Supporting Information

Facile and scalable design of light-emitting and ROS-generating hybrid materials made of polyurea gels embedding a molybdenum cluster-based salt

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Table S1. Characteristics of the Hydrogen-bonded carbonyl bands in the FTIR Spectra (amide I region) of the polyurea containing different amounts of Mo cluster

Cluster content	H-bond C=O band (*d*)		isocyanurate ring		H-bond C=O band (*d*)		H-bond C=O band (*o*)	
	freq (cm^{-1})	width (cm^{-1})	freq (cm^{-1})	width (cm^{-1})	freq (cm^{-1})	width (cm^{-1})	freq (cm^{-1})	width (cm^{-1})
0 (PUr)	1716	16.7	1689	20.5	1670	35.4	1639	30.4
1 (PUr-1)	1717	20.7	1689	20.3	1673	31.8	1643	34.8
3 (PUr-3)	1717	18.6	1689	20.2	1672	32.5	1643	33.0
5 (PUr-5)	1715	27.5	1689	21.1	1672	33.7	1643	38.4
10 (PUr-10)	1716	18.3	1689	20.5	1670	35.5	1640	29.4

*d = disordered, o = ordered, width = full width measured at half-height

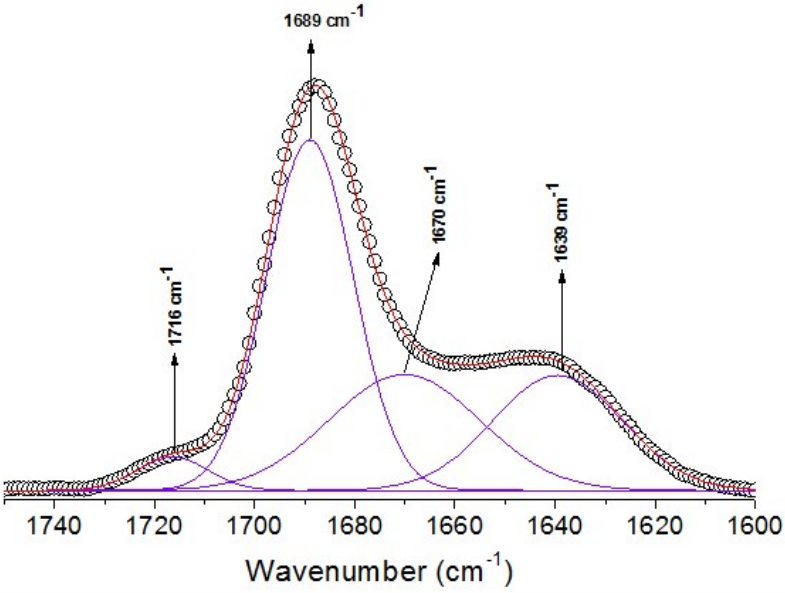

FIGURE S1: FTIR spectra and corresponding Gaussian curve-fits of the amide I region of unloaded polyurea-PUr.

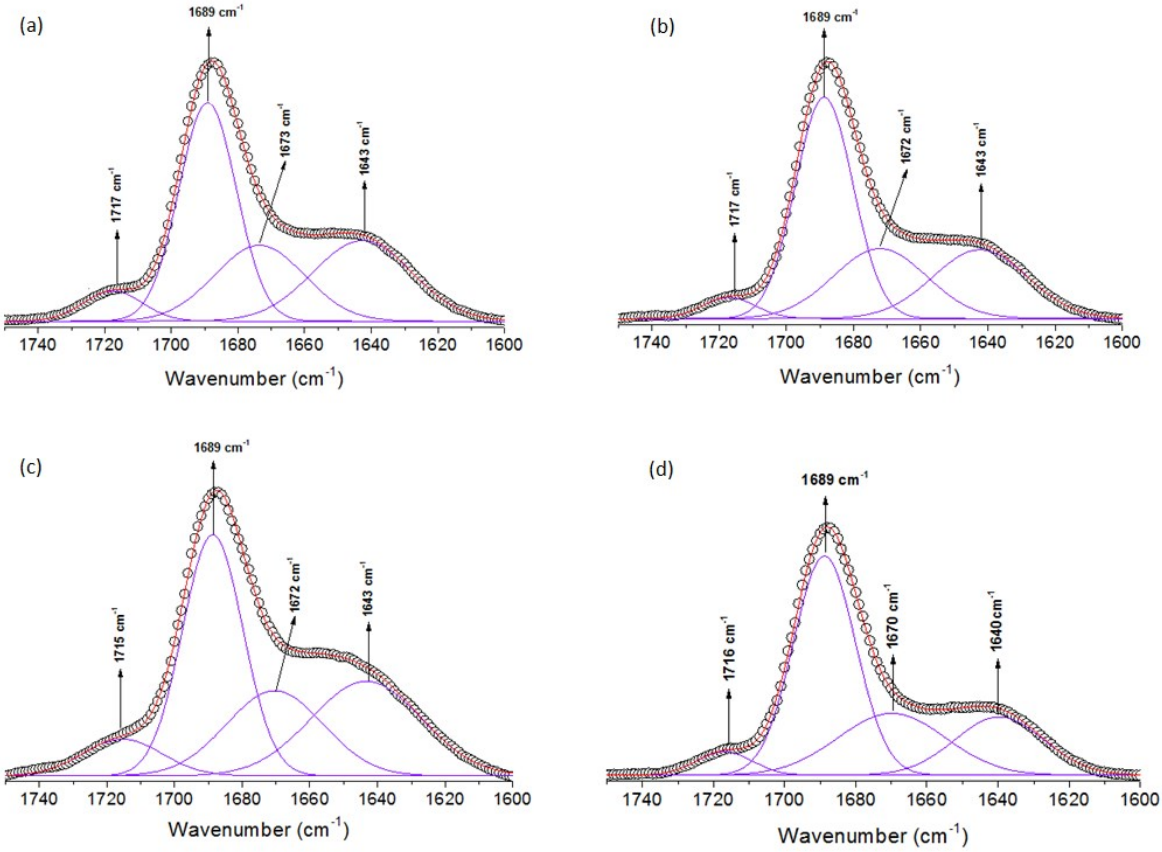

FIGURE S2: FTIR spectra and corresponding Gaussian curve-fits of the amide I region of loaded polyurea containing (a) 1 wt% , (b) 3 wt%, (c) 5 wt%, (d) 10 wt% of Mo cluster respectively..

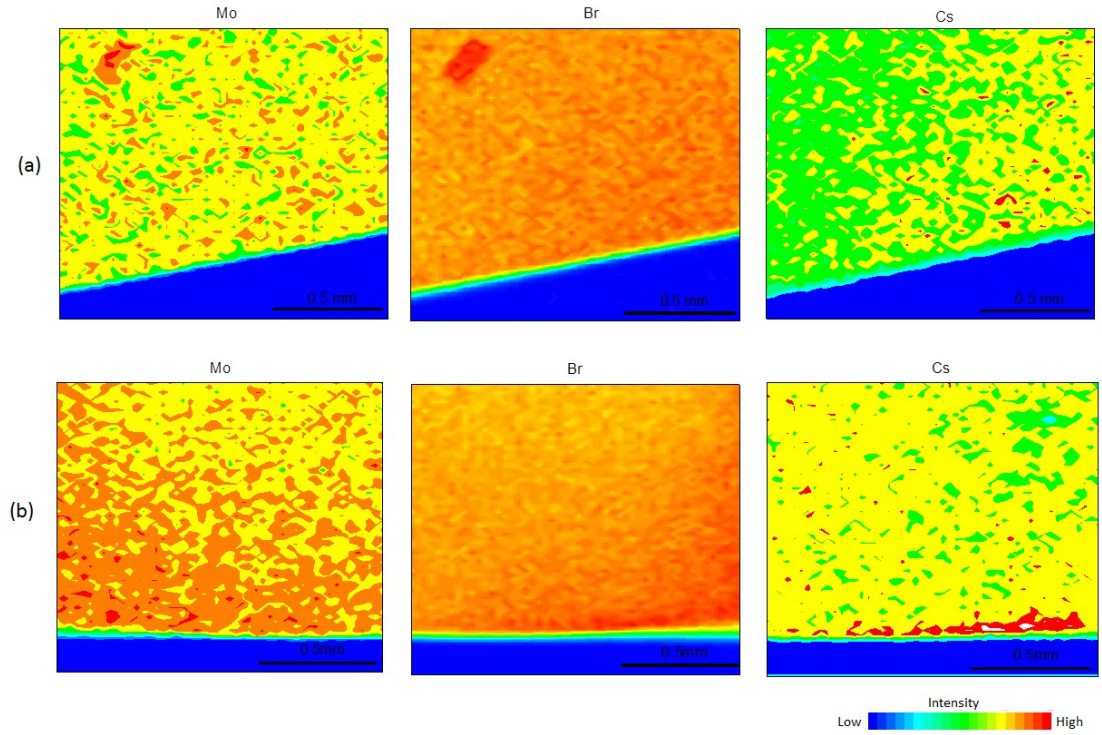

FIGURE S3: Intensity maps of Mo (first column), Br (second column) and Cs (third columm) collected by confocal micro-X-ray fluorescence imaging for loaded PUr membrane containing (a) 3 wt% and (b) 5 wt% of $Cs_2Mo_6Br_{14}$ cluster.

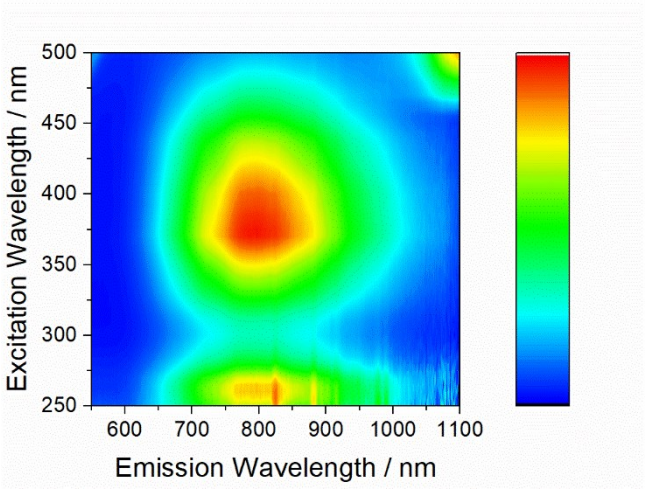

Figure S4. Emission *vs* excitation map of PUr-1

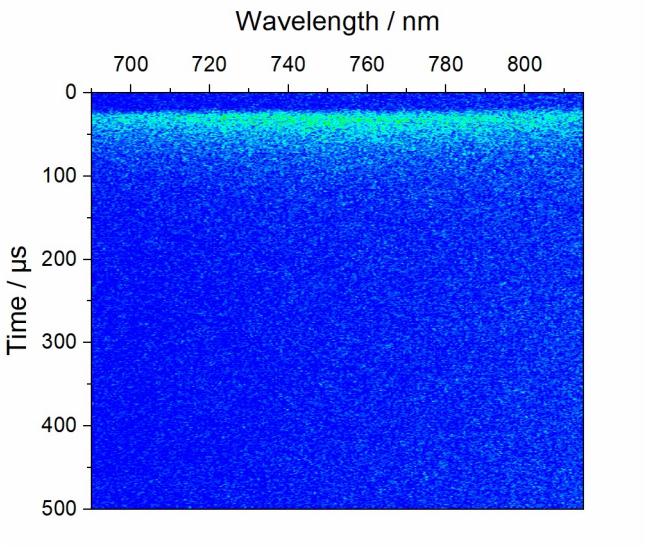

Figure S5. Emission decay map recorded at λ_{exc} = 375 nm for PUr-1.

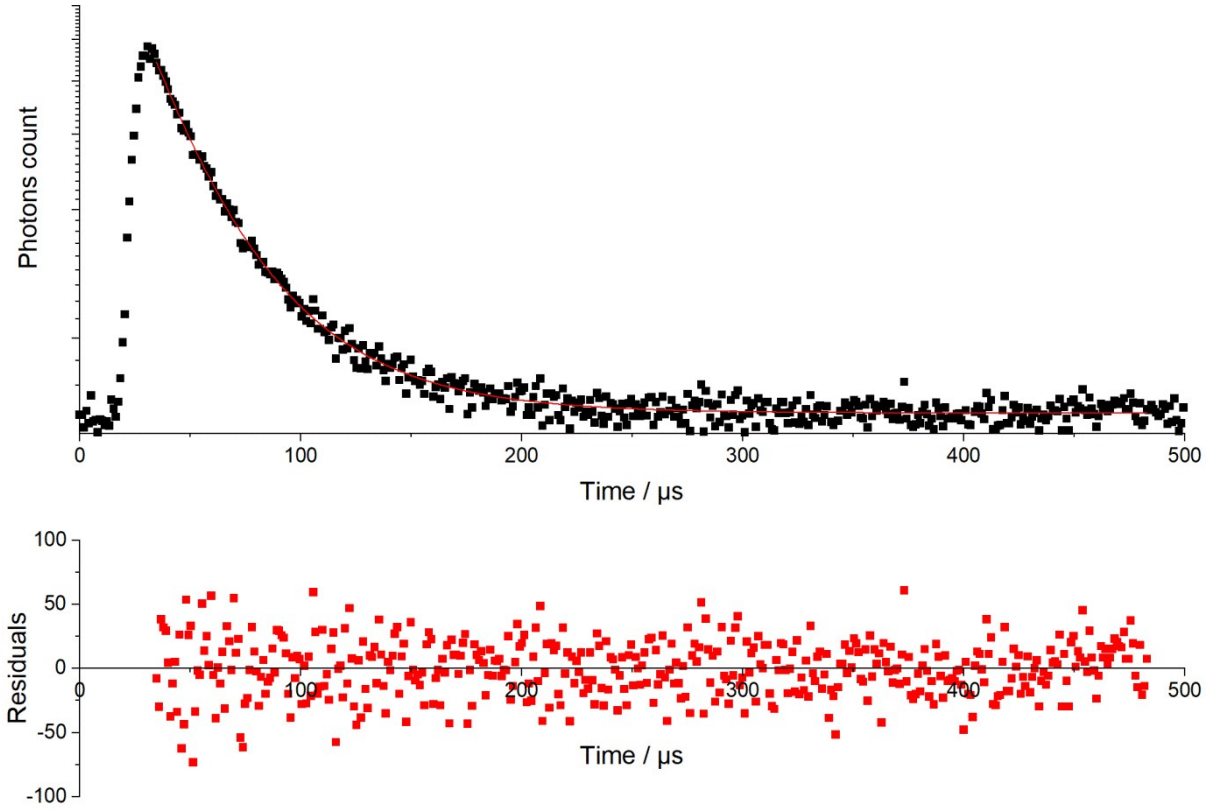

Figure S6. Integrated emission decay profile recorded for PUr-1 (λ_{exc} =375 nm) and residual plot of the calculated fit.

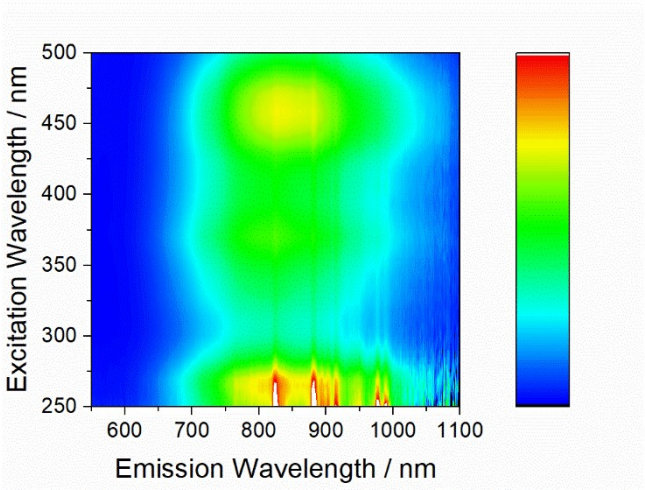

Figure S7. Emission *vs* excitation map of PUr-3.

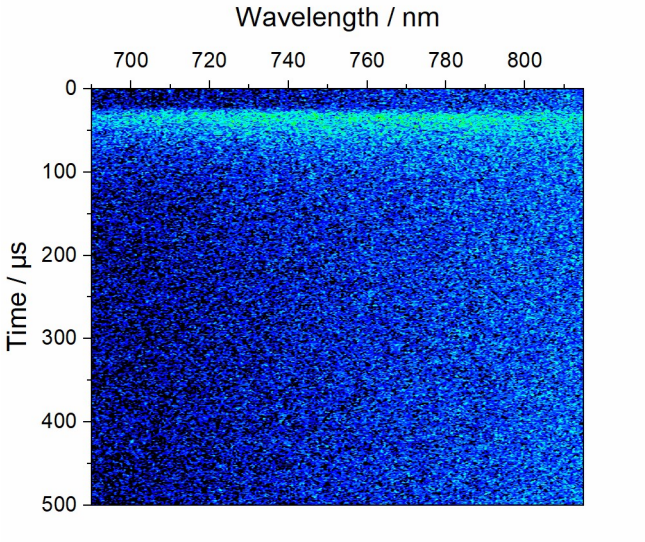

Figure S8. Emission decay map recorded at λ_{exc} = 375 nm for PUr-3.

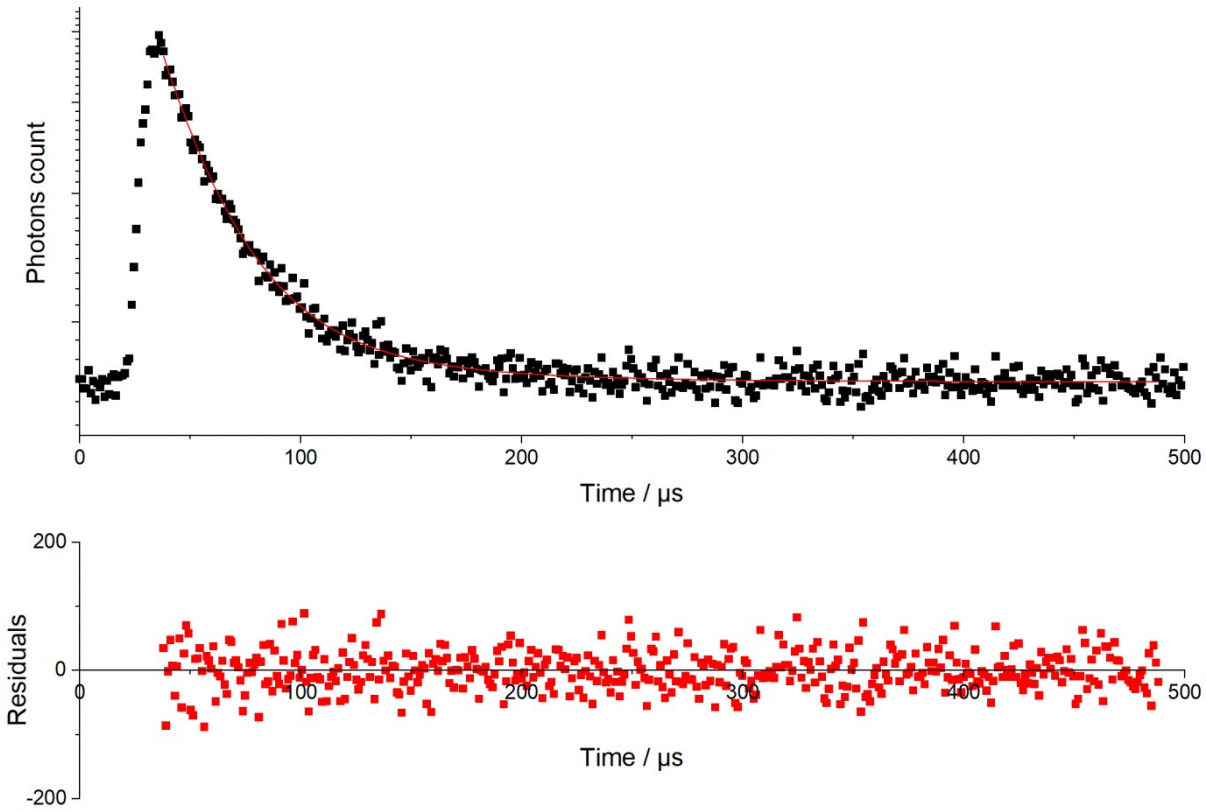

Figure S9. Integrated emission decay profile recorded for PUr-3 (λ_{exc} =375 nm) and residual plot of the calculated fit.

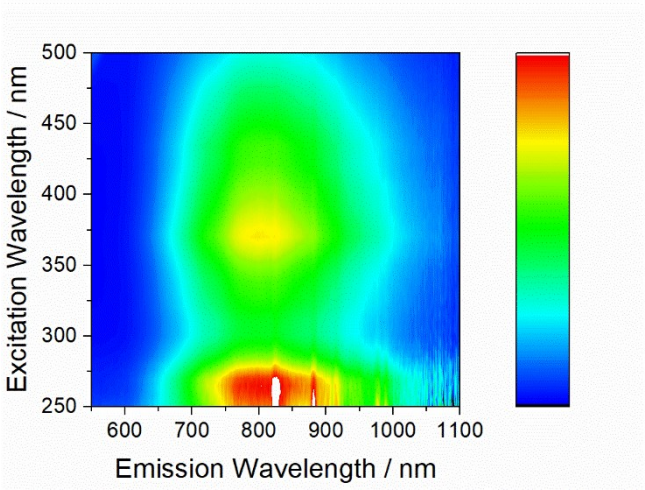

Figure S10. Emission *vs* excitation map of PUr-5.

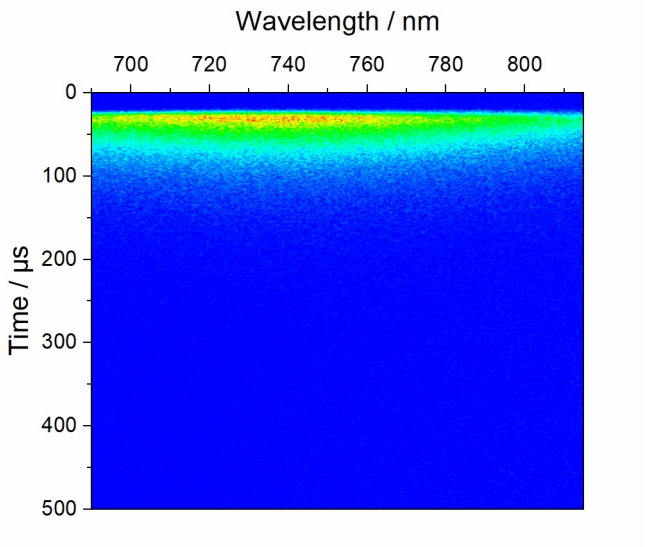

Figure S11. Emission decay map recorded at λ_{exc} = 375 nm for PUr-5.

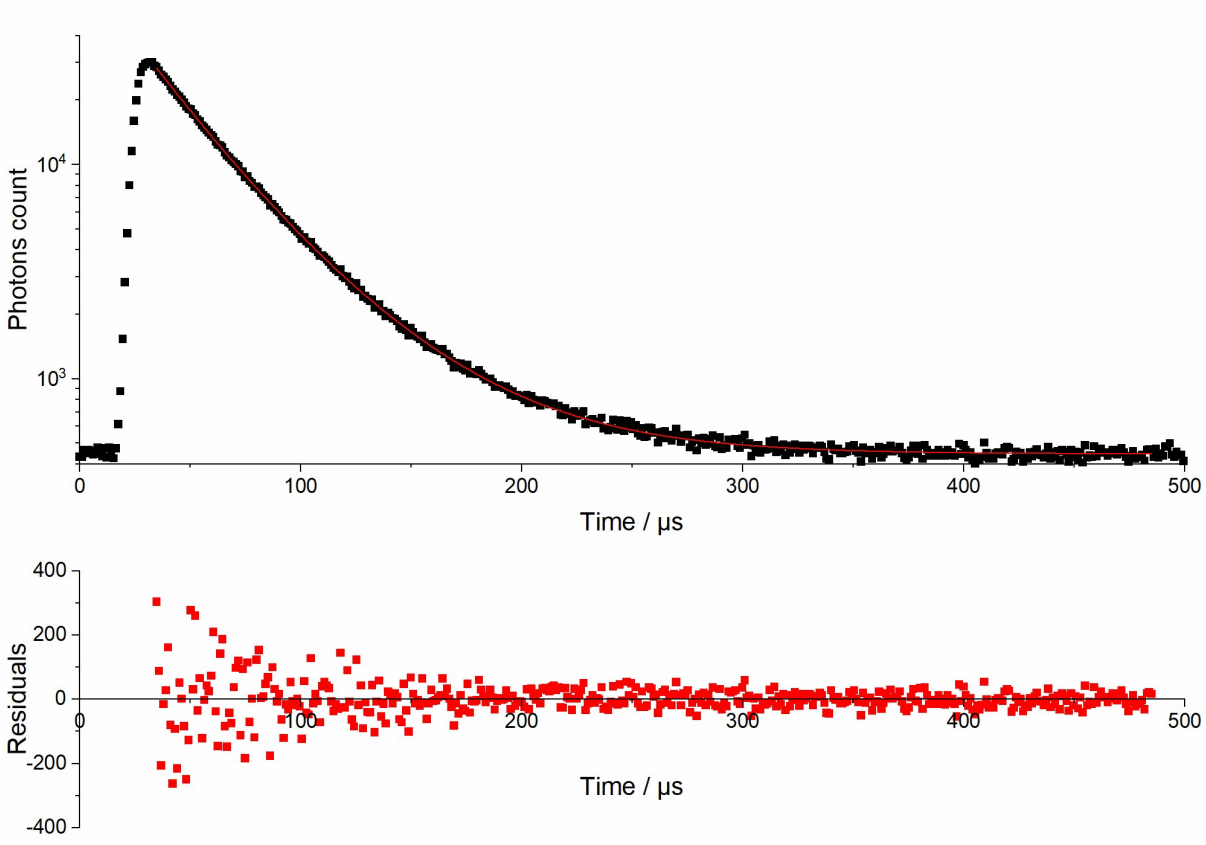

Figure S12. Integrated emission decay profile recorded for PUr-5 (λ_{exc} =375 nm) and residual plot of the calculated fit.

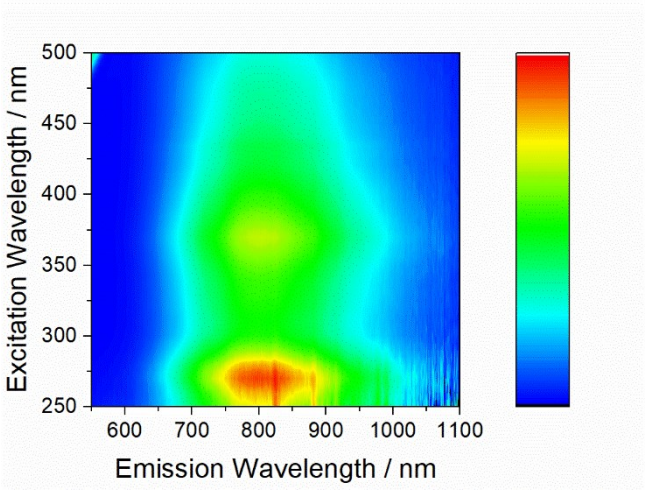

Figure S13. Emission *vs* excitation map of PUr-10.

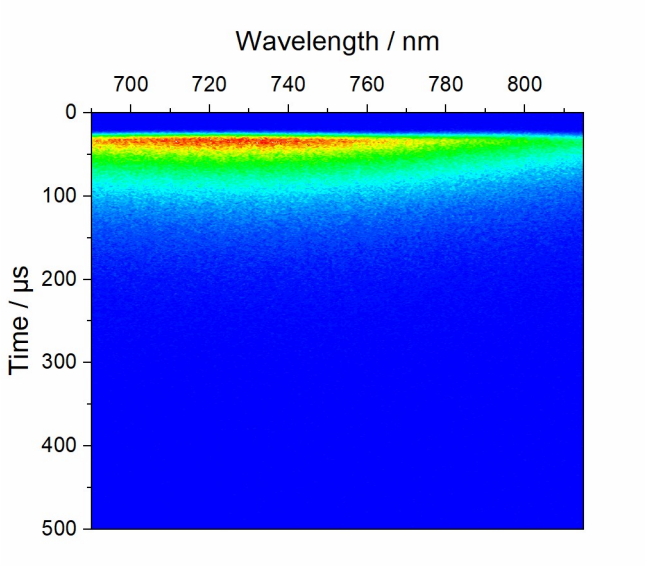

Figure S14. Emission decay map recorded at λ_{exc} = 375 nm for PUr-10.

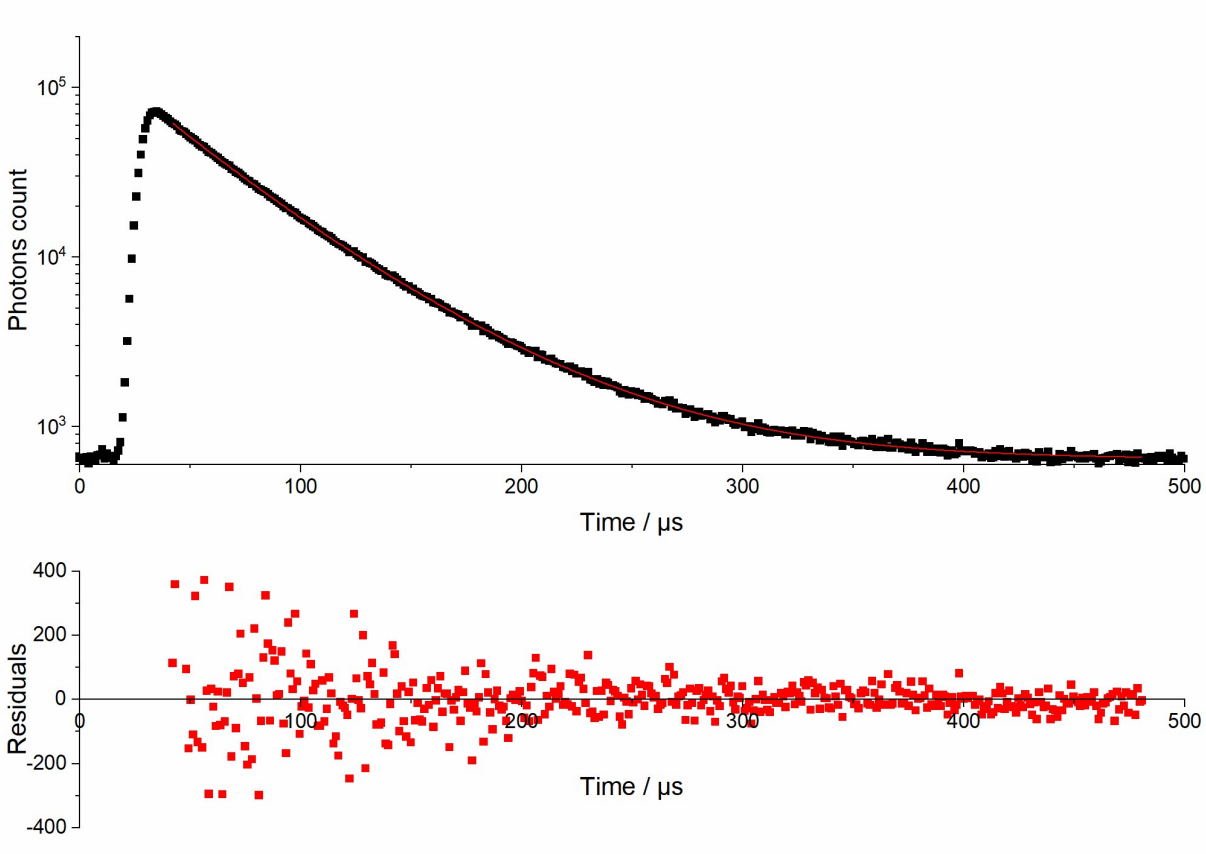

Figure S15. Integrated emission decay profile recorded for PUr-10 (λ_{exc} =375 nm) and residual plot of the calculated fit.

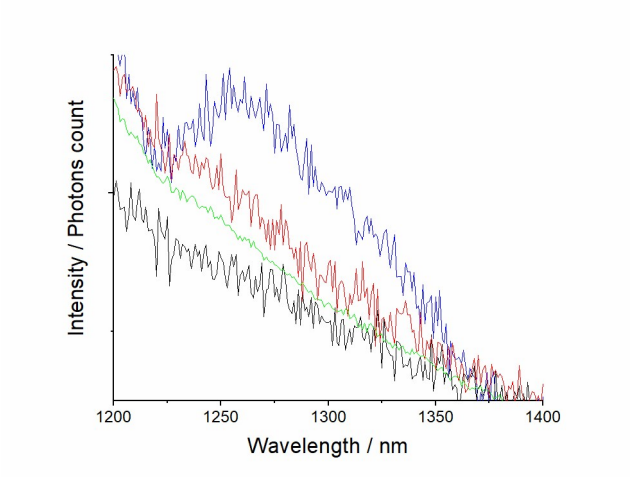

Figure S16. $^1\Delta_g$ O_2 emission spectra observed for PUr-1 (black), PUr-3 (red), PUr-5 (green) and PUr-10 (blue) by exciting samples at 375 nm.