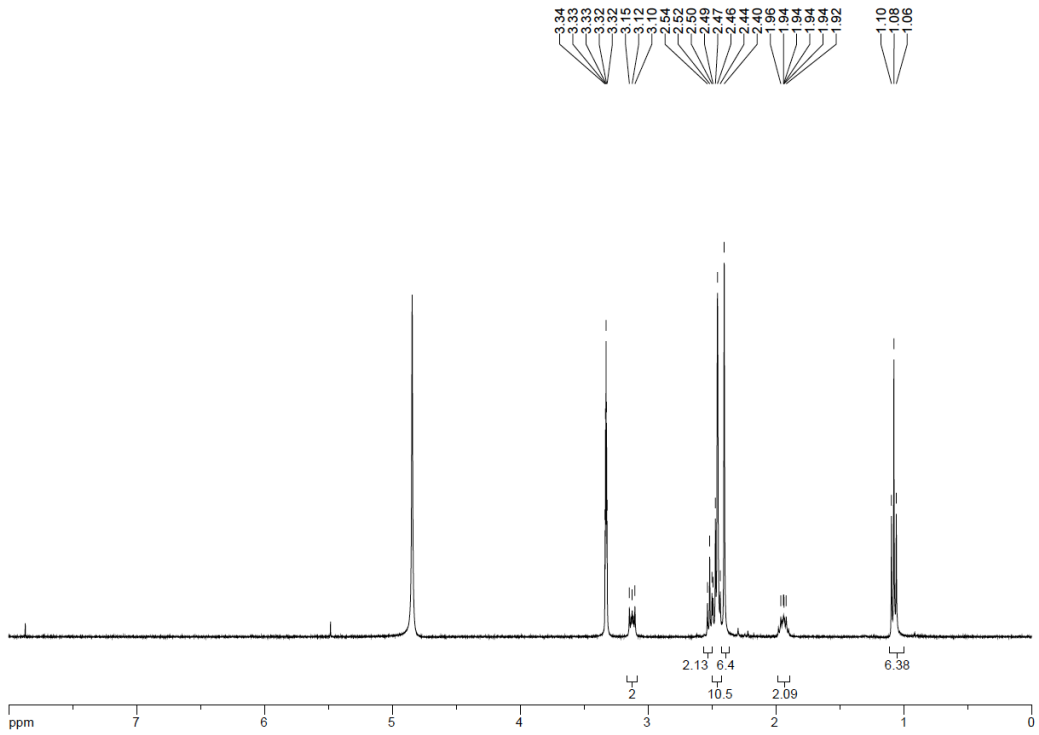
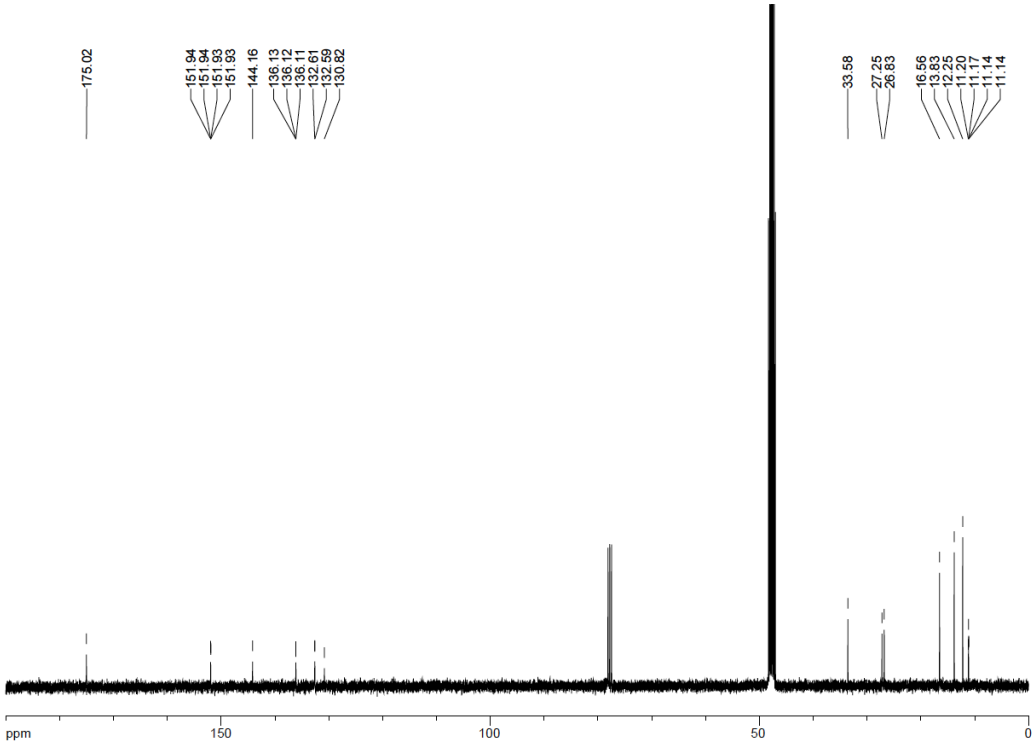
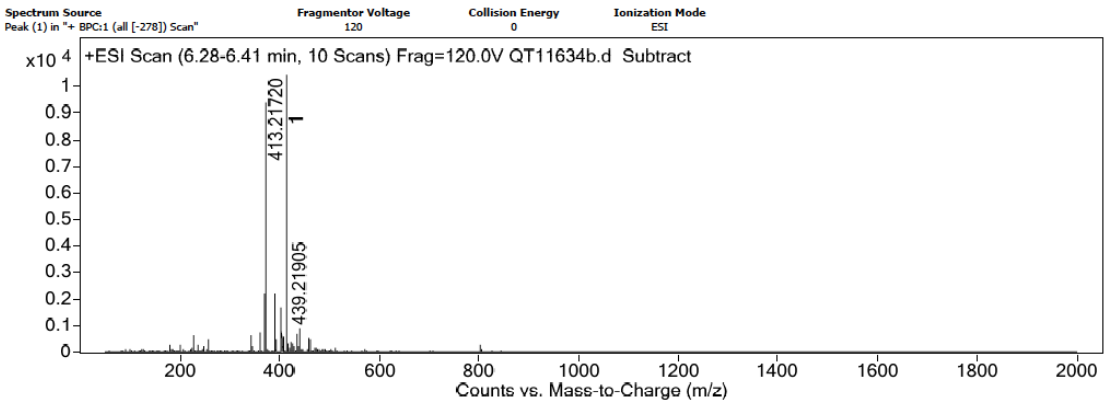
NMR and mass spectra



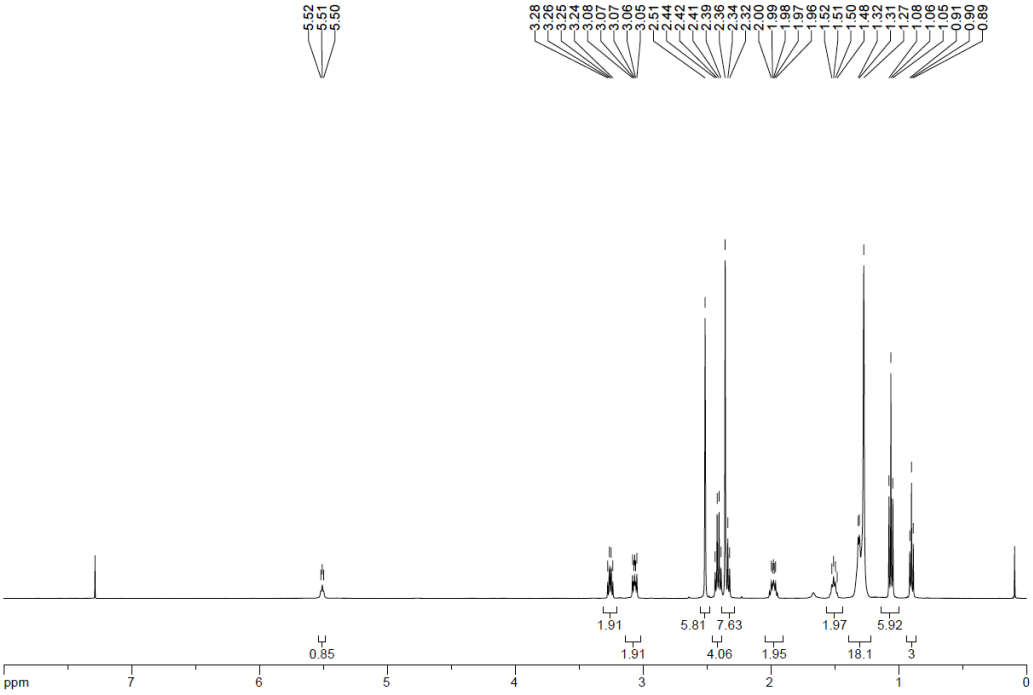
1H spectrum of **1**



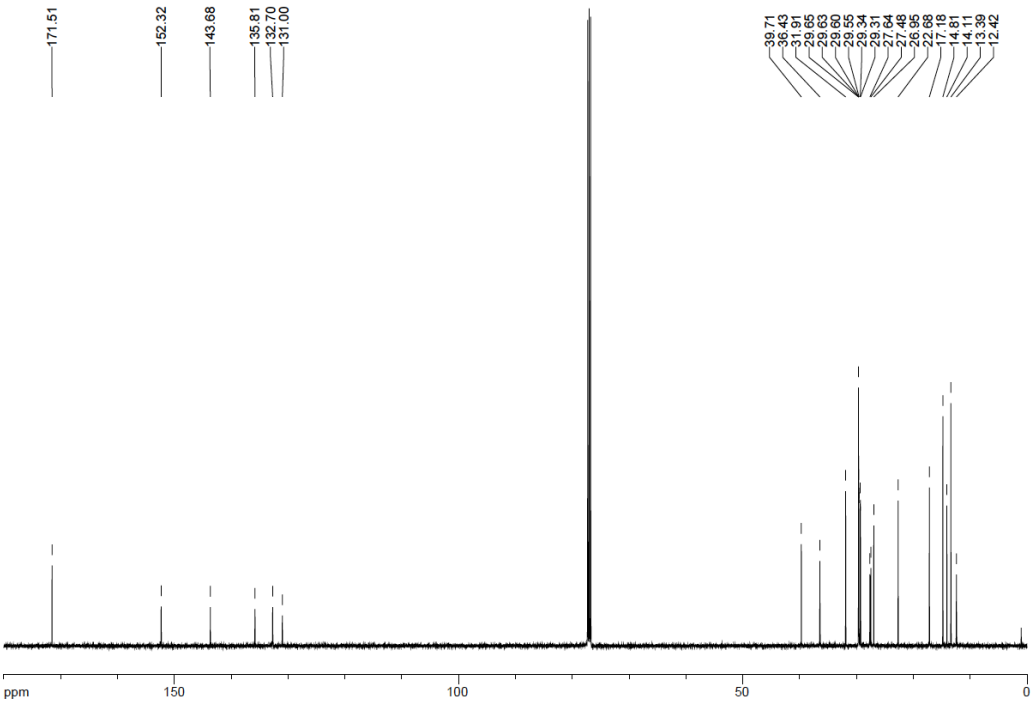
13C spectrum of **1**



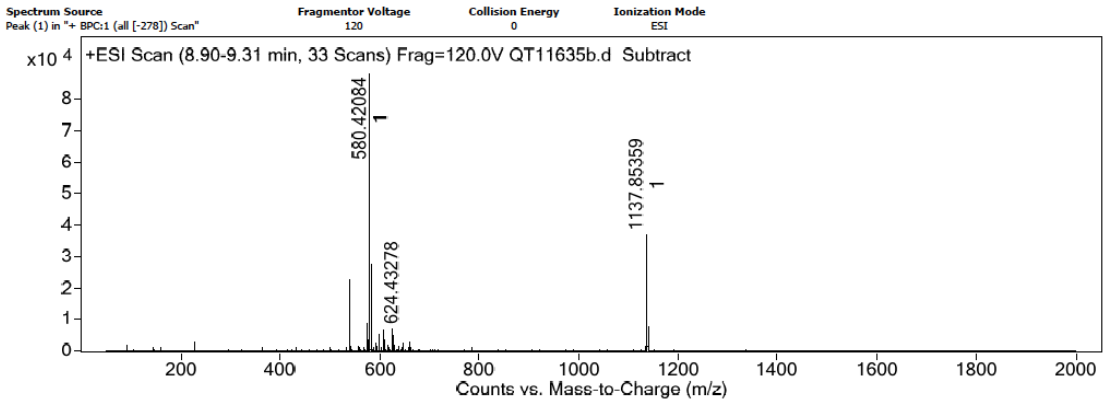
HRMS spectrum of **1**



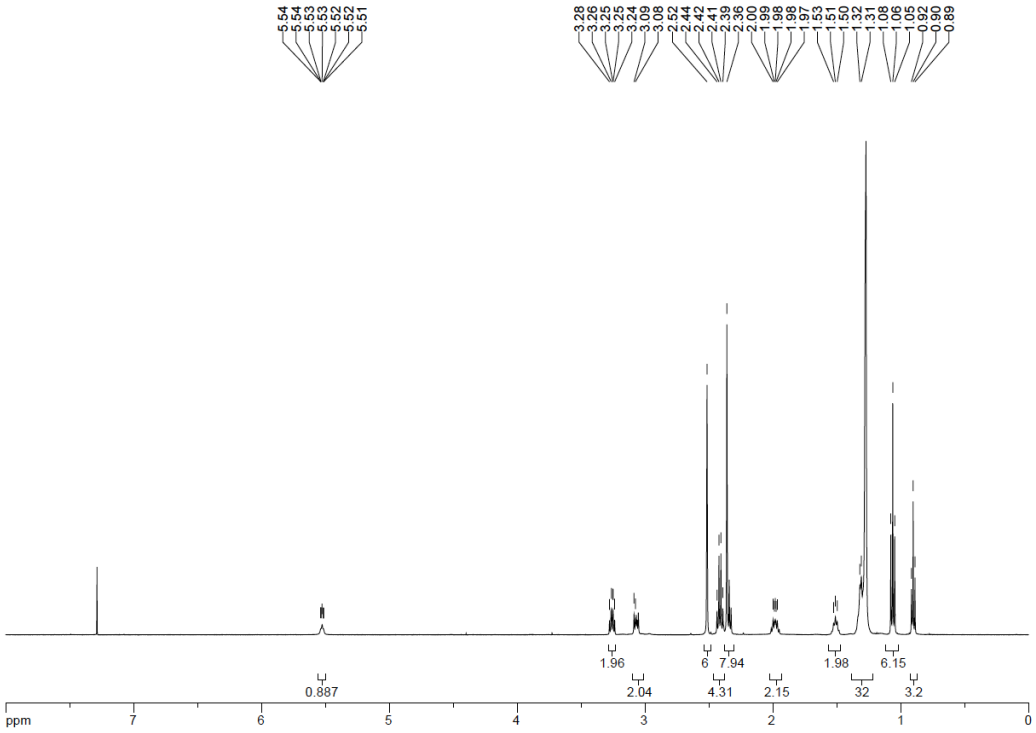
1H spectrum of B-C12



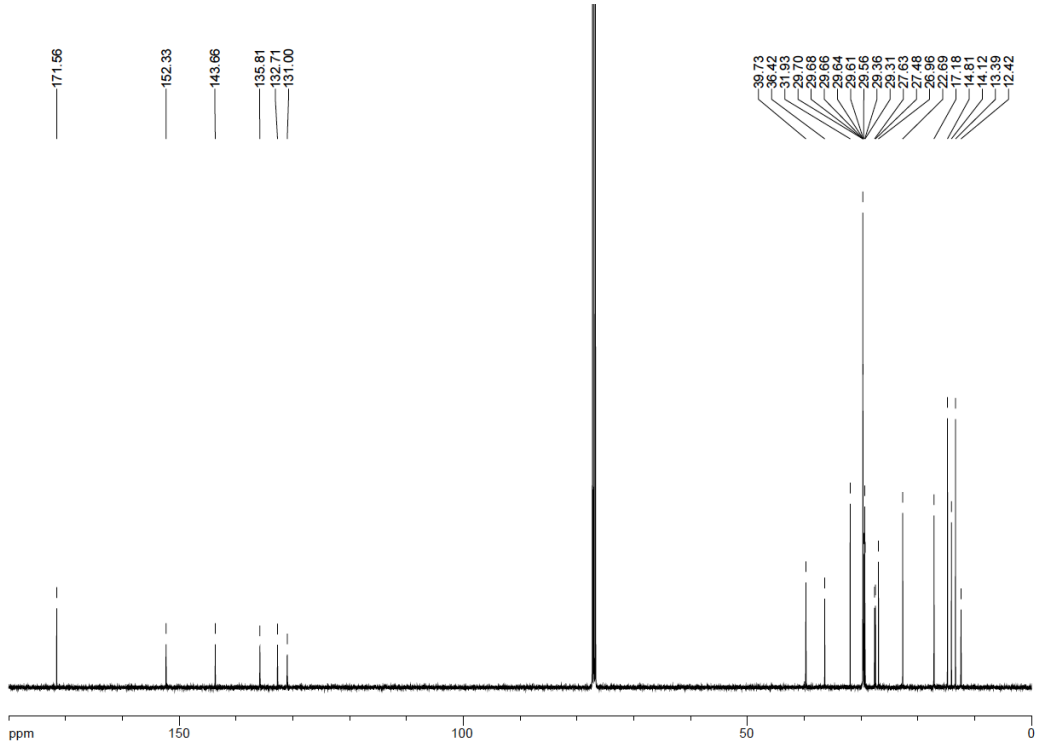
13C spectrum of B-C12



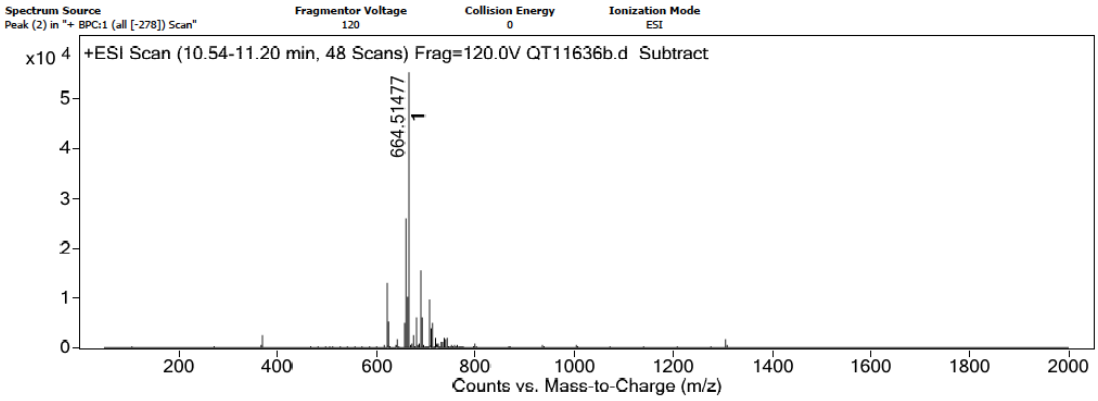
HRMS spectrum of B-C12



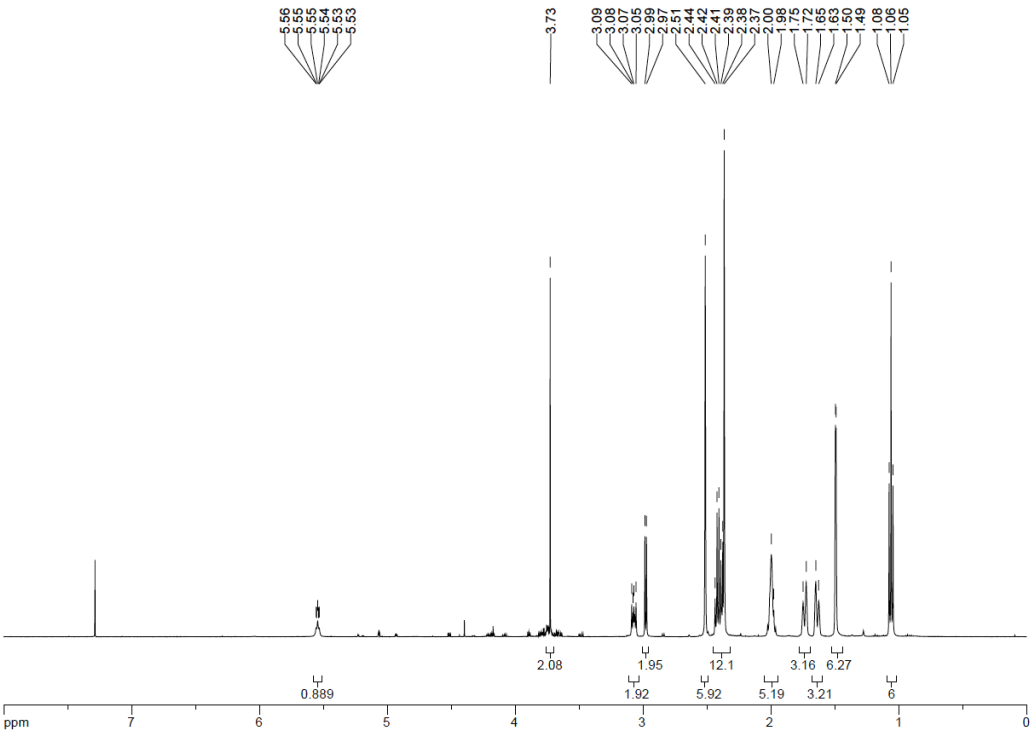
1H spectrum of B-C18



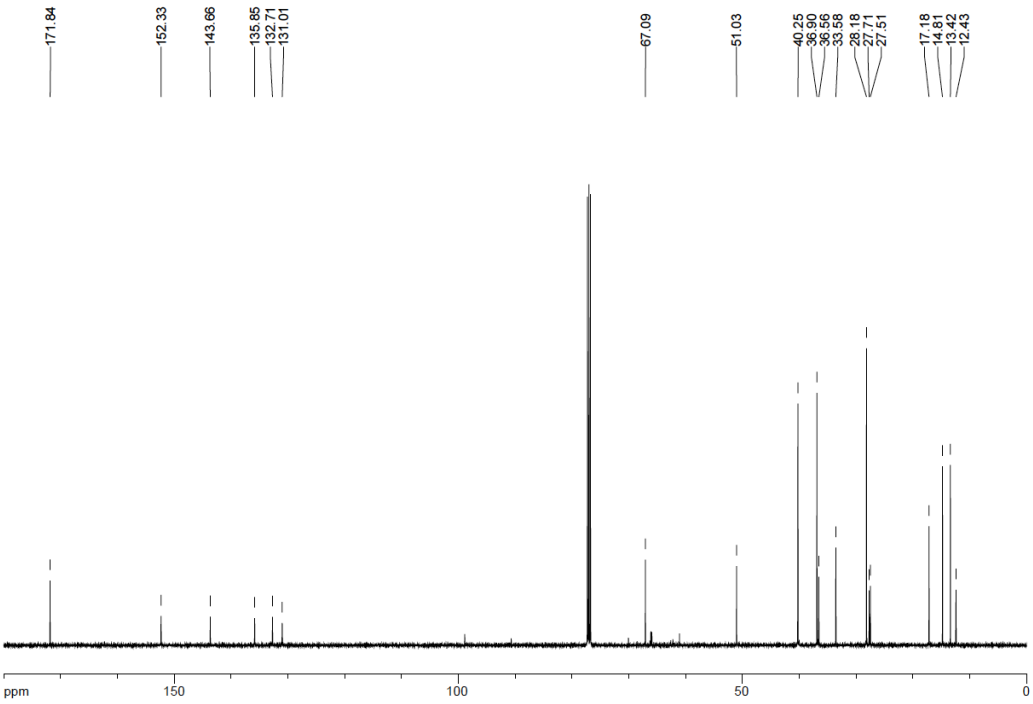
13C spectrum of B-C18



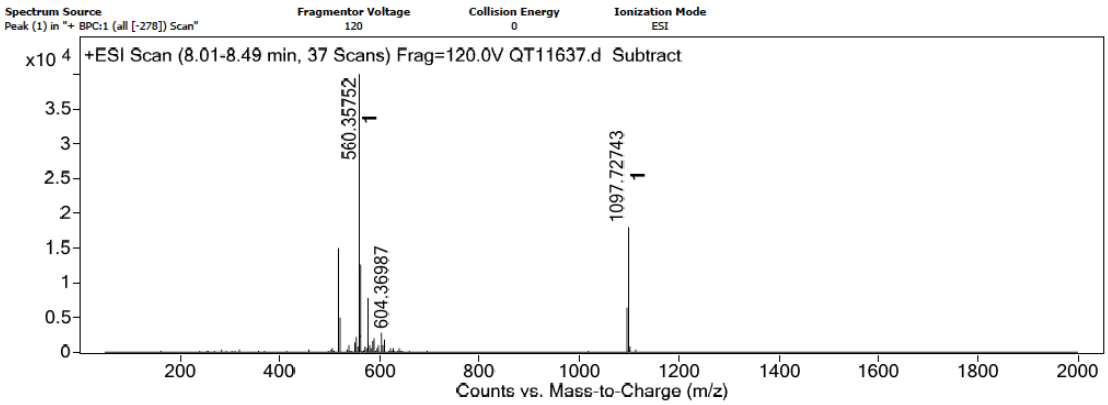
HRMS spectrum of B-C18



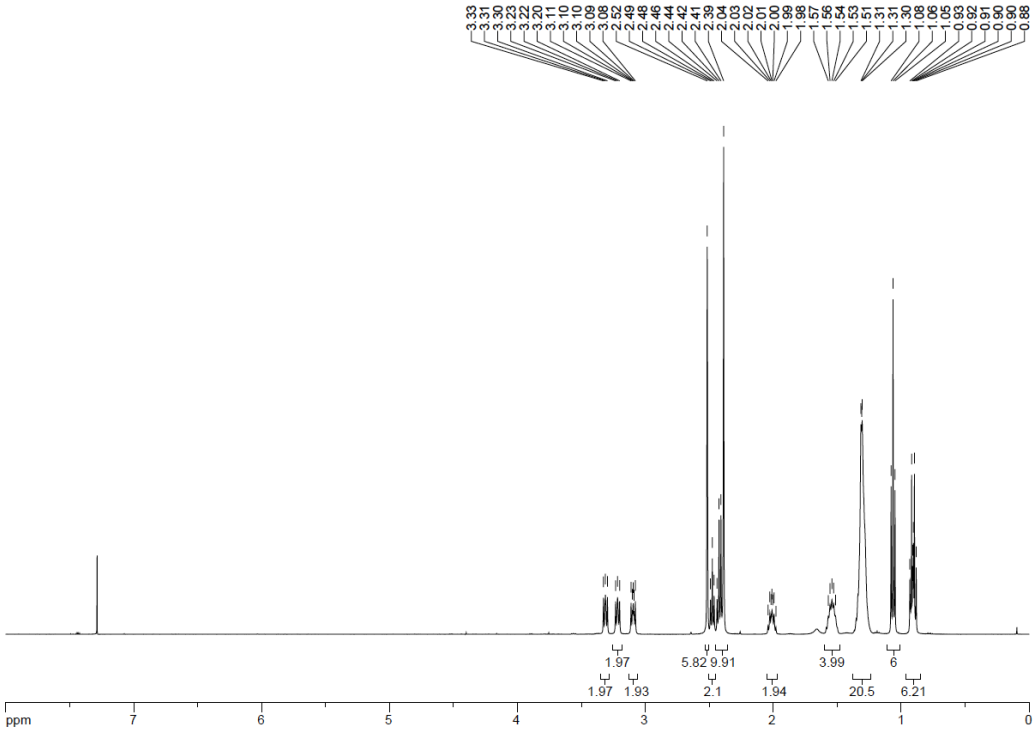
1H spectrum of B-Ad



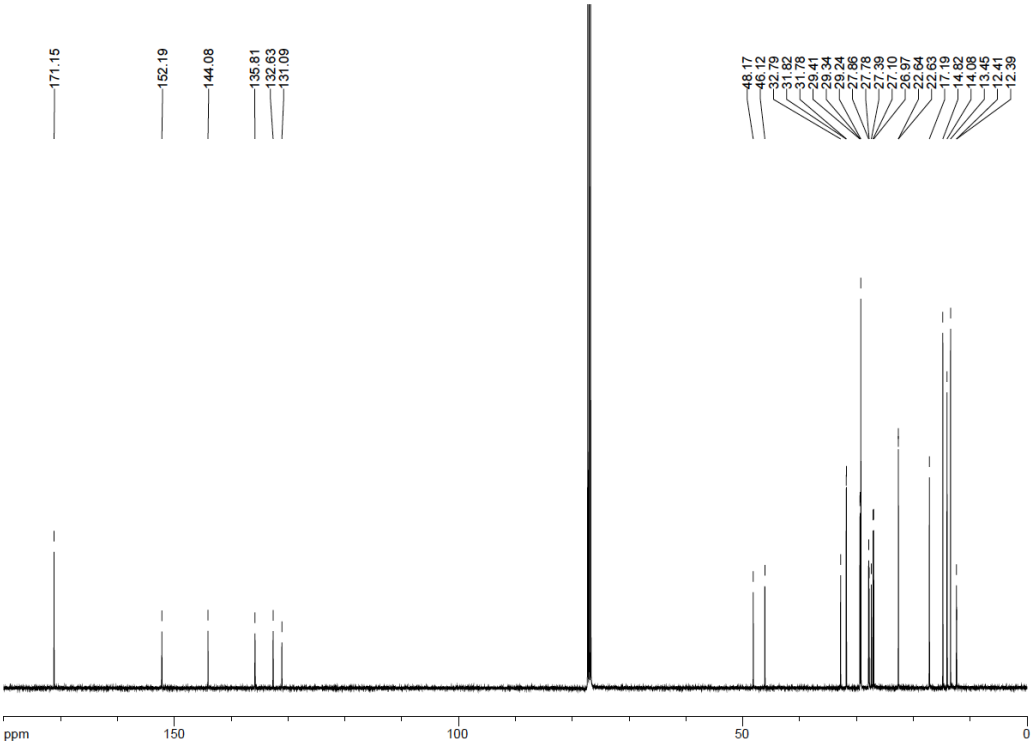
13C spectrum of B-Ad



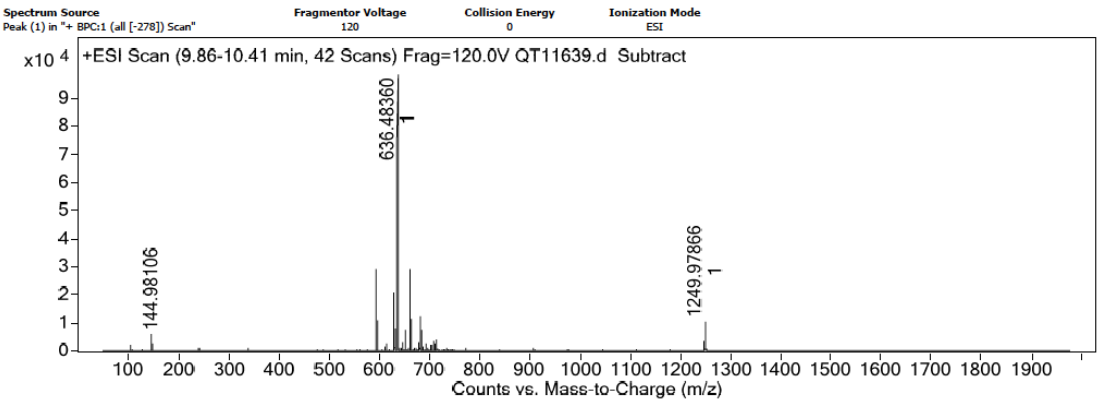
HRMS spectrum of B-Ad



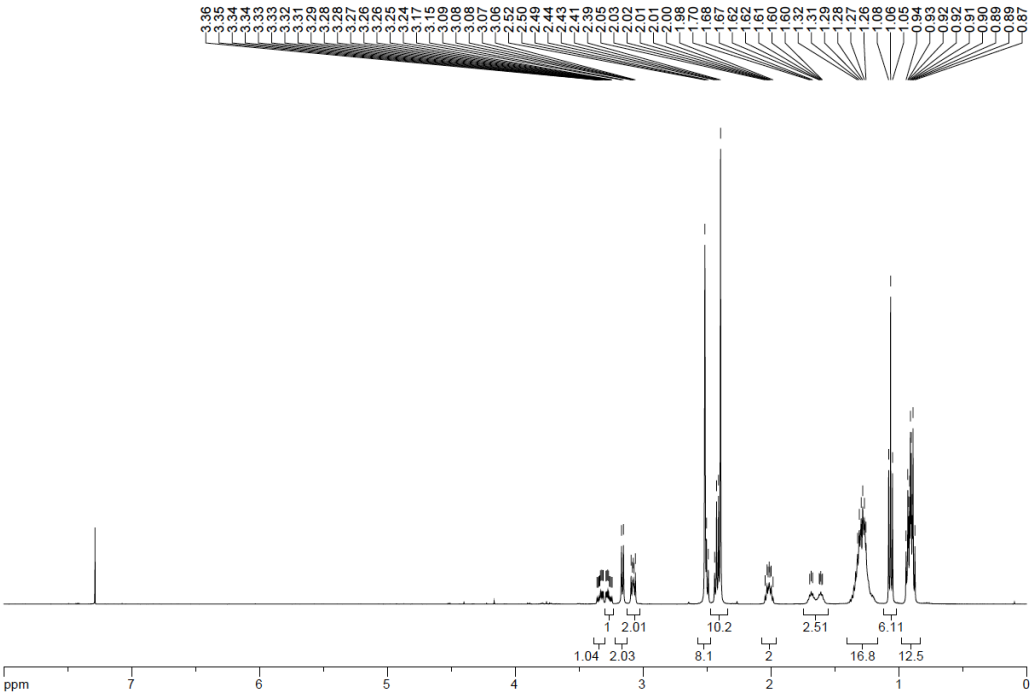
1H spectrum of B-2C8



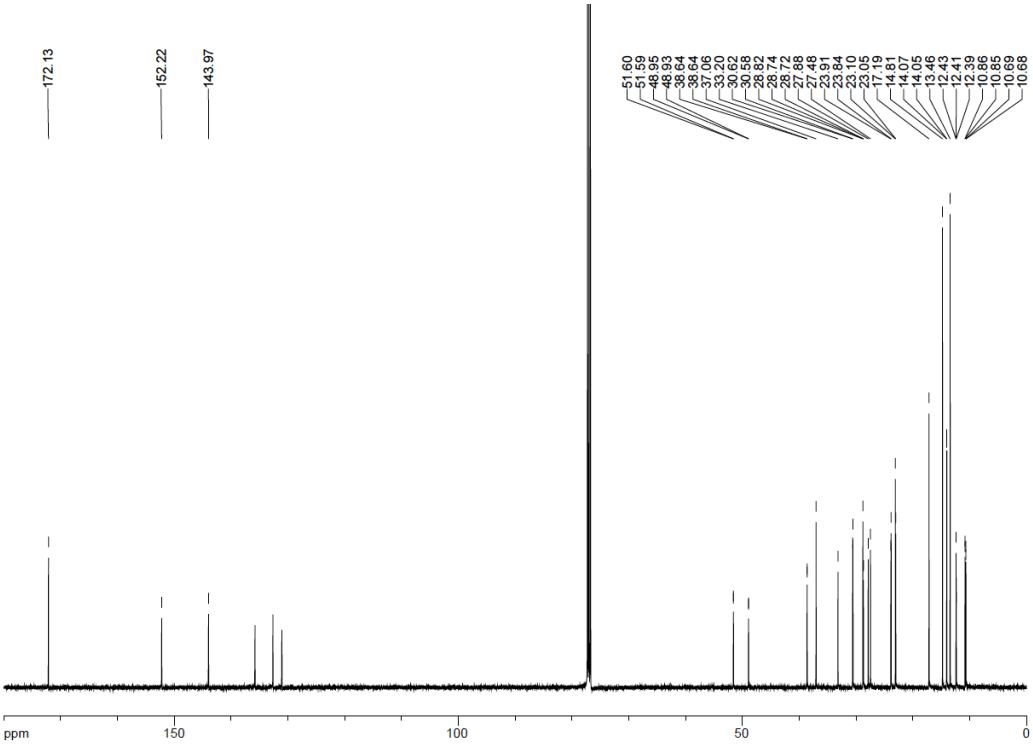
13C spectrum of B-2C8



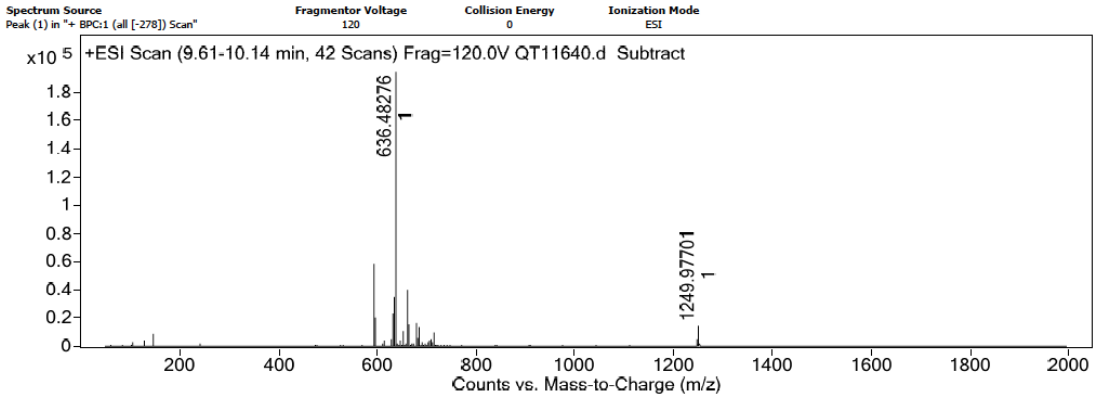
HRMS spectrum of B-2C8



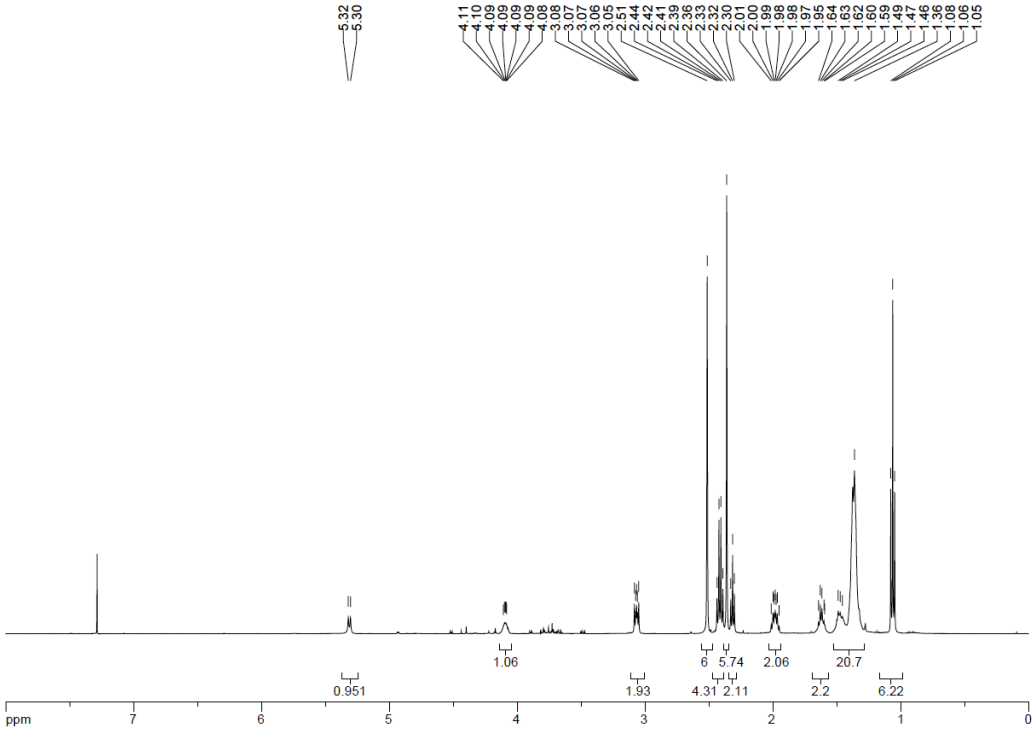
1H spectrum of B-b2C8



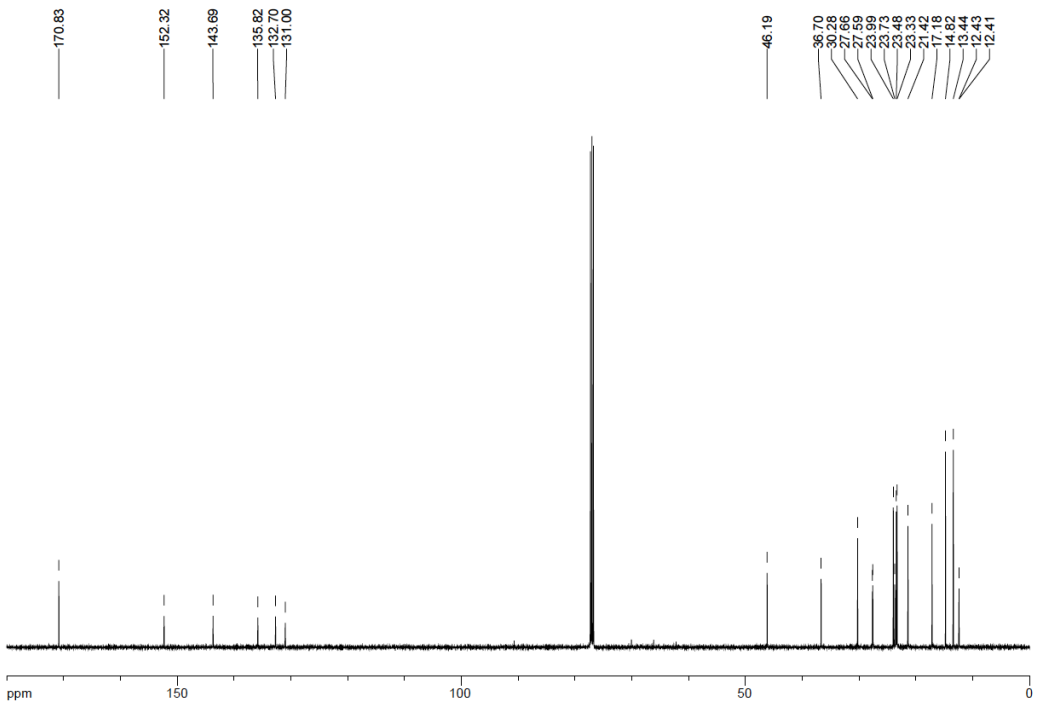
13C spectrum of B-b2C8



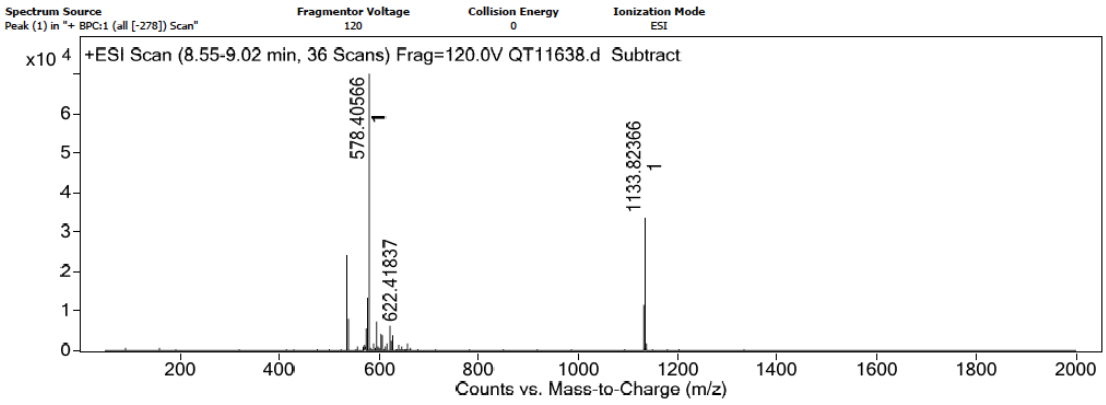
HRMS spectrum of B-b2C8



1H spectrum of B-cC12



13C spectrum of B-cC12



HRMS spectrum of B-cC12

Spectroscopic studies

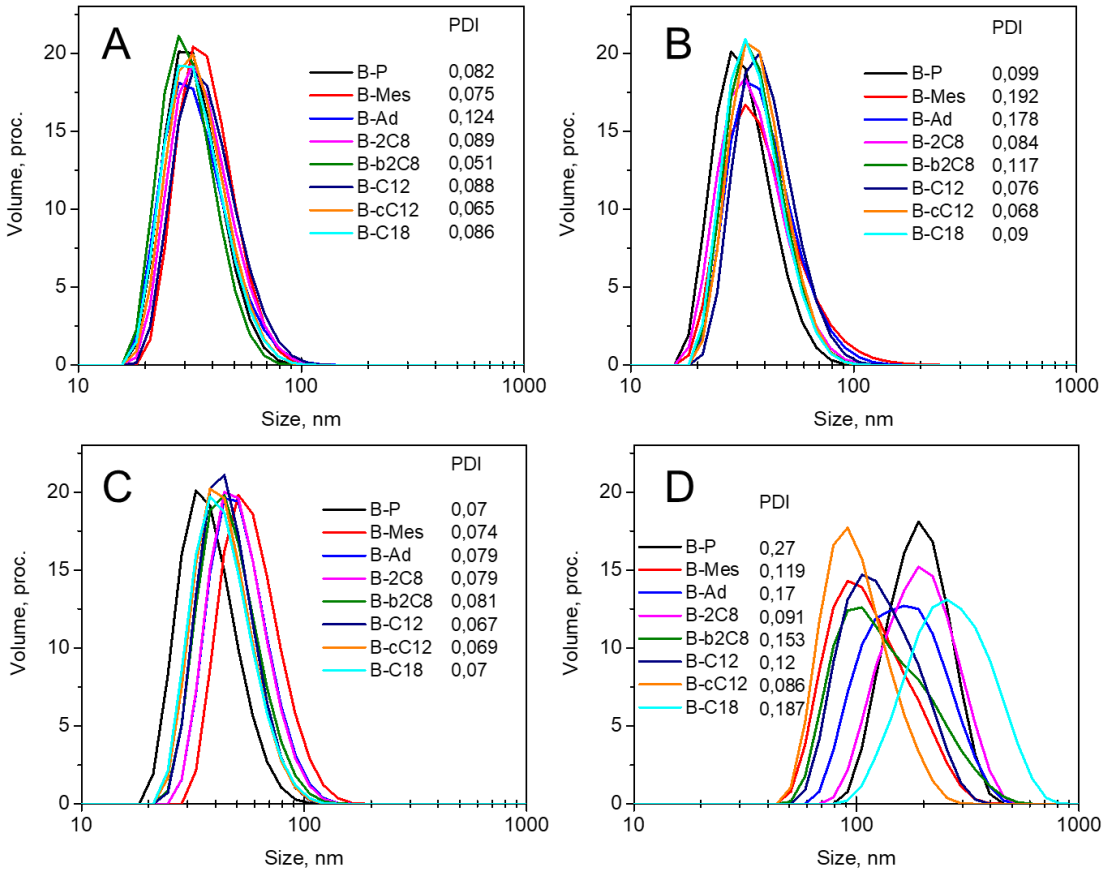


Figure S1. Volume size distribution of BODIPY PLGA NPs at different dye loadings measured by DLS: A -20 mM, B-100 mM, C-200 mM. D – Volume size distribution of BODIPY aggregates without polymer obtained in the same way as NPs solutions, using concentration corresponding to 100 mM loading.

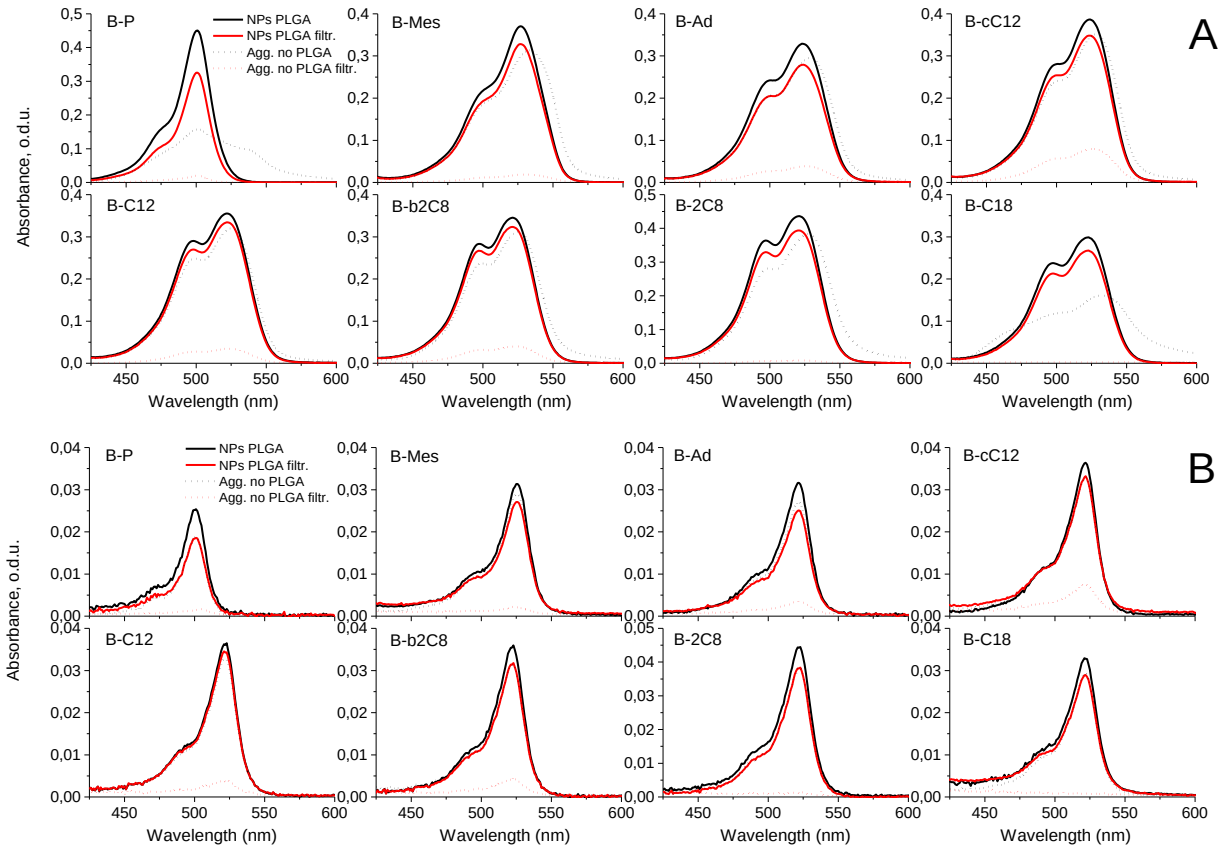


Figure S2. Absorption spectra of PLGA NPs loaded with different BODIPY dyes (200 mM loading) before (solid black line) and after filtration through PTFE filter (pore size 200 nm) (solid red line) in phosphate buffer (A) and diluted (20x) in dioxane (B). Absorption spectra before (back dots) and after filtration (red dots) of BODIPY aggregates without PLGA, obtained by the same nanoprecipitation protocol, are shown for comparison in buffer (A) and diluted (20x) in dioxane (B).

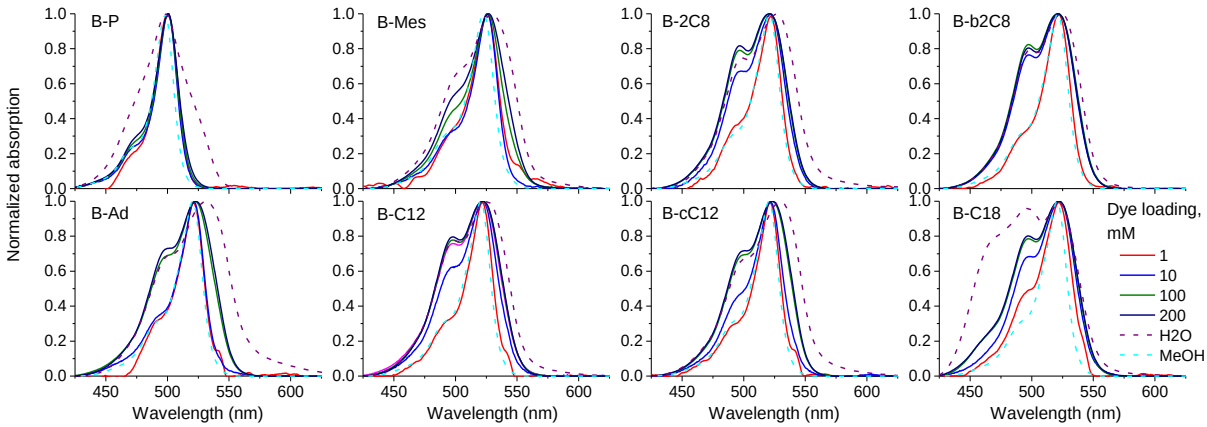


Figure S3. Normalized absorption spectra of PLGA NPs loaded with different BODIPY dyes.

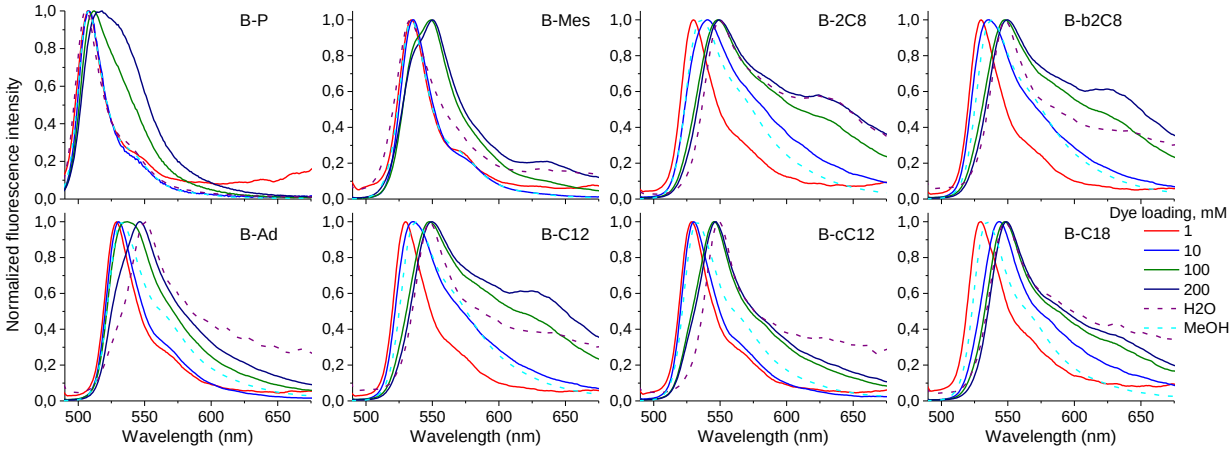
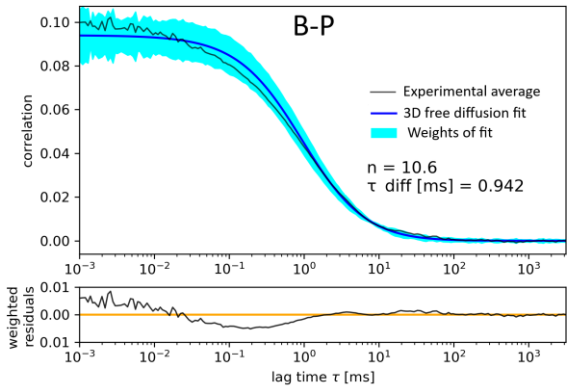
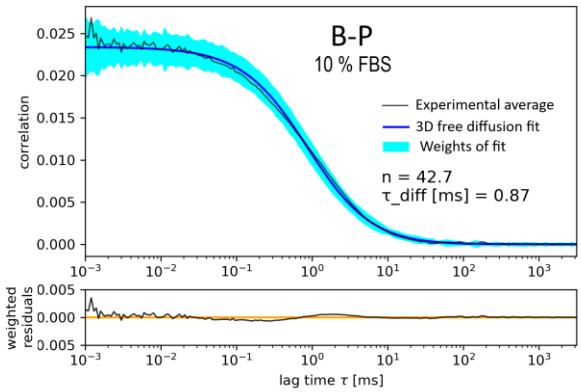
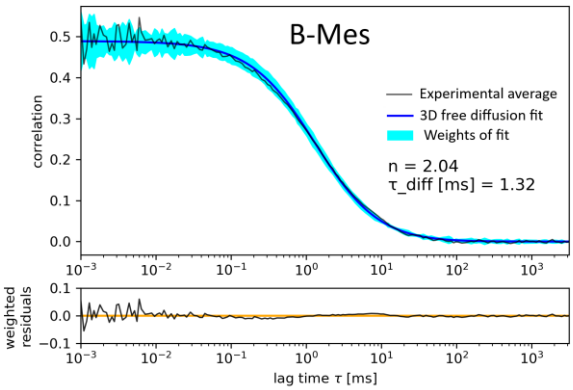
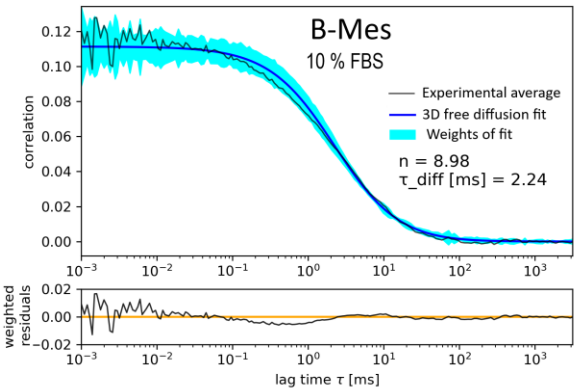


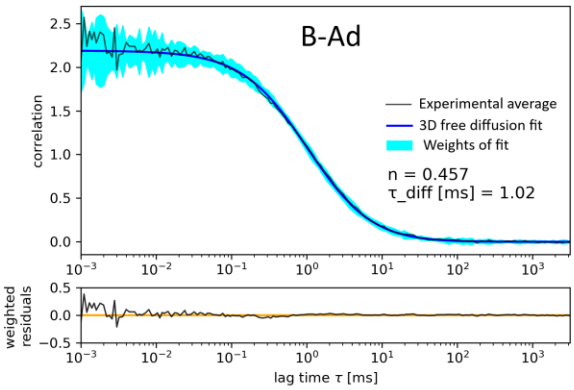
Figure S4. Normalized emission spectra of PLGA NPs loaded with different BODIPY dyes.

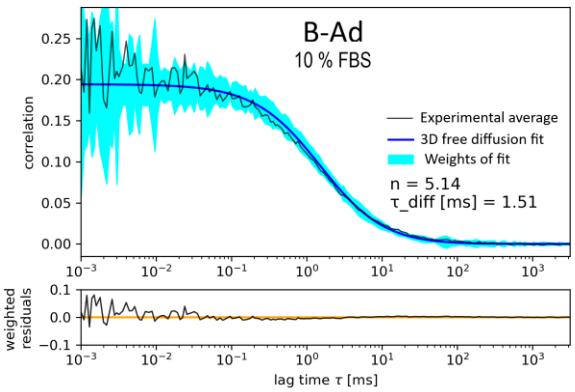

B-P
Experimental average
3D free diffusion fit
Weights of fit
n = 10.6
τ diff [ms] = 0.942
correlation
weighted residuals
lag time τ [ms]

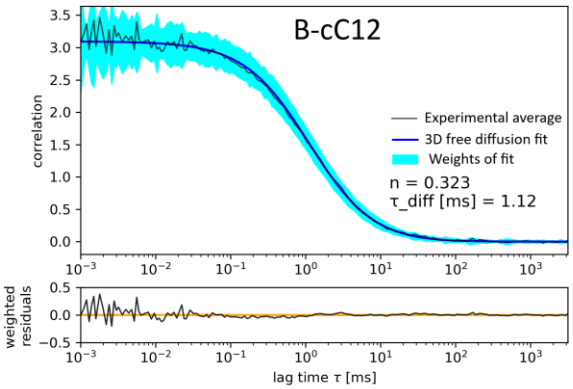

B-P
10 % FBS
Experimental average
3D free diffusion fit
Weights of fit
n = 42.7
τ_diff [ms] = 0.87
correlation
weighted residuals
lag time τ [ms]

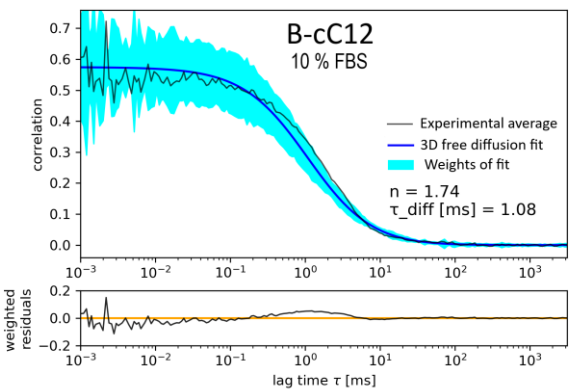

B-Mes
Experimental average
3D free diffusion fit
Weights of fit
n = 2.04
τ_diff [ms] = 1.32
correlation
weighted residuals
lag time τ [ms]


B-Mes
10 % FBS
Experimental average
3D free diffusion fit
Weights of fit
n = 8.98
τ_diff [ms] = 2.24
correlation
weighted residuals
lag time τ [ms]


B-Ad
Experimental average
3D free diffusion fit
Weights of fit
n = 0.457
τ_diff [ms] = 1.02
correlation
weighted residuals
lag time τ [ms]


B-Ad
10 % FBS
Experimental average
3D free diffusion fit
Weights of fit
n = 5.14
τ_diff [ms] = 1.51
correlation
weighted residuals
lag time τ [ms]


B-cC12
Experimental average
3D free diffusion fit
Weights of fit
n = 0.323
τ_diff [ms] = 1.12
correlation
weighted residuals
lag time τ [ms]


B-cC12
10 % FBS
Experimental average
3D free diffusion fit
Weights of fit
n = 1.74
τ_diff [ms] = 1.08
correlation
weighted residuals
lag time τ [ms]

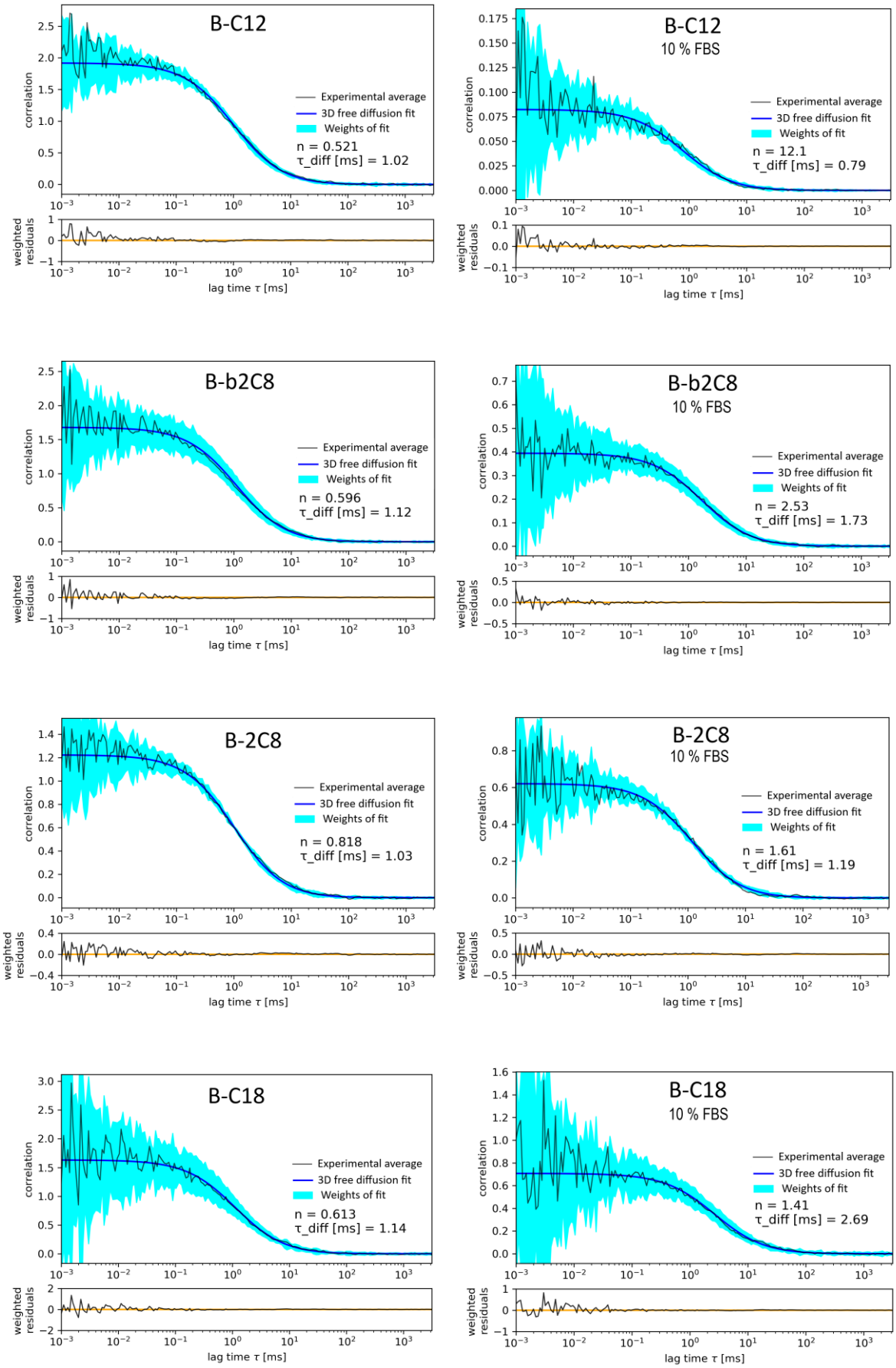
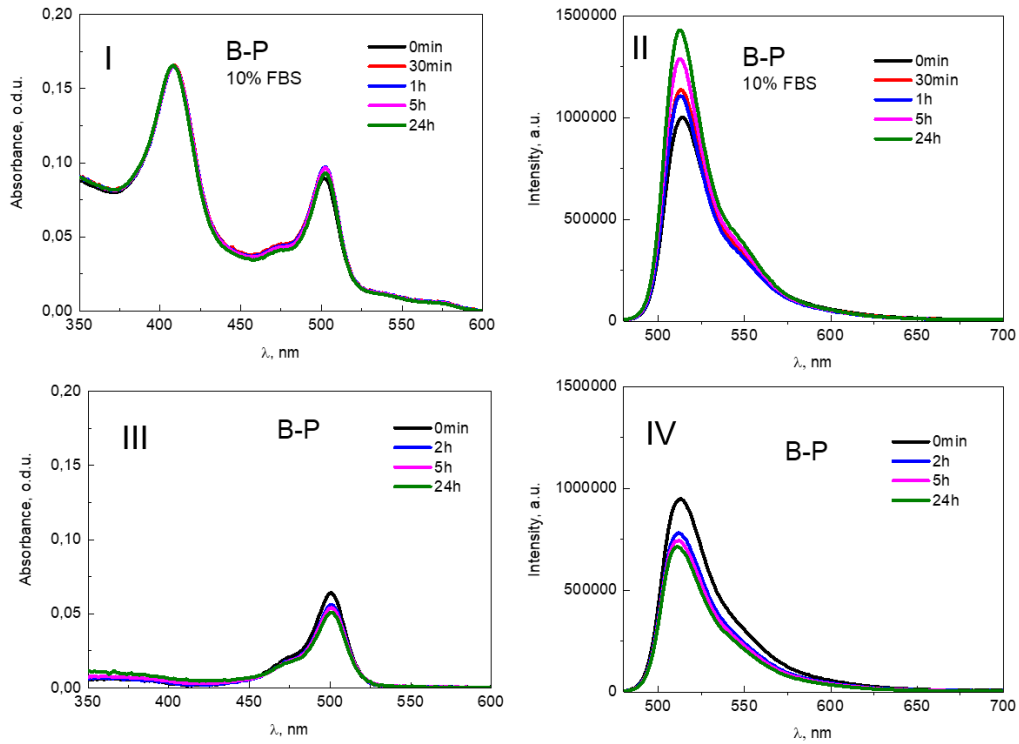
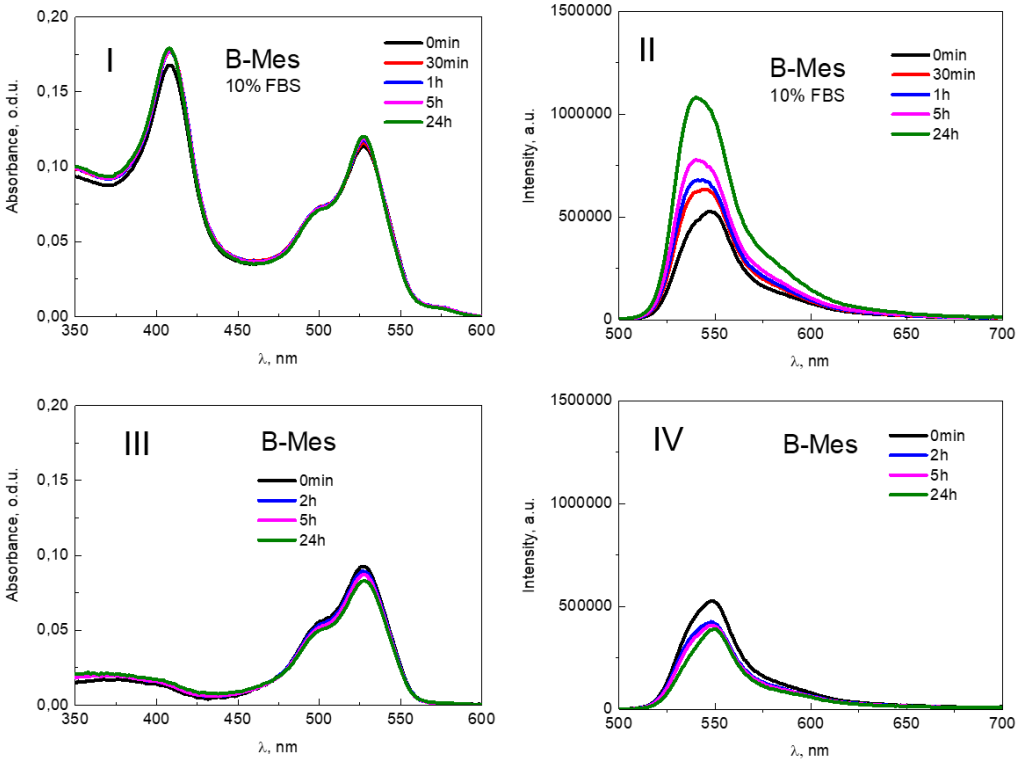


Figure S5. Fluorescence autocorrelation curves (experimental average of 10 measurements and theoretical fit using three-dimensional free diffusion model), plot of weighted residuals of different BODIPY PLGA NPs without FBS (left column) and in the presence of 10% FBS (right column).

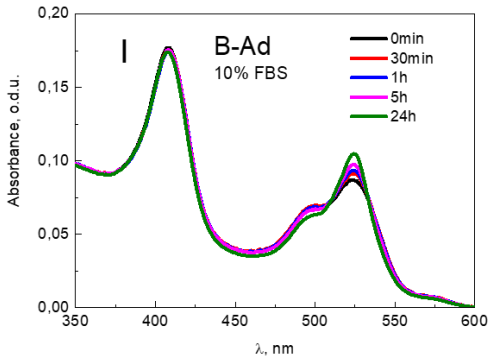
A

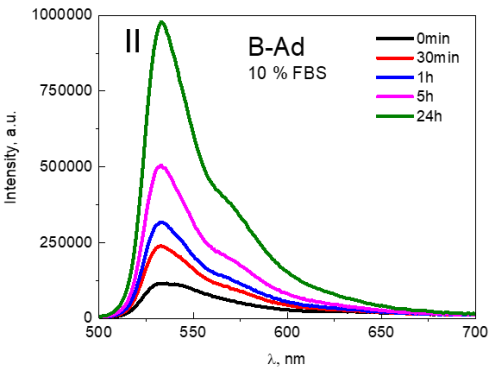

I
B-P
10% FBS
0min
30min
1h
5h
24h
Absorbance, o.d.u.
λ, nm
II
B-P
10% FBS
0min
30min
1h
5h
24h
Intensity, a.u.
λ, nm
III
B-P
0min
2h
5h
24h
Absorbance, o.d.u.
λ, nm
IV
B-P
0min
2h
5h
24h
Intensity, a.u.
λ, nm

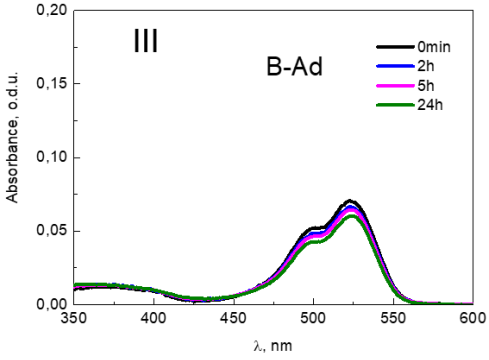
B

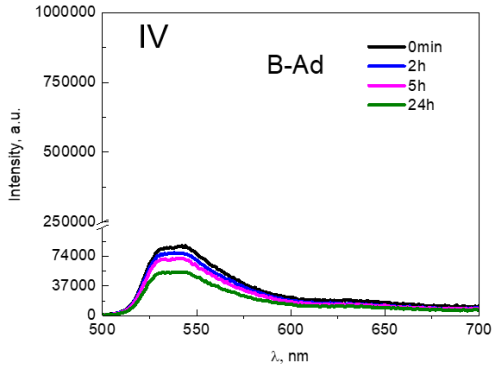

I
B-Mes
10% FBS
0min
30min
1h
5h
24h
Absorbance, o.d.u.
λ, nm
II
B-Mes
10% FBS
0min
30min
1h
5h
24h
Intensity, a.u.
λ, nm
III
B-Mes
0min
2h
5h
24h
Absorbance, o.d.u.
λ, nm
IV
B-Mes
0min
2h
5h
24h
Intensity, a.u.
λ, nm

C

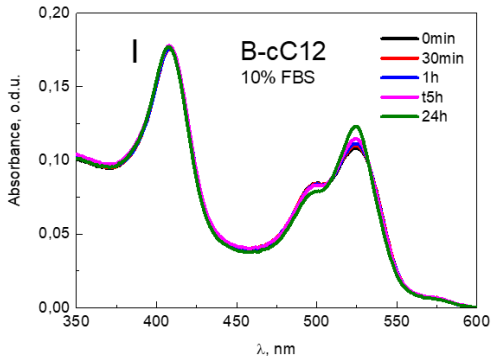

I
B-Ad
10% FBS
0min
30min
1h
5h
24h
Absorbance, o.d.u.
λ, nm

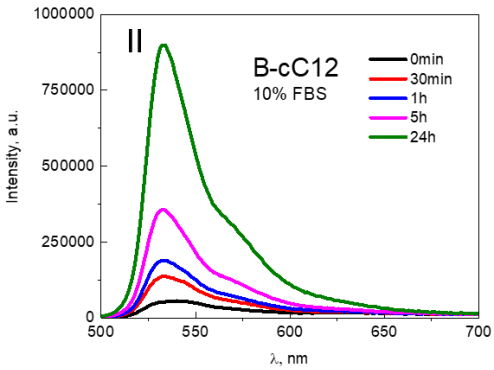

II
B-Ad
10 % FBS
0min
30min
1h
5h
24h
Intensity, a.u.
λ, nm

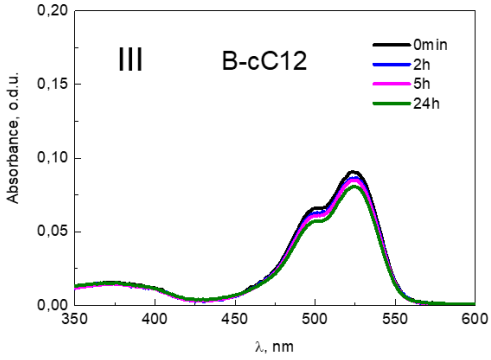

III
B-Ad
0min
2h
5h
24h
Absorbance, o.d.u.
λ, nm

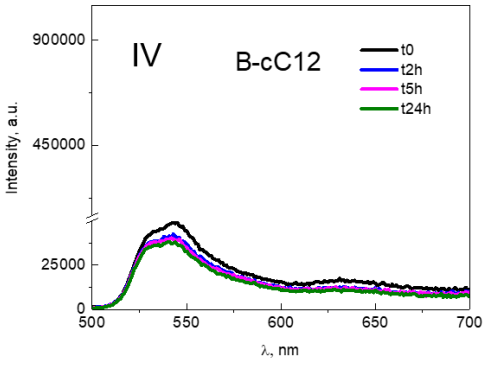

IV
B-Ad
0min
2h
5h
24h
Intensity, a.u.
λ, nm

D

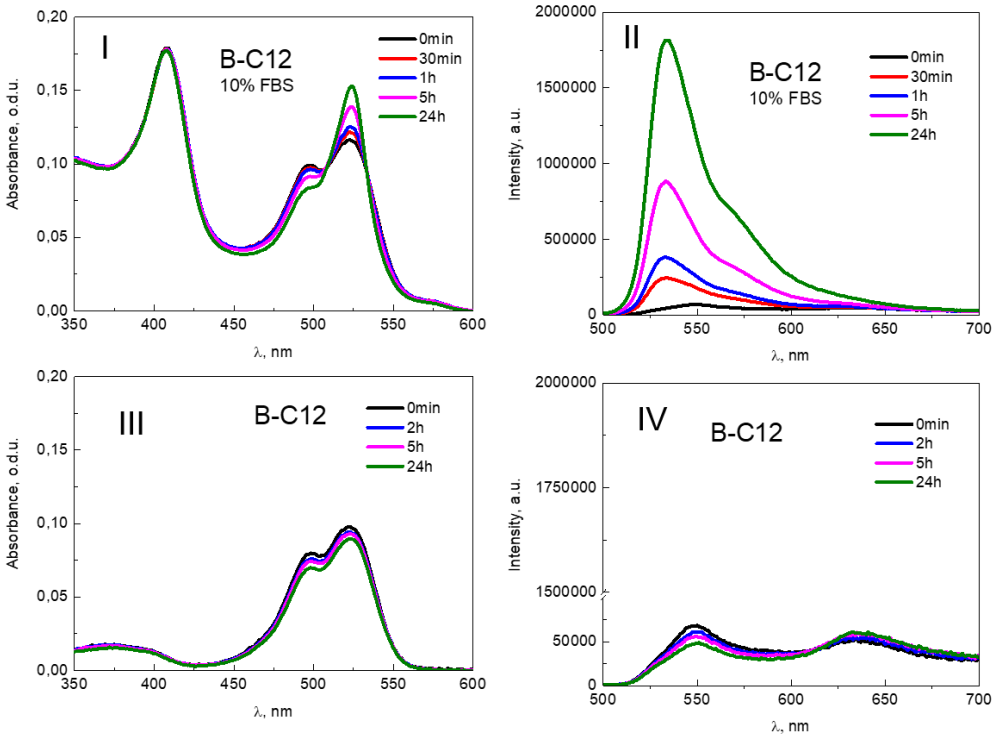

I
B-cC12
10% FBS
0min
30min
1h
t5h
24h
Absorbance, o.d.u.
λ, nm


II
B-cC12
10% FBS
0min
30min
1h
5h
24h
Intensity, a.u.
λ, nm

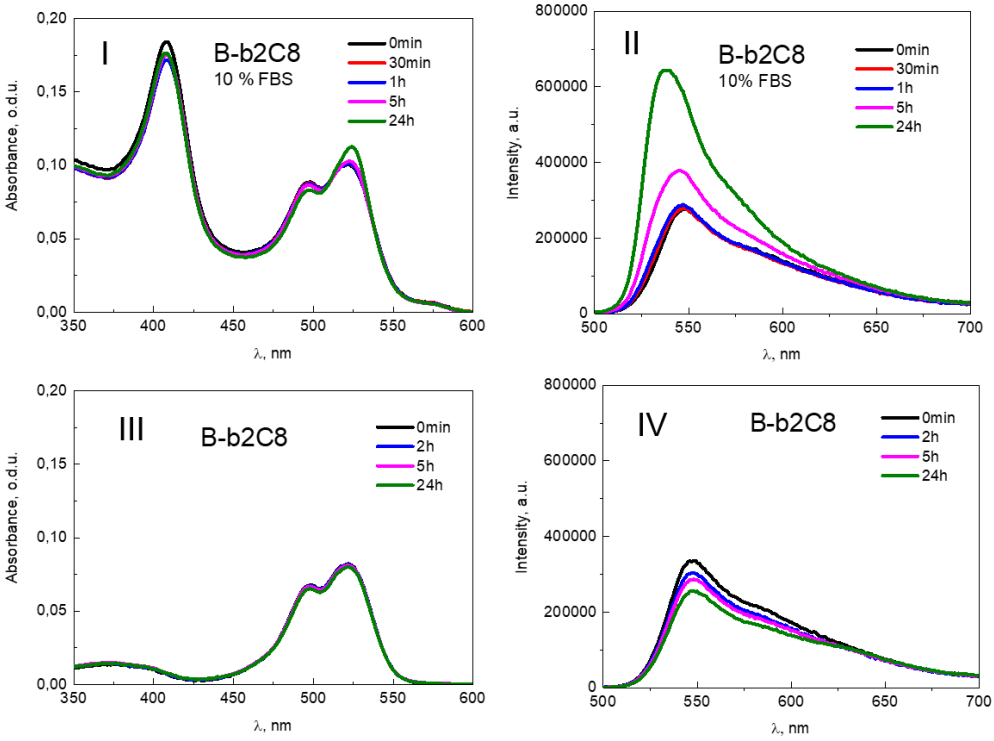

III
B-cC12
0min
2h
5h
24h
Absorbance, o.d.u.
λ, nm


IV
B-cC12
t0
t2h
t5h
t24h
Intensity, a.u.
λ, nm

E


I
B-C12
10% FBS
0min
30min
1h
5h
24h
Absorbance, o.d.u.
λ, nm
II
B-C12
10% FBS
Intensity, a.u.
III
B-C12
2h
IV
B-C12

F


I
B-b2C8
10 % FBS
0min
30min
1h
5h
24h
Absorbance, o.d.u.
λ, nm
II
B-b2C8
10% FBS
Intensity, a.u.
III
B-b2C8
2h
IV

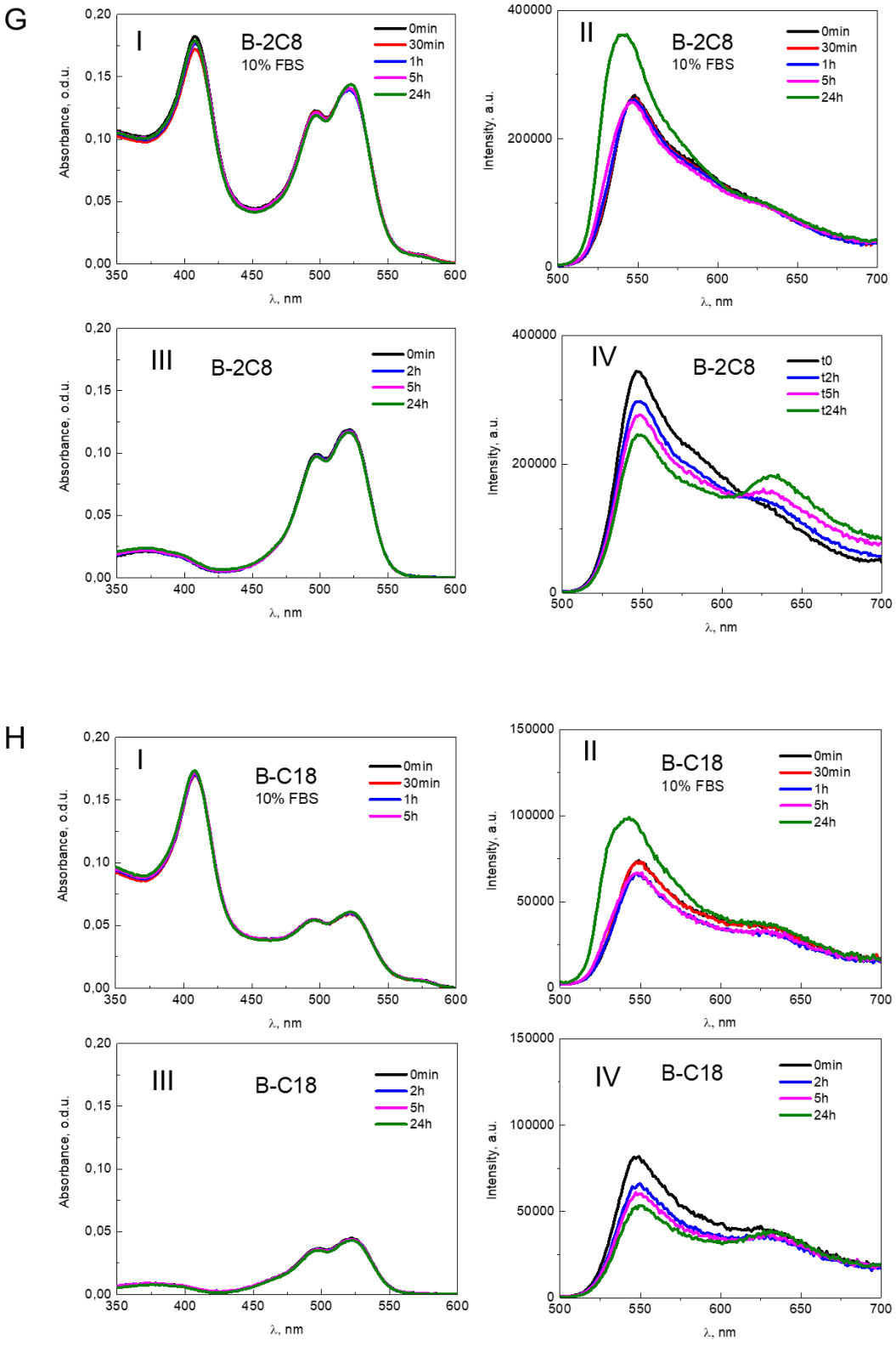


Figure S6. Time changes in absorption and emission spectra of BODIPY PLGA NPs (B-P (A) B-Mes (B), B-Ad (C), B-cC12 (D), B-C12 (E), B-b2C8 (F), B-2C8 (G), B-C18 (H)) (200 mM loading) in the presence of 10% FBS (I, II, respectively) and without FBS (III, IV, respectively). For the emission measurements λ_{ex} at 490 nm was used for all NPs, except for B-P - λ_{ex} =470 nm.