Electronic supplementary information

Alcohol- and water-soluble bis(*tpy*)quaterthiophenes with phosphonium side groups: new conjugated units for metallo-supramolecular polymers

Pavla Štenclová, Kristýna Šichová, Ivana Šloufová, Jiří Zedník, Jiří Vohlídal* and Jan Svoboda *

Charles University in Prague, Faculty of Science, Department of Physical and Macromolecular Chemistry, Hlavova 2030, CZ-128 40, Prague 2, Czech Republic.
Fax:+420 224919752; Tel:+420 221951310;

E-mail: jan.svoboda@natur.cuni.cz (J. Svoboda)
jiri.vohlidal@natur.cuni.cz (J. Vohlídal)

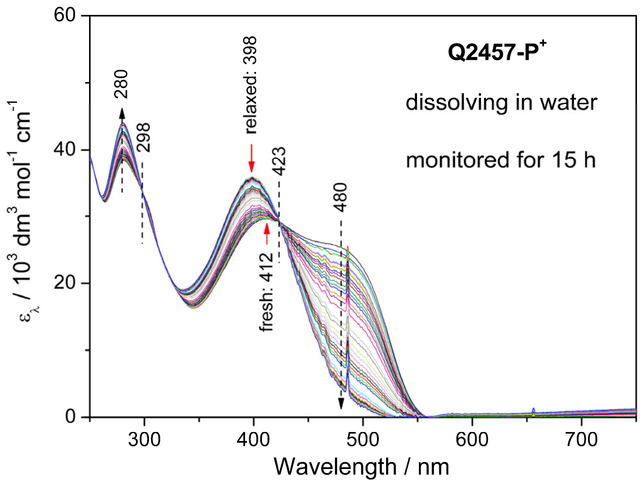


Figure S1. Time-development of the UV/vis spectra during the dissolution of **Q2457-P$^+$** in water. Room temperature, $2{\cdot}10^{-5}$M

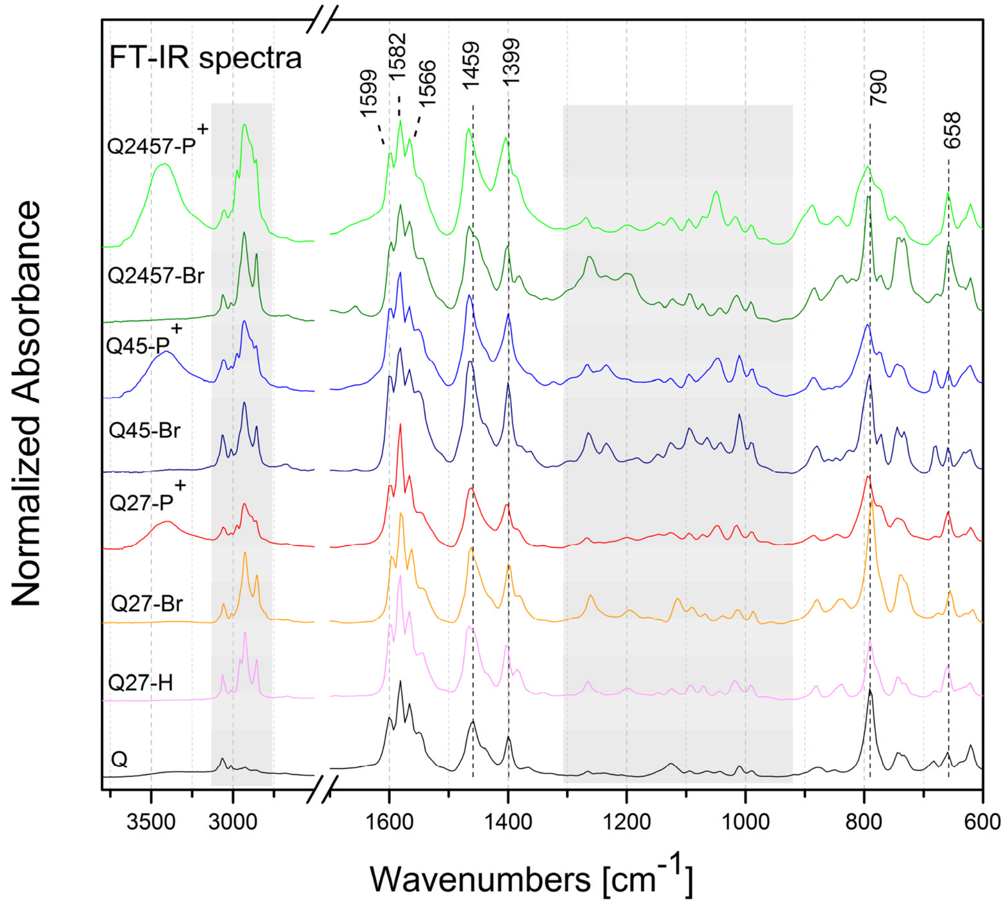
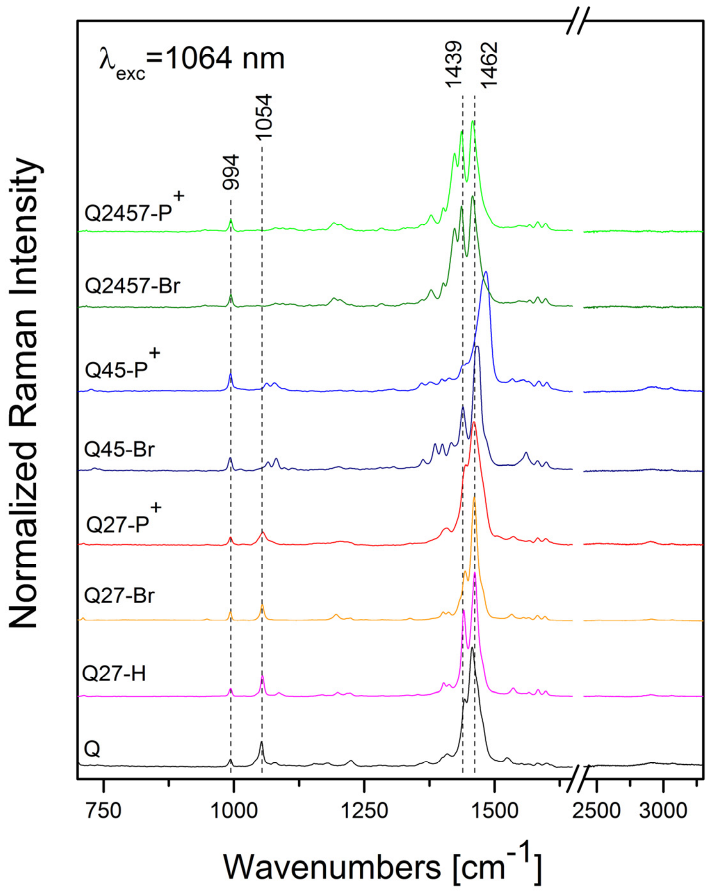


Figure S2. Infrared spectra of prepared unimers.



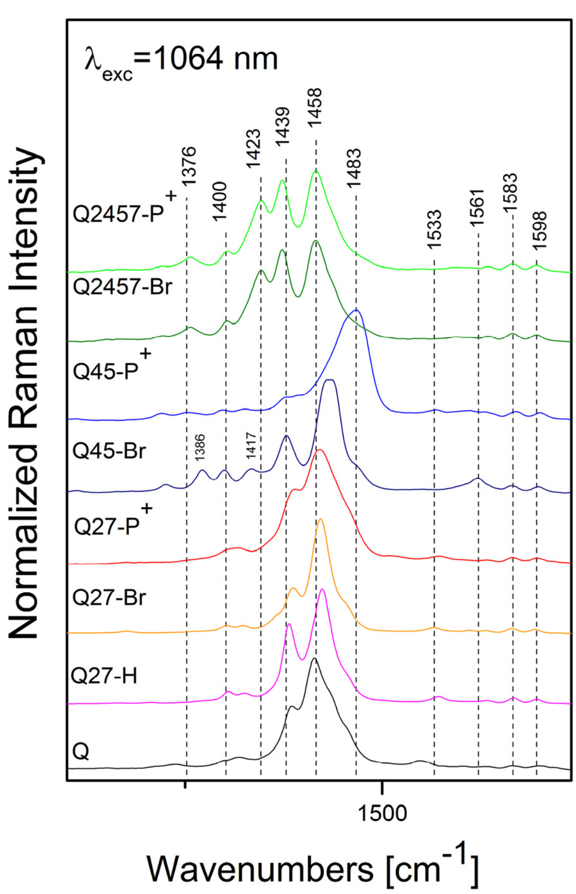


Figure S3. Off-resonance Raman spectra of prepared unimers (λ_{exc} = 1064 nm).

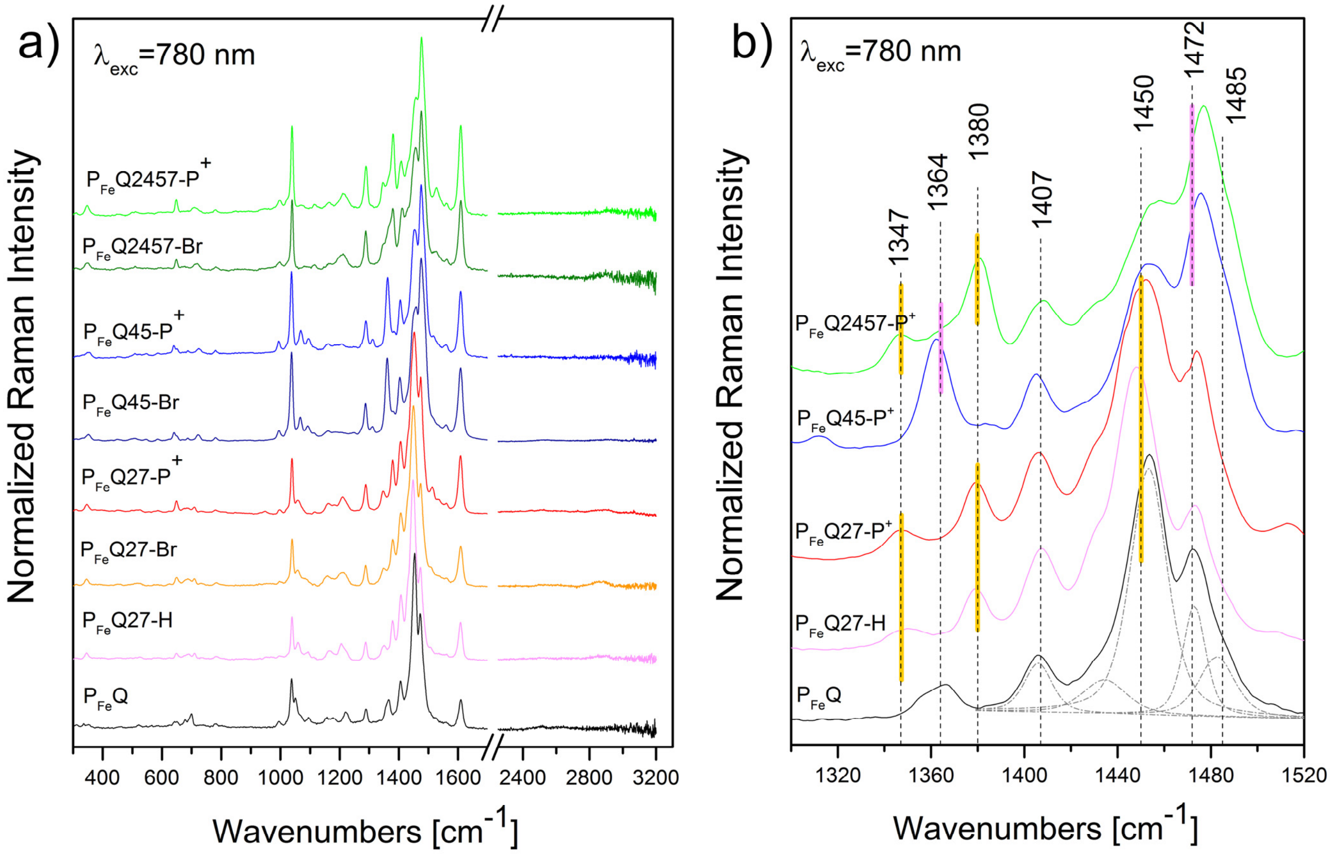


Figure S4. Off-resonance Raman spectra of Fe-polymers at λ_{exc} = 780 nm (a) and deconvolution of spectra (b).

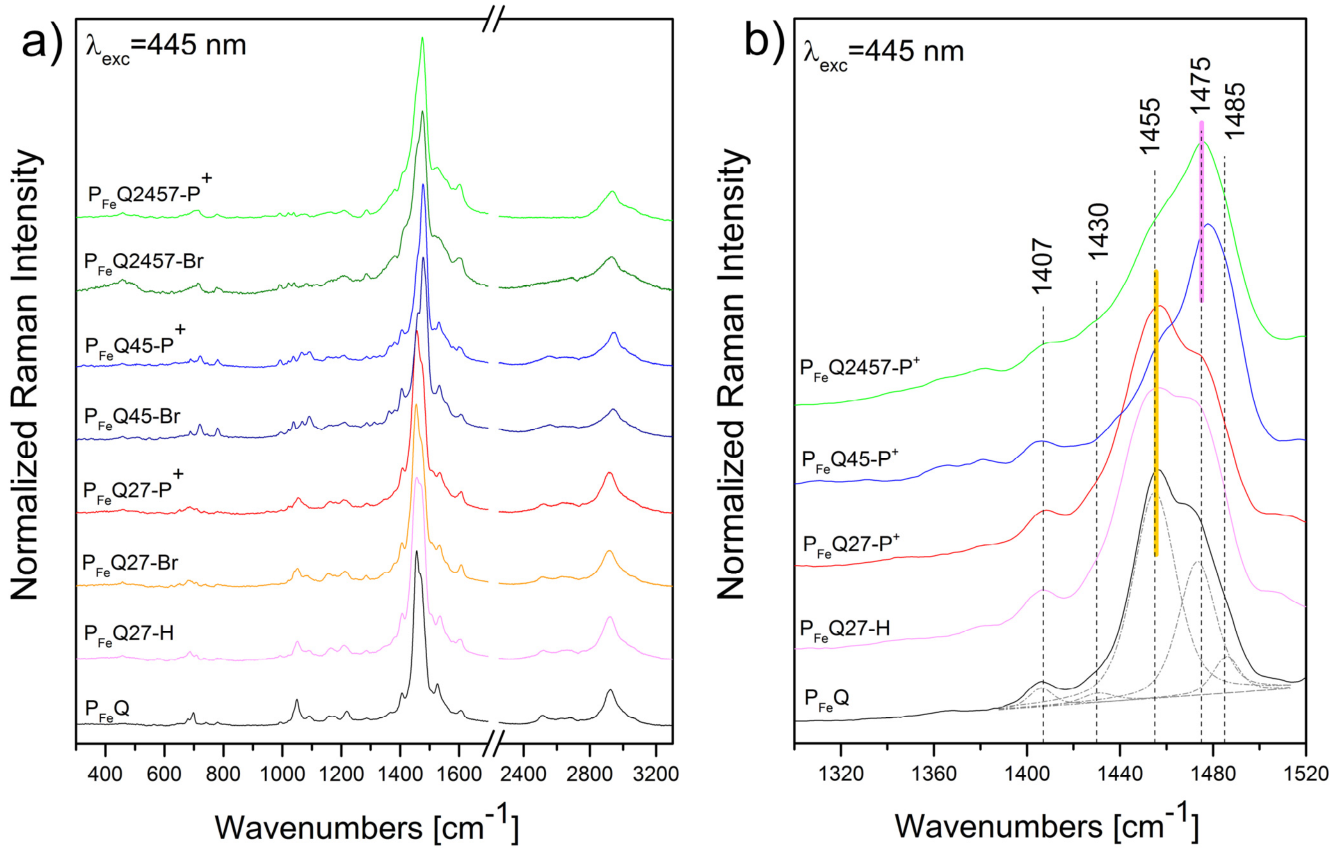


Figure S5. Off-resonance Raman spectra of Fe-polymers at λ_{exc} = 445 nm (a) and deconvolution of spectra (b).

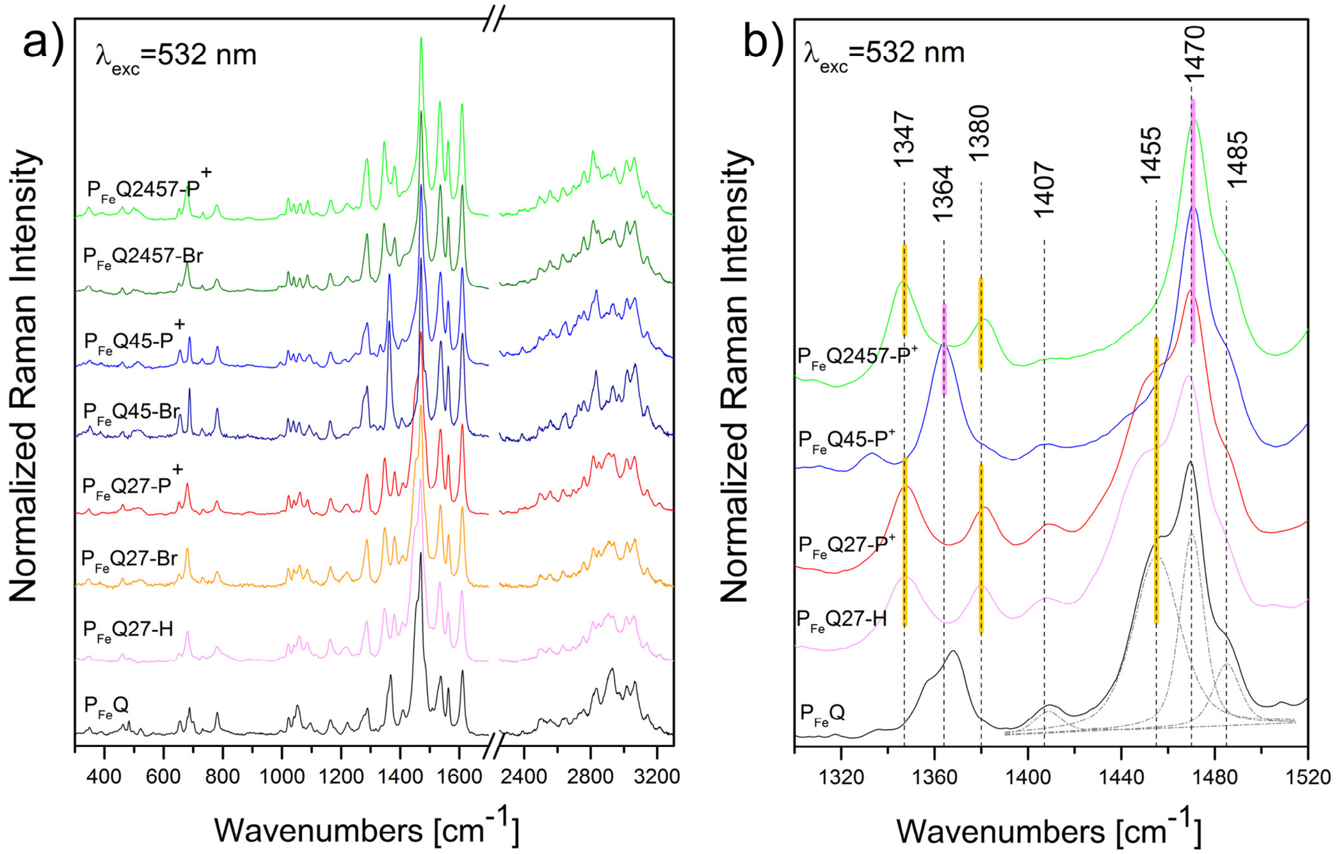


Figure S6. Off-resonance Raman spectra of Fe-polymers at λ_{exc} = 532 nm (a) and deconvolution of spectra (b).

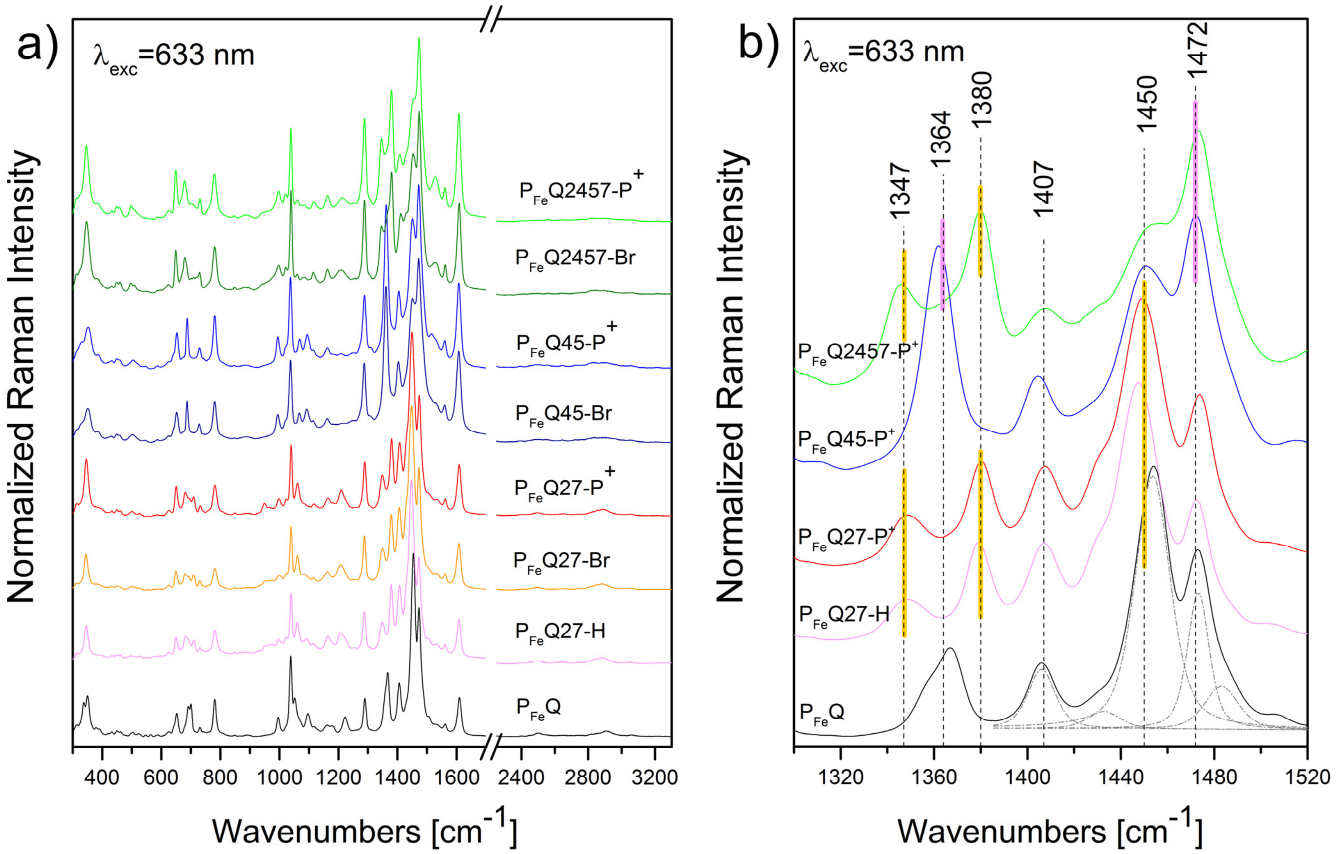


Figure S7. Off-resonance Raman spectra of Fe-polymers at λ_{exc} = 633 nm (a) and deconvolution of spectra (b).

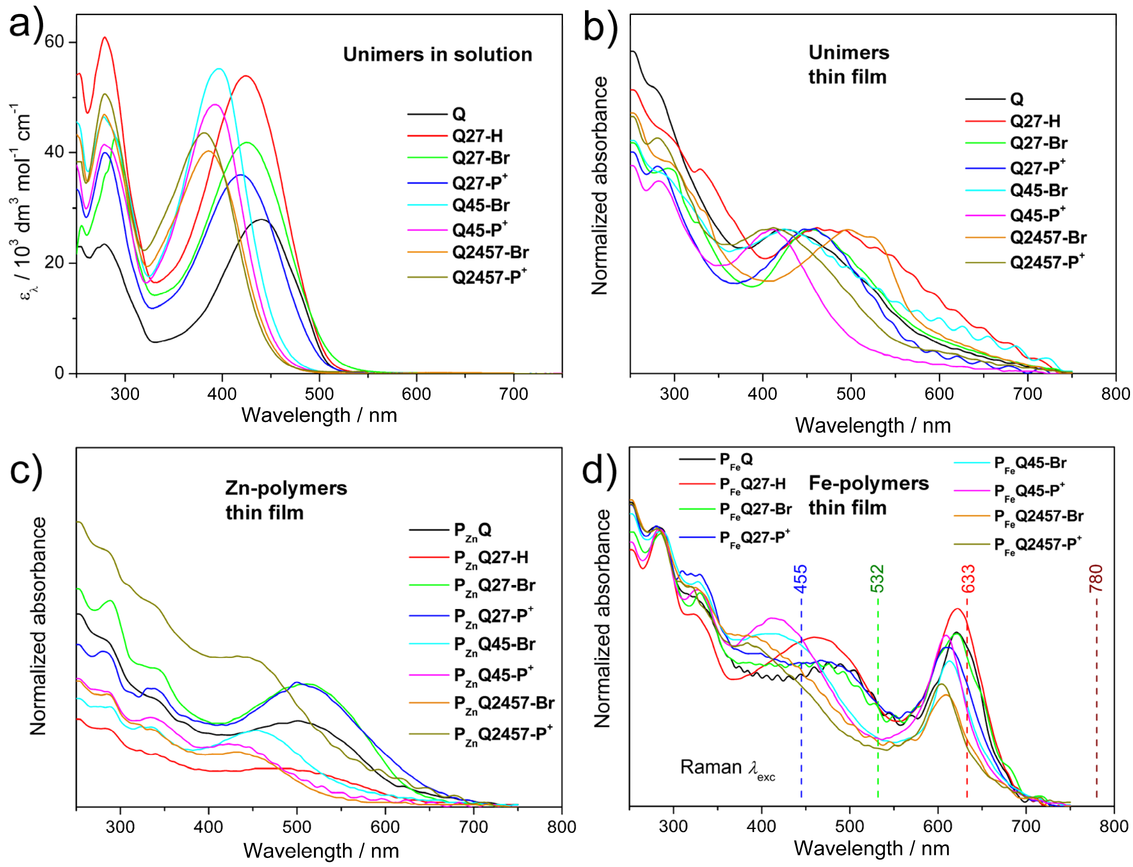


Figure S8. UV/vis spectra of prepared unimers and polymers.

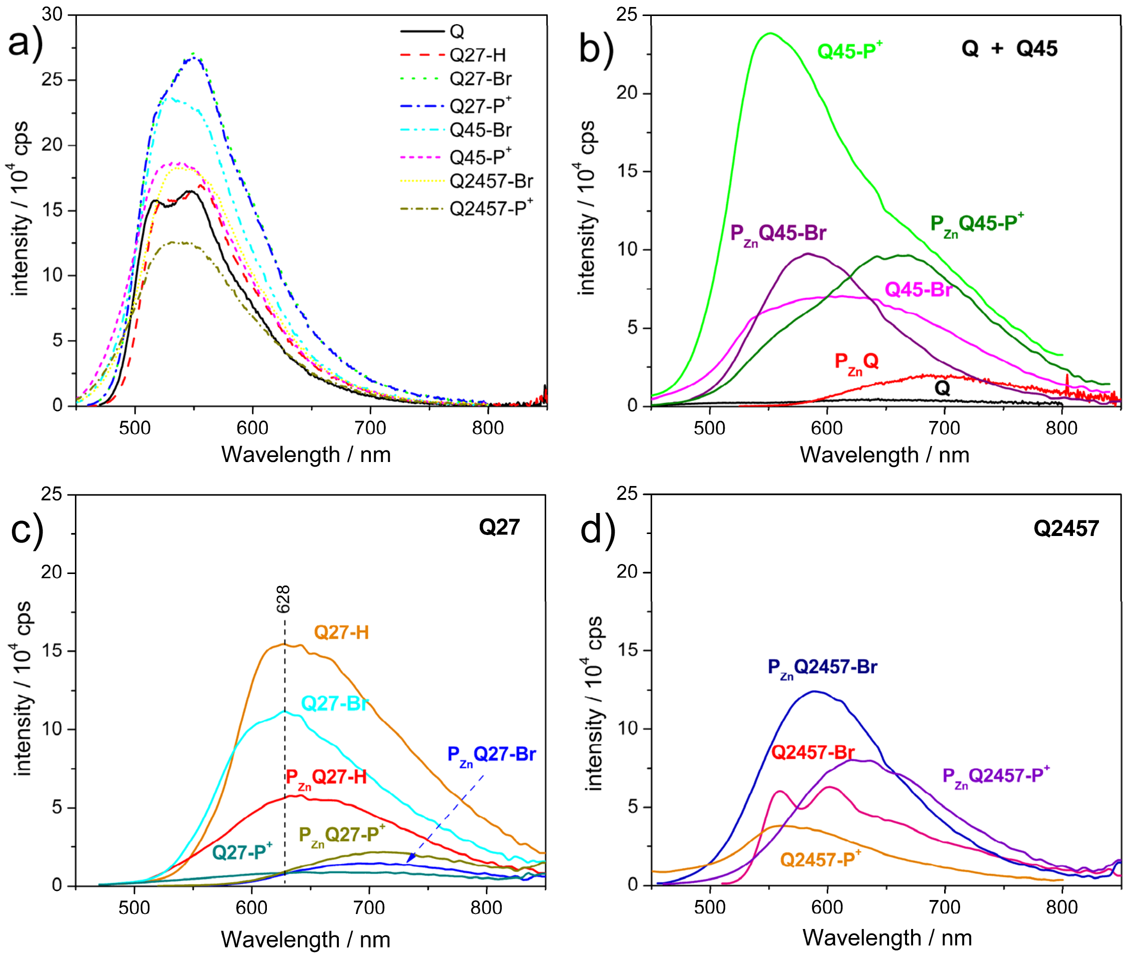


Figure S9. Luminescence spectra of prepared unimers in solution (a) and unimers and Zn-polymers in thin film (b-d).

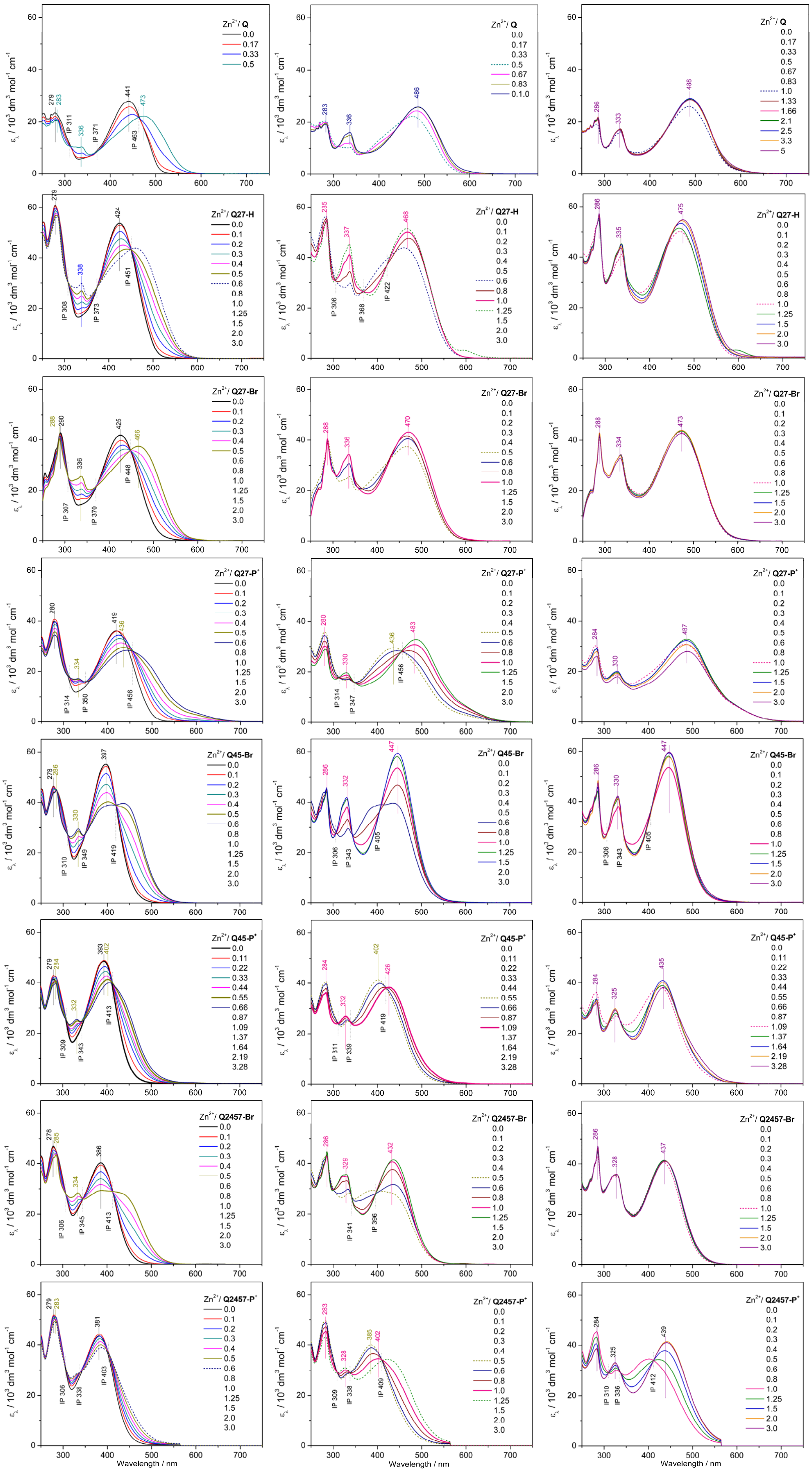


Figure S10. Complete set of UV/vis spectra accompanying the titration of non-ionic and ionic unimers with Zn^{2+} ions. Initial unimer concentration $2 \cdot 10^{-5}$M in chloroform/acetonitrile (non-ionic species) or methanol (ionic unimers), room temperature. Each column depicts the particular stage of assembling.

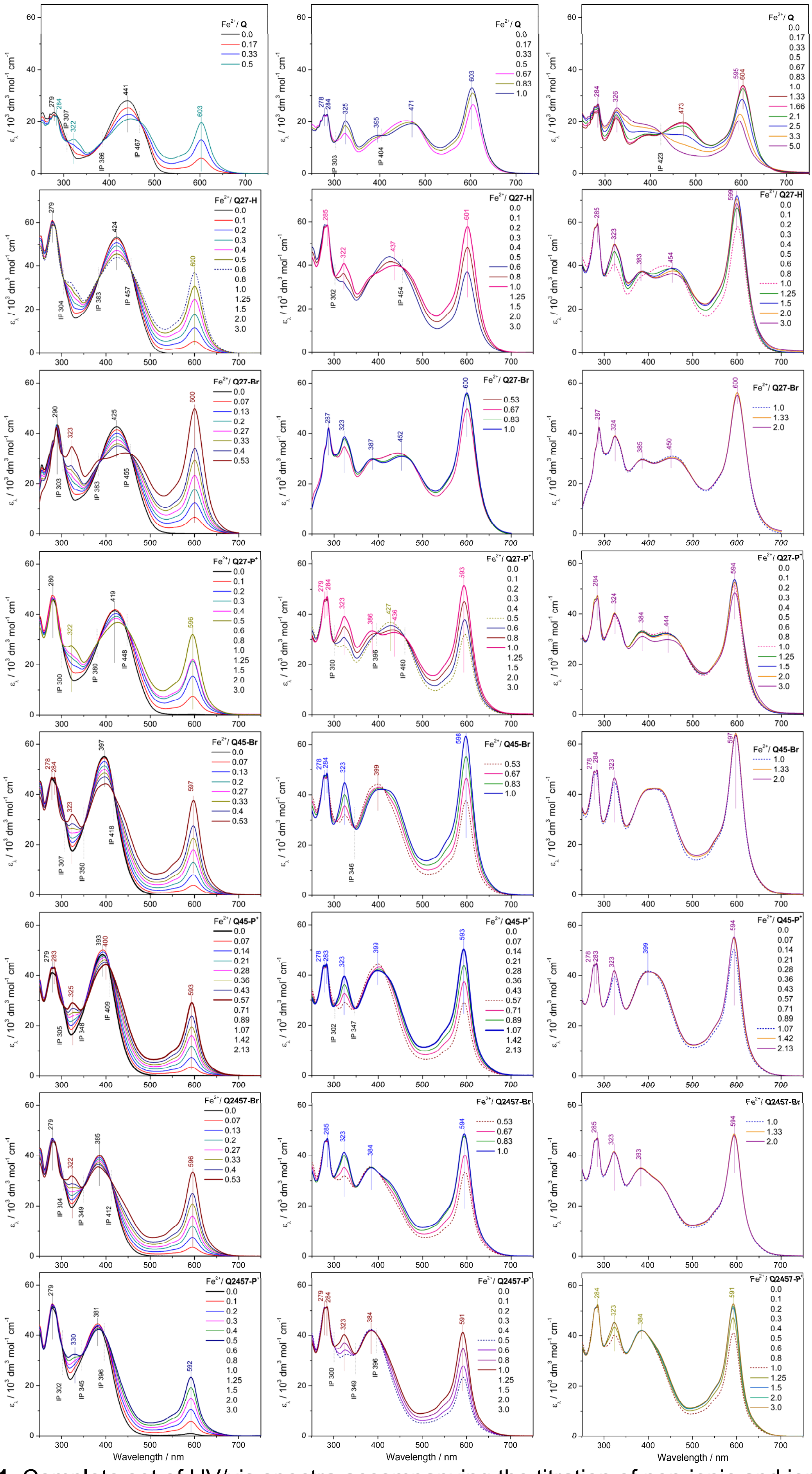


Figure S11. Complete set of UV/vis spectra accompanying the titration of non-ionic and ionic unimers with Fe^{2+} ions. Initial unimer concentration $2\cdot10^{-5}$M in chloroform/acetonitrile (non-ionic species) or methanol (ionic unimers), room temperature. Each column depicts the particular stage of assembling.

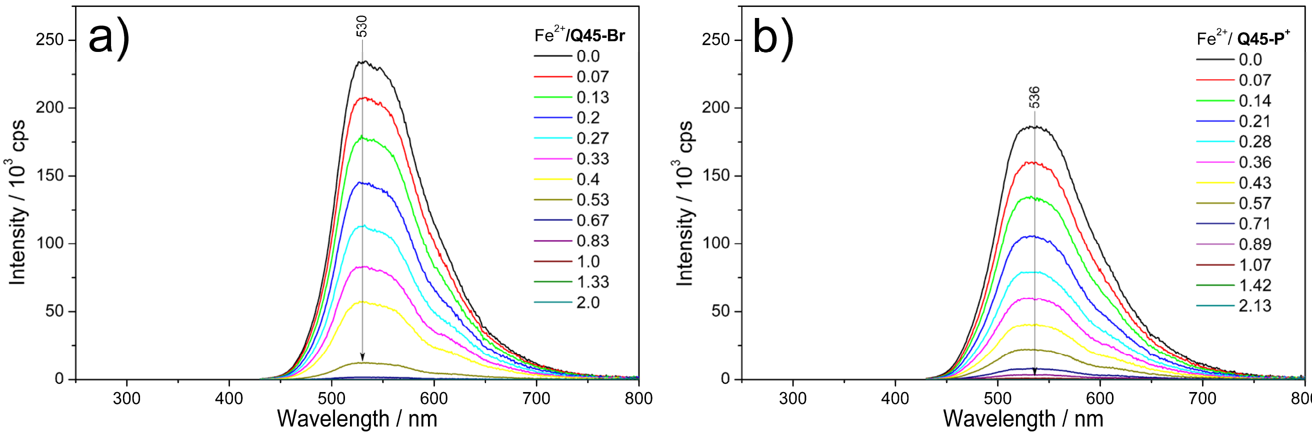


Figure S12. Changes in photoluminescence spectra accompanying titration of unimers **Q45-Br** (a) and **Q45-P$^+$** (b) with Fe^{2+} in chloroform/acetonitrile (a) or methanol (b).

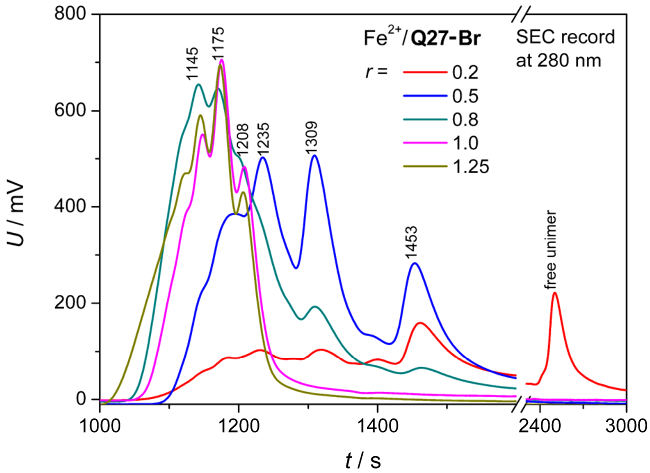


Figure S13. The SEC records of the Fe^{2+}/**Q27-Br** systems of different composition.

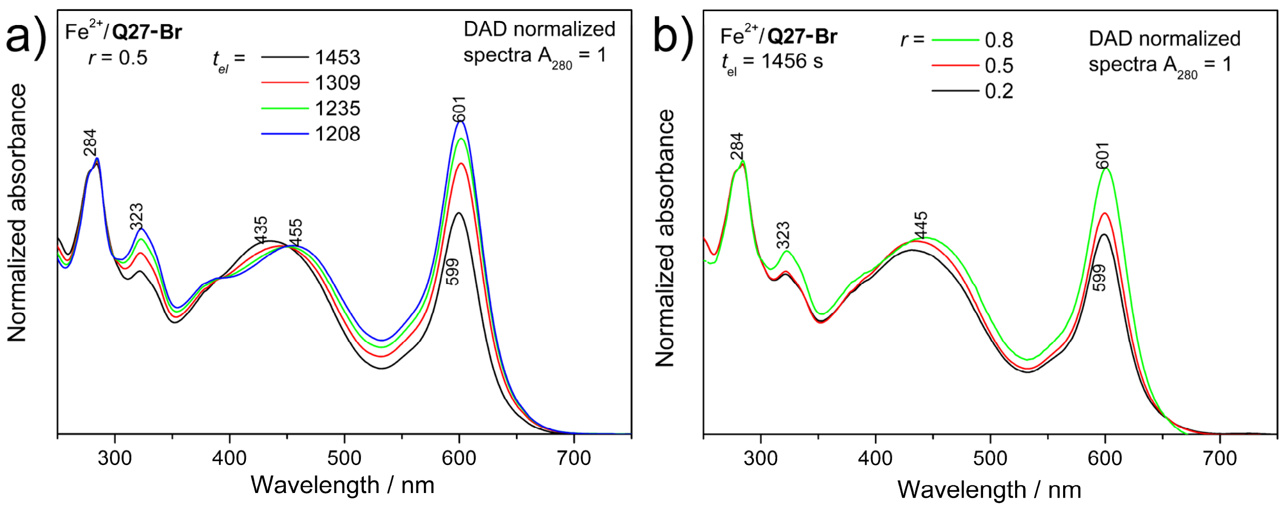


Figure S14. The DAD spectra at different elution time t_{el} (a) and the UV/vis spectra of SEC fractions (t_{el} = 1456 s) of Fe^{2+} / **Q27-Br** systems of different composition (b).

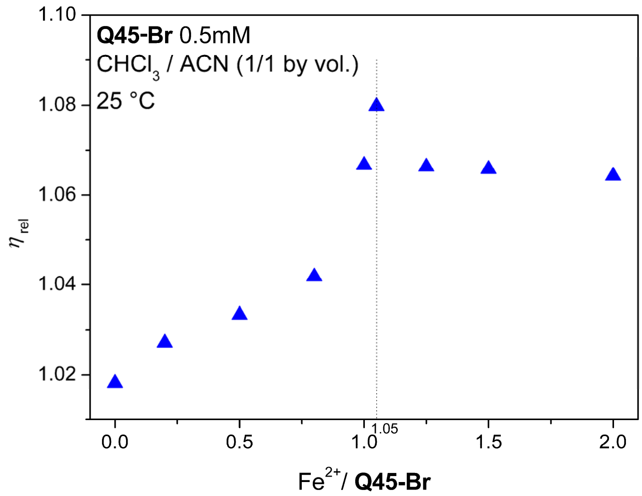


Figure S15. Relative viscosity of solution of the system Fe^{2+}/**Q45-Br** as a function of composition.

Table S1. The photoluminescence maxima, λ_F, in solution and in thin film, photoluminescence quantum yield, Φ, and lifetime of excited states, τ. Solvent: methanol for ionic unimers and polymers (suffix **-P⁺**); acetonitrile/chloroform (1/1 by vol.) for all the other unimers and polymers.

Sample	λ_F, nm (ϕ, %) solution	film	τ, ns solution	film
Unimers				
Q	514,546 (30%)	645 (<1%)	0.79 (100%)	0.24 (35%) 0.98 (49%) 3.71 (16%)
Q27-H	554 (26%)	630 (1%)	0.62 (94%) 1.53 (6%)	0.15 (56%) 0.51 (38%) 1.84 (6%)
Q27-Br	554 (31%)	630 (1%)	0.57 (85%) 1.20 (15%)	0.13 (54%) 0.50 (36%) 1.98 (10%)
Q27-P⁺	550 (18%)	~650 (<1%)	0.69 (100%)	0.15 (35%) 0.83 (43%) 2.54 (22%)
Q45-Br	530 (14%)	610 (1%)	0.43 (9%) 0.55 (91%)	0.18 (51%) 0.75 (39%) 3.82 (10%)
Q45-P⁺	536 (11%)	550 (1%)	0.31 (33%) 0.57 (67%)	0.08 (62%) 0.40 (30%) 2.27 (8%)
Q2457-Br	536 (14%)	560,603 (3%)	0.37 (44%) 0.50 (56%)	0.07 (79%) 0.42 (16%) 1.84 (5%)
Q2457-P⁺	536 (10%)	560 (1%)	0.39 (57%) 0.56 (43%)	0.07 (74%) 0.39 (22%) 1.84 (4%)
Zn-polymers				
P_{Zn}Q	656	~690 (1%)		0.27 (53%) 0.92 (34%) 2.51 (13%)
P_{Zn}Q27-H	673	~640 (2%)		0.18 (41%) 0.91 (44%) 3.54 (15%)
P_{Zn}Q27-Br	675	~710 (1%)		0.16 (57%) 0.72 (36%) 3.05 (7%)
P_{Zn}Q27-P⁺	550	~705 (<1%)		0.11 (47%) 0.54 (42%) 1.92 (11%)
P_{Zn}Q45-Br	673	585 (3%)		0.21 (45%) 0.98 (39%) 3.63 (16%)
P_{Zn}Q45-P⁺	536	660 (1%)		0.06 (79%) 0.29 (17%) 1.98 (4%)
P_{Zn}Q2457-Br	668	590 (3%)		0.15 (43%) 0.71 (42%) 3.24 (15%)
P_{Zn}Q2457-P⁺	552	625 (1%)		0.15 (56%) 0.56 (36%) 2.05 (8%)