Electronic Supplementary Information (ESI)

Two Chelating-Amine-Functionalized Lanthanide Metal-Organic Frameworks for Adsorptions and Catalysis

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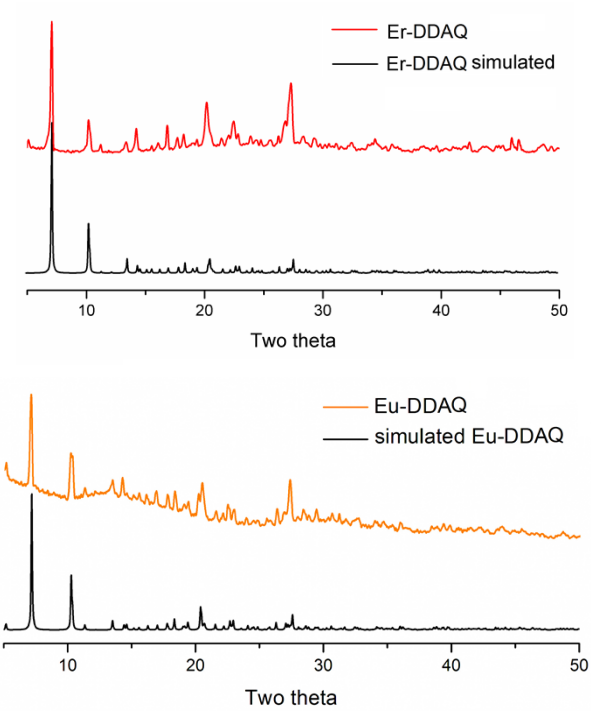

Fig S1. PXRD patterns of Er-DADQ and Eu-DADQ.

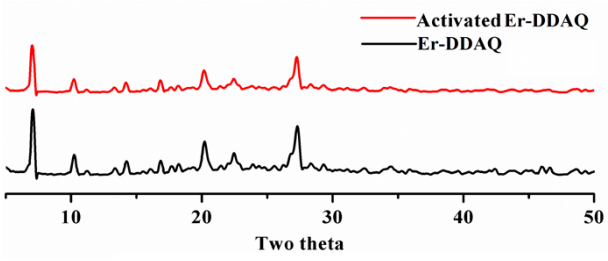

Fig S2. PXRD patterns of activated Er-DADQ.

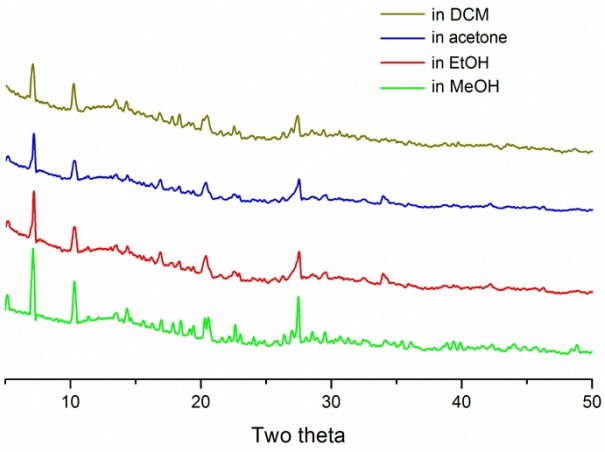

Fig S3. PXRD patterns of Er-DADQ after immersing in different solvents for one week.

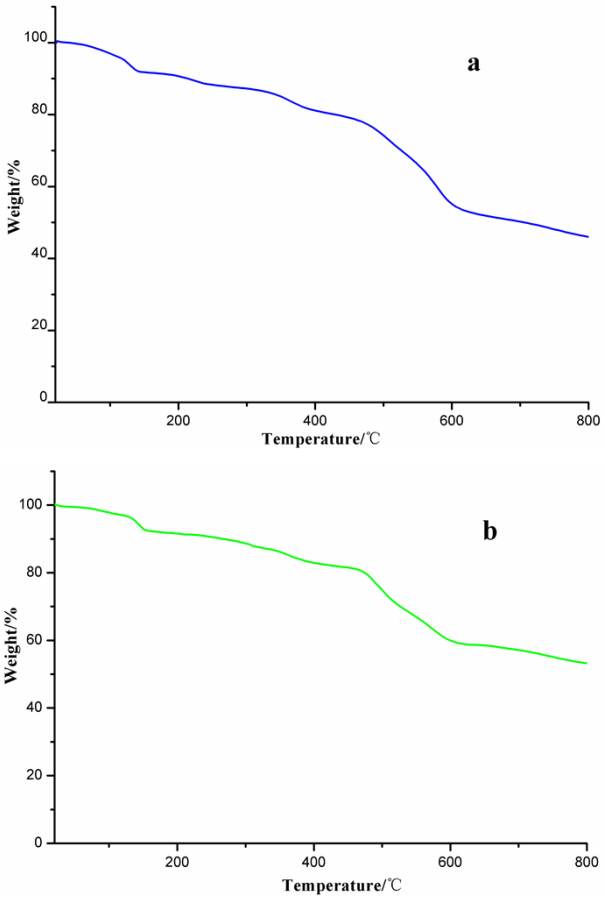

Fig S4. TG profiles of Er-DADQ (a) and Eu-DADQ (b)

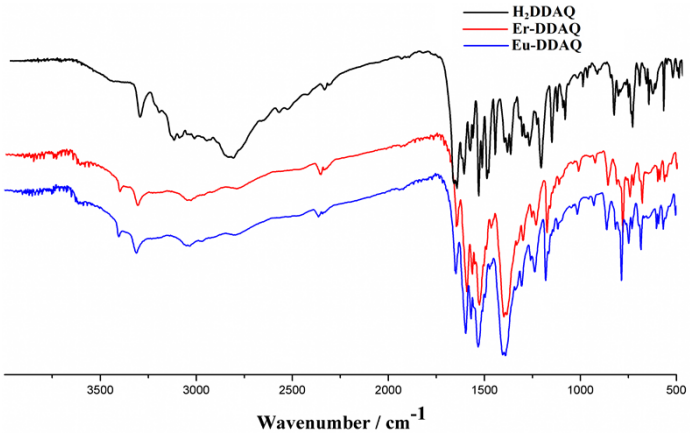

Fig S5. IR spectra of H_2DADQ, Er-DADQ and Eu-DADQ.

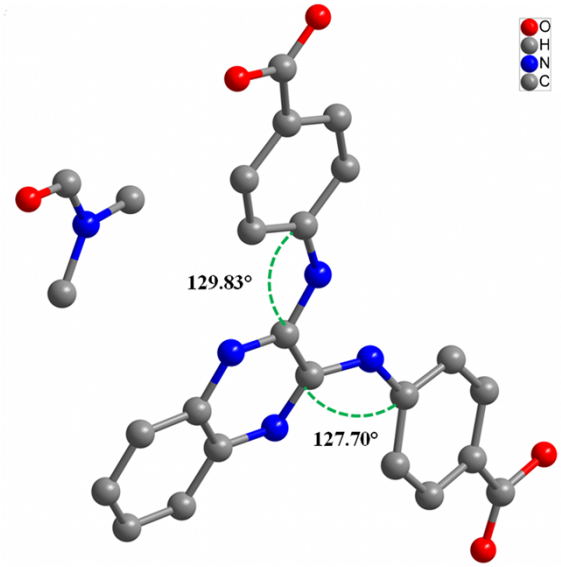

Fig S6. Molecular structure of H_2DDQ, and H atoms were omitted for clarity.

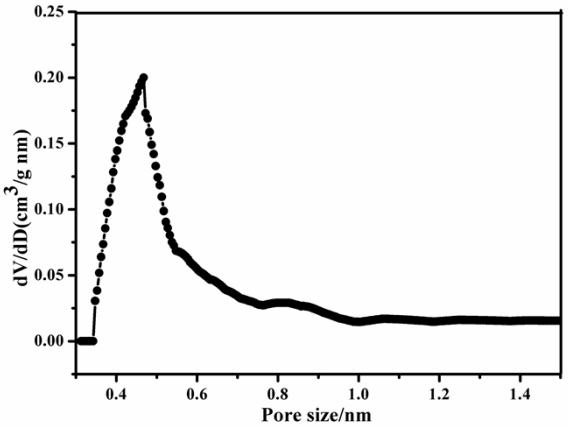

Fig S7. Pore size distribution of Er-DDAQ.

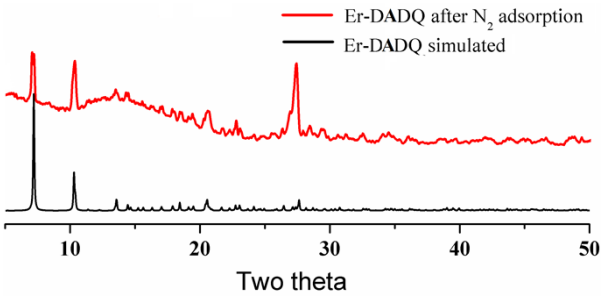

Fig S8. PXRD pattern of Er-DADQ after the N_2 adsorption.

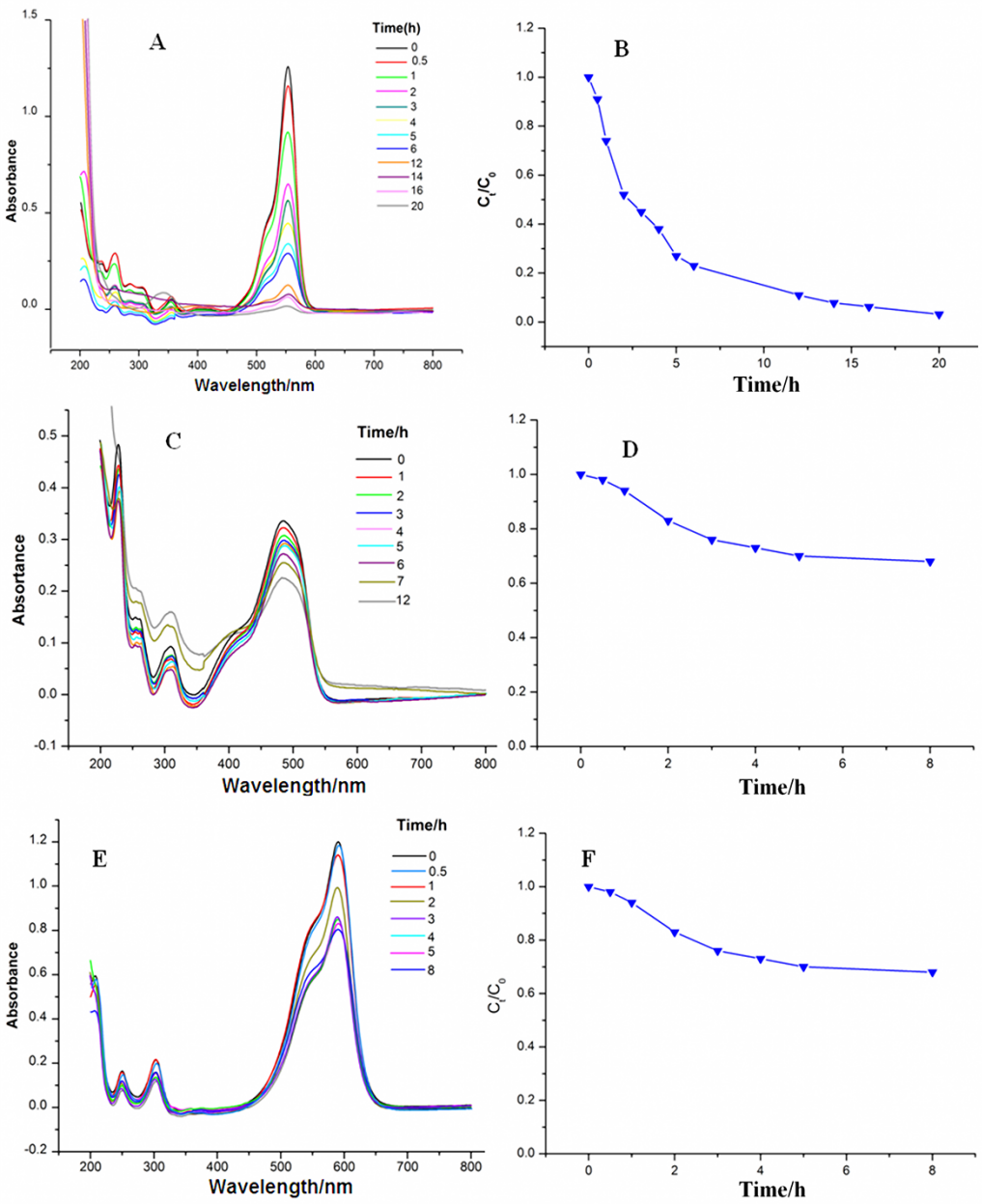

Fig S9. (A, C and E) UV-vis absorption spectra of RhB, MO and CV solutions in the presence of Er-DADQ. (B, D and E) the relationship between C_t/C_0 and reaction time (t) in the absorption of RhB, MO and CV.

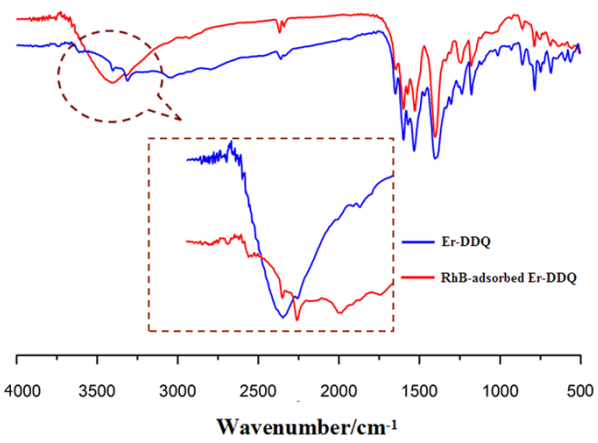

Fig S10. Comparison of IR spectra between Er-DADQ and RhB absorbed Er-DADQ.

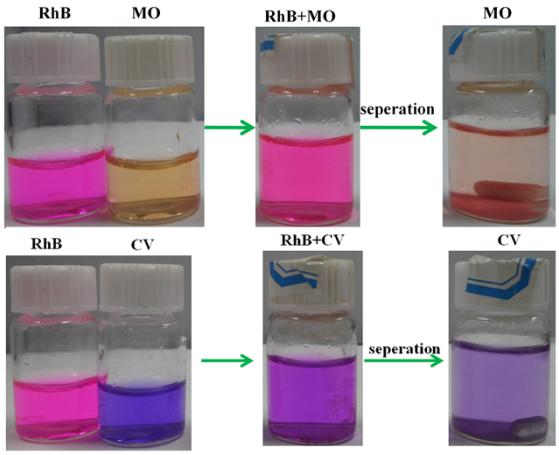

Fig S11. Separations process of two equal-mass dyes mixtures in Er-DADQ.

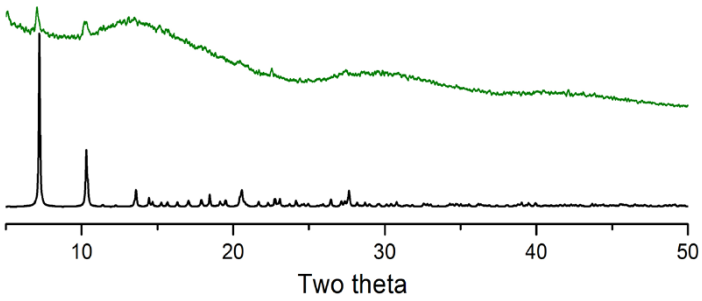

Fig S12. PXRD pattern of RhB absorbed Er-DADQ(green) and simulated Er-DADQ(black).

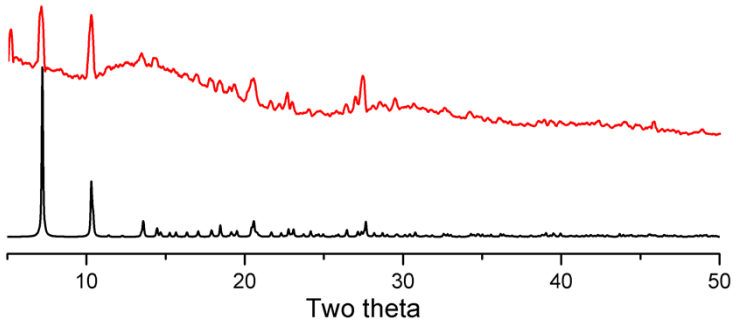

Fig S13. PXRD pattern of retrieved ER-DADQ as catalyst (red) and simulated Er-DADQ (black).

Table S1. Crystal data and structure refinements for the three compounds

Compound	H_2DADQ	Er-DADQ	Eu-DADQ
Formula	$C_{25}H_{25}N_5O_6$	$C_{44}H_{43}ErN_8O_{15}$	$C_{44}H_{43}EuN_8O_{15}$
Formula weight	491.50	1091.12	1075.82
Crystal size / mm	0.34 × 0.26 × 0.22	0.26 × 0.22 ×0.20	0.28 × 0.24 ×0.20
Crystal system	triclinic	orthorhombic	orthorhombic
Space group	$P\bar{1}$	*P*ccn	*P*ccn
a (Å)	9.826 (2)	13.138 (3)	13.166(3)
b (Å)	11.358 (2)	33.947 (7)	34.112(7)
c (Å)	11.609 (2)	10.013 (2)	10.078(2)
α (°)	66.07 (3)	90.00	90.00
β (°)	84.95 (3)	90.00	90.00
γ (°)	78.63 (3)	90.00	90.00
D_c(g cm^{-3})	1.406	1.623	1.579
Z	2	4	4
F(000)	516	2204	2184
Reflections collected	8826	13058	10771
Unique reflections	4152	4268	3787
μ (mm$^{-1)}$	0.103	1.960	1.465
R_1 [I>2σ(I)]	0.0442	0.0466	0.0764
wR_2 [I>2σ(I)]	0.1092	0.1221	0.1858
max/min (e Å^{-3})	0.208/-0.190	0.726/-0.867	0.946/-1.261
Goodness-of-fit on F^2	1.058	1.070	1.005

Table S2. Selected bond lengths (Å) and angles (°) for the three compounds

H_2DADQ					
O1-C20	1.314(2)	O2-C20	1.224(2)	O3-C21	1.229(2)
O4-C21	1.317(2)	N1-C7	1.303(2)	N1-C5	1.376(2)
N2-C8	1.305(2)	N2-C6	1.376(2)	N3-C7	1.376(2)
N1-C5-C1	120.20(15)	N1-C5-C6	120.79(15)	C7-N1-C5	118.29(14)
C8-N4-C22	127.63(14)	C7-N3-C16	129.84(14)	N2-C6-C5	120.39(15)
Er-DADQ					
Er1-O1 $^{\#1}$	2.253(4)	Er1-O2 $^{\#2}$	2.317(4)	Er1-O4 $^{\#4}$	2.447 (4)
Er1-O5 $^{\#1}$	2.403(4)				
O1-Er1-O1$^{\#1}$	92.05(19)	O1-Er1-O2$^{\#2}$	141.73(14)	O1-Er1-O2$^{\#3}$	89.98(13)
O1-Er1-O5	80.48(14)	O1$^{\#1}$-Er1-O5	148.33(14)	O2$^{\#2}$-Er1-O5	78.03(14)
O2$^{\#3}$-Er1-O5	69.48(14)	O5-Er1-O5$^{\#1}$	120.83(18)	O1-Er1-O4$^{\#4}$	74.80(13)
O1$^{\#1}$-Er1-O4$^{\#4}$	72.58(14)	O2$^{\#2}$-Er1-O2$^{\#3}$	111.19(18)	O2$^{\#2}$-Er1-O4$^{\#4}$	141.27(14)
O2$^{\#3}$-Er1-O4$^{\#4}$	71.15(13)	O5-Er1-O4$^{\#4}$	132.98(14)	O5$^{\#1}$-Er1-O4$^{\#4}$	73.60(14)
Eu-DADQ					
Eu1-O1 $^{\#1}$	2.309(7)	Eu1-O2$^{\#2}$	2.372(7)	Eu1-O4 $^{\#5}$	2.505(8)
Eu1-O5$^{\#1}$	2.436(9)				
O1-Eu1-O1$^{\#1}$	91.9(4)	O1-Eu1-O2$^{\#2}$	142.1(3)	O1$^{\#1}$-Eu1-O2$^{\#2}$	88.7(2)
O2$^{\#2}$-Eu1-O2$^{\#3}$	113.2(4)	O1-Eu1-O5	81.5(3)	O1$^{\#1}$-Eu1-O5	148.2(3)
O2$^{\#2}$-Eu1-O5	784(3)	O2-Eu1-O5$^{\#3}$	69.2 (3)	O5-Eu1-O5$^{\#1}$	119.3(4)
O1-Eu1-O4$^{\#5}$	72.5(3)	O1$^{\#1}$-Eu1-O4$^{\#5}$	75.8(3)	O2$^{\#2}$-Eu1-O4$^{\#5}$	71.0(3)
O2$^{\#3}$-Eu1-O4$^{\#5}$	139.3(3)	O5-Eu1-O4$^{\#5}$	72.5(3)	O5$^{\#1}$-Eu1-O4$^{\#5}$	134.1(3)

$^{\#1}$ -*x*+1/2, -*y*+3/2, *z*; $^{\#2}$ *x*, -*y*+3/2, *z*-1/2; $^{\#3}$ -*x*+1/2, *y*, *z*-1/2; $^{\#4}$ *x*+1/2, -*y*+2, -*z*+1/2; $^{\#5}$ -*x*, *y*-1/2, -*z*+1/2

Table S3 Recycling tests for cyanosilylation of benzaldehyde catalyzed by desolvated Er-DADQ for the same reaction time.

Run	Conversion (%)
1st	98.2
2nd	97.9
3rd	98.0
4th	97.7
5th	96.9

Table S4 Test of heterogeneity of the reaction [b]

Catalyzed reaction		reacting after filtration	
Time(min)	Yield (%)	Time(min)	Yield (%)
10	37	240	39

[b] The catalyzed reaction was carried out for 10 min with Er-DDAQ ultrasonically. Then after filtration of the catalyst, the reaction was continued for another 4h. The yields were determined by GC-MS.