Supplementary Information

Supramolecular assemblies of triblock copolymers with hexanuclear molybdenum clusters for sensing antibiotics in aqueous solutions via energy transfer

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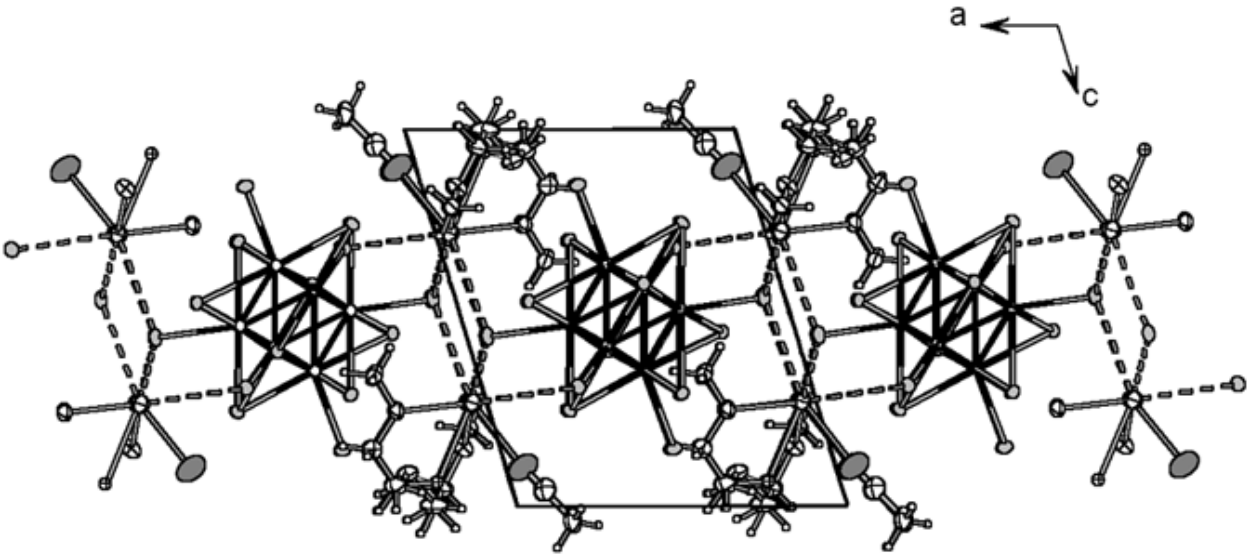

Figure S1. Section of a layer connecting $\{K(dyglime)(CH_3CN)\}_2^{2+}$ and $[Mo_6I_{14}]^{2-}$ in the crystal structure of **1**. Contacts between K^+ and I^- are shown as dashed lines.

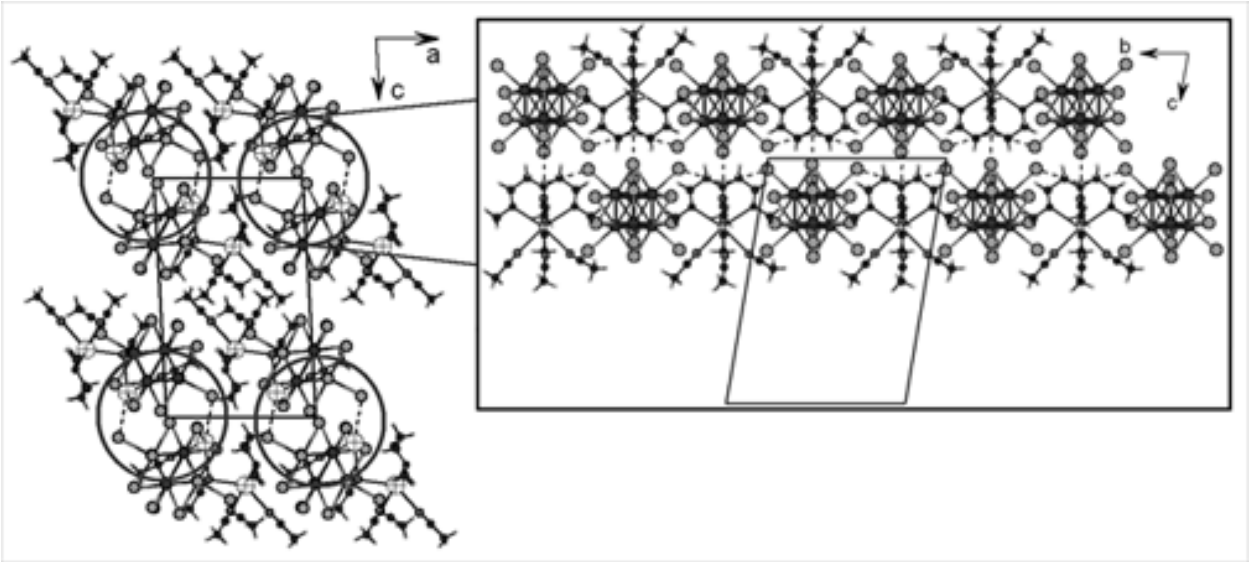

Figure S2. Infinite column built of $\{(CH_3CN)_3K(dyglime)(\mu\text{-}CH_3CN)K(CH_3CN)\}^{2+}$ cations and anions of $[Mo_6I_{14}]^{2-}$ in the crystal structure of **2**.

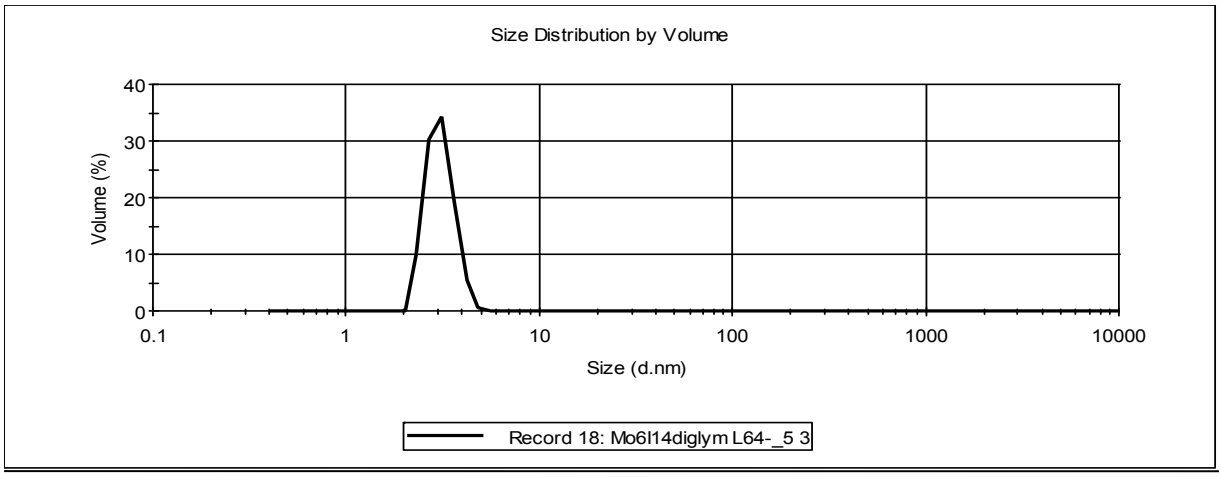

Fig.S3 Size distribution in solutions of L64 (C=0. 35-10 mM) and **1** (0.035 mM), t=25 °C, PDI=0.1-0.3.

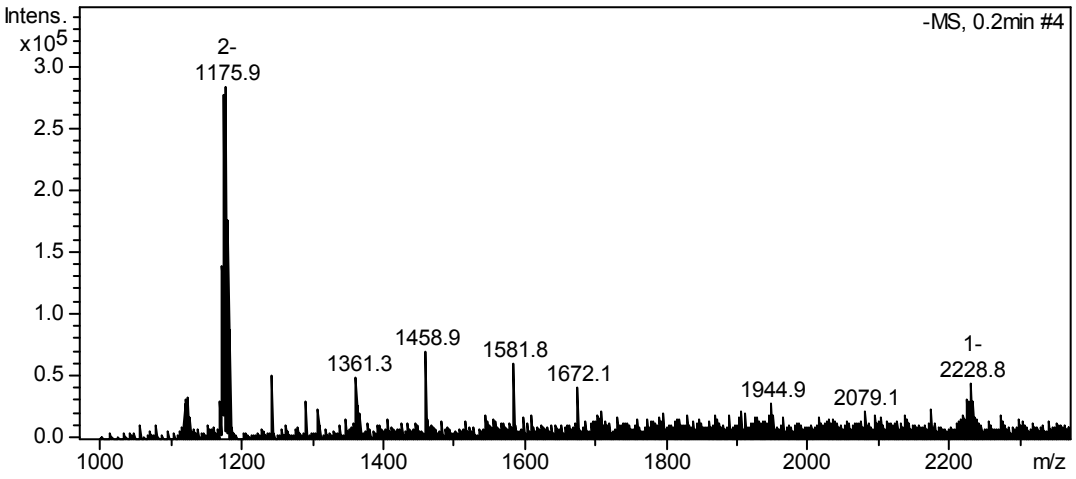

Fig.S4. ESI spectra of **1** (0.01 mM) in aqueous solutions of P123, pH 6.

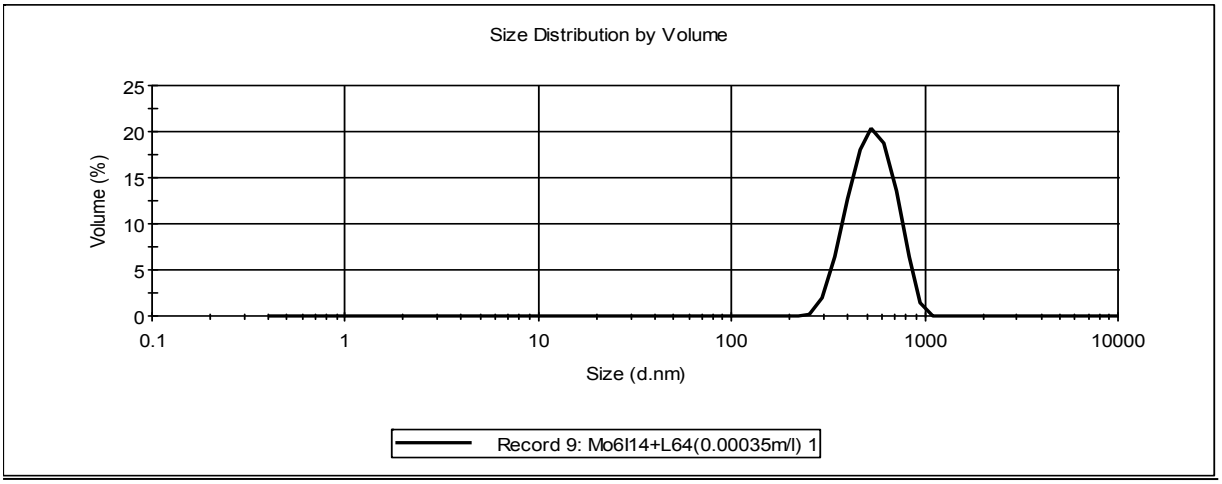

Fig.S5. Size distribution in solutions of L64 (10 mM) and **1** (0.035 mM), 2-3 hours after the sample preparation , t=25 °C, PDI=0.1.

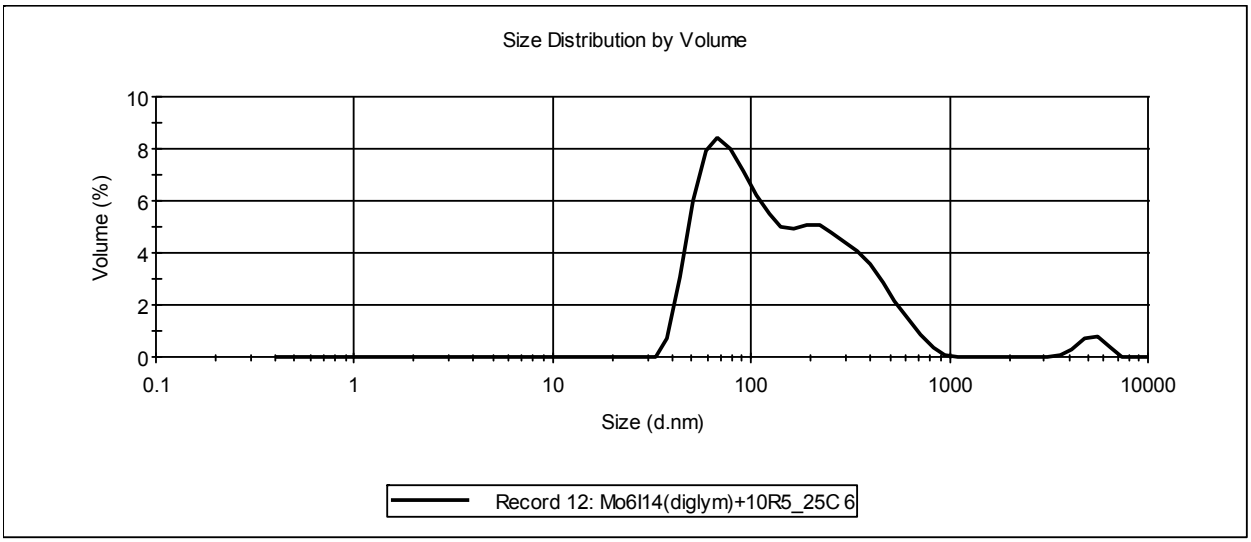

Fig.S6. Size distribution in solutions of **1** (0.035 mM) and 10R5 (10 mM), t=25 °C, PDI=0.26.

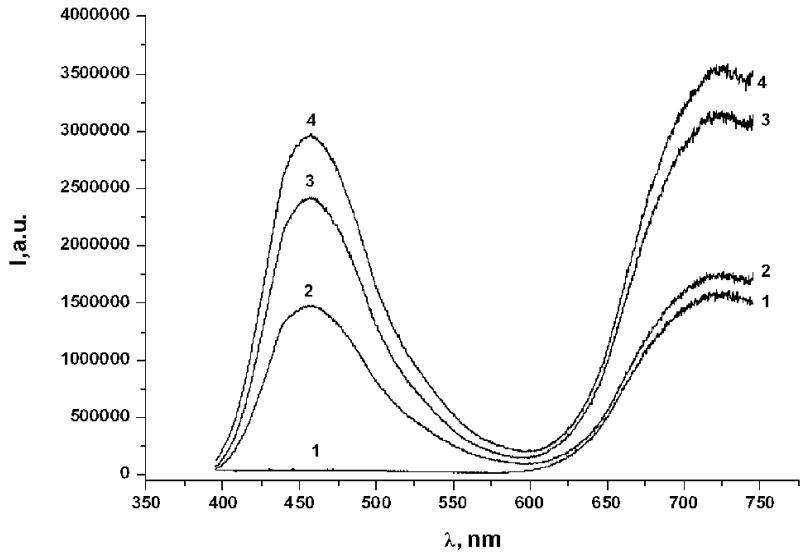

Fig.S7. Luminescence spectra of **1** (0.035 mM) itself (1) and in the presence of difloxacin: 0.02 mM - (2), 0.035 mM – (3), 0.07 mM – (4) in aqueous solutions of L64 (0.35 mM) at pH within 5.0-5.5, λ_{ex}=380 nm..

Table S1. Experimental details

Parameters	**1**	**2**
Chemical formula	$C_{16}H_{34}I_{14}K_2Mo_6N_2O_6$	$C_{16}H_{29}I_{14}K_2Mo_6N_5O_3$
M_r	2780.89	2769.88
Crystal system, space group	Triclinic, $P\bar{1}$	Triclinic, $P\bar{1}$
Temperature (K)	150	150
a, b, c (Å)	10.4798 (3), 11.0059 (3), 13.2185 (3)	11.1975 (4), 13.0620 (4), 18.1803 (8)
α, β, γ (°)	113.459 (1), 99.171 (1), 103.312 (1)	80.332 (1), 86.953 (1), 89.764 (1)
V (Å^3)	1306.09 (6)	2617.58 (17)
Z	1	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	9.86	9.84
Crystal size (mm)	0.15 × 0.07 × 0.05	0.20 × 0.20 × 0.10
Diffractometer	Bruker X8Apex	Bruker X8Apex
Absorption correction	Empirical (using intensity measurements) based on intensities (*SADABS*, Bruker, 2005)	Empirical (using intensity measurements) based on intensities (*SADABS*, Bruker, 2005)
T_{min}, T_{max}	0.202, 0.338	0.055, 0.102
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13307, 6541, 5856	31131, 14221, 10578
R_{int}	0.028	0.034
θ values (°)	θ_{max} = 31.4, θ_{min} = 3.1	θ_{max} = 31.6, θ_{min} = 2.2
Range of h, k, l	$-13 \le h \le 15$, $-15 \le k \le 9$, $-15 \le l \le 17$	$-16 \le h \le 16$, $-16 \le k \le 11$, $-25 \le l \le 26$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.050, 1.04	0.041, 0.093, 1.04
No. of reflections, parameters, restraints	6541, 215, 0	14221, 422, 0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0141P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 11.015P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.08, -0.80	1.96, -1.43

Computer programs: Apex2 V.1.27 (Bruker, 2005), *SHELXS97* (Sheldrick, 1990), *SHELXL97* (Sheldrick, 1997), *SHELXTL* V6.22 (Bruker, 2000-2005), local programs.

Table S2. Geometry of $\{Mo_6(\mu_3\text{-}I)_8\}^{4+}$ clusters

Complex	Mo-Mo	Mo - μ_3I	Mo-X[a]	Reference
1	2.6666(4) - 2.6935(4)	2.7696 (4) - 2.7862(4)	X = I; 2.8337(4) - 2.8684(3)	This work
2	2.6758(8) - 2.6822(9)	2.7663 (8) - 2.7821(7)	X = I; 2.8394(8) - 2.8639(8)	This work
$(NBu_4)_2[Mo_6I_8(NCS)_6]$	2.660-2.673	2.778-2.789	X = NCS; 2,141-2,150	[1]
$(NBu_4)_2[\{Mo_6I_8\}F_6]$	2.650	2.798	X = F; 2.008	[2]
$(NBu_4)_2[\{Mo_6I_8\}Cl_6]$	2.655	2.775	X = Cl; 2.460	-//-
$(NBu_4)_2[\{Mo_6I_8\}Br_6]$	2.670	2.775	X = Br; 2.616	-//-
$(NBu_4)_2[\{Mo_6I_8\}I_6]$	2.675	2.767	X = I; 2.846	-//-
$(NBu_4)_2[Mo_6I_8(C_3F_7COO)_6]$	2.6604(4)	2.7740(4)	X = C_3F_7COO; 2.132(2)	[3]

References

[1] M. Höhling, M. K. Simsek, W. Preetz // Z. anorg. allg. Chem. 624 (1998) 1171-1174
[2] P. Brückner, W. Preetz, M. Pünjer // Z. anorg. allg. Chem. 623 (1997) 8-17
[3] M.N. Sokolov, M. A. Mihailov, E.V. Peresypkina, K.A. Brylev, N. Kitamura, V.P. Fedin // Dalton Trans., 2011, 40, 6375