Europium (III) β-Diketone Complex as Portable Luminescent Chemosensor for Naked Eye Cu^{2+} Detection and Recyclable On–Off–On Vapor Response

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Supporting Information

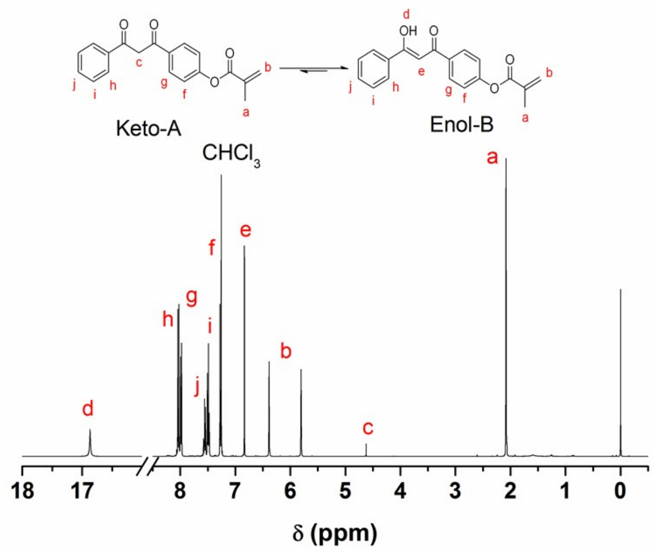


Figure S1. ^{1}H NMR spectrum of DKMA monomer.

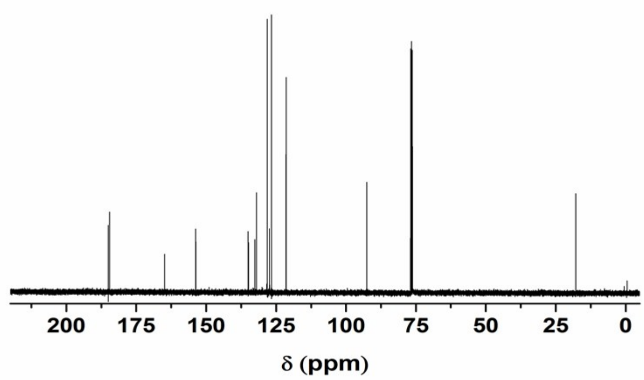
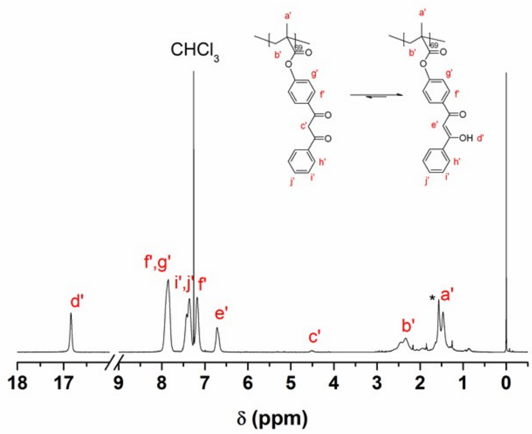
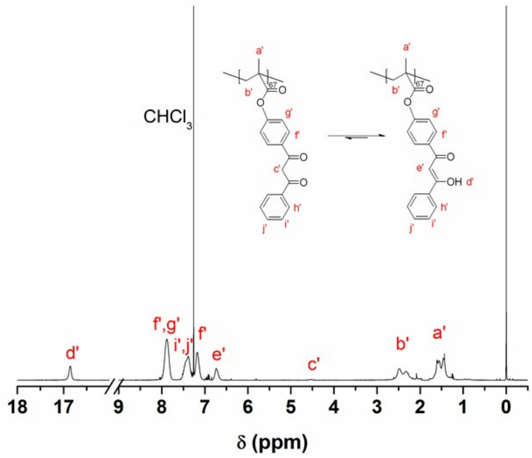
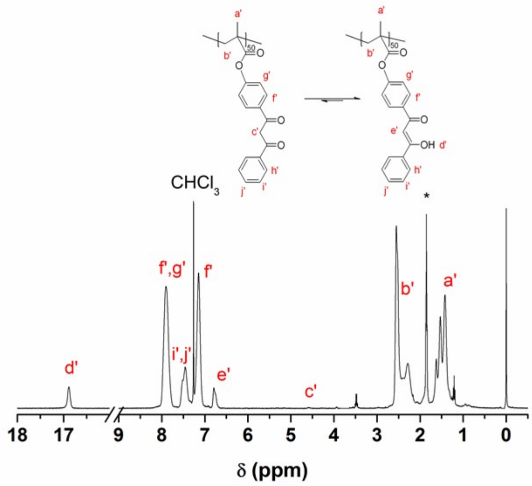


Figure S2. ^{13}C NMR spectrum of DKMA monomer.


CHCl$_3$
d'
f',g'
i',j'
f'
e'
c'
b'
a'
*
δ (ppm)


CHCl$_3$
d'
f',g'
i',j'
f'
e'
c'
b'
a'
δ (ppm)


CHCl$_3$
d'
f',g'
i',j'
f'
e'
c'
b'
a'
*
δ (ppm)

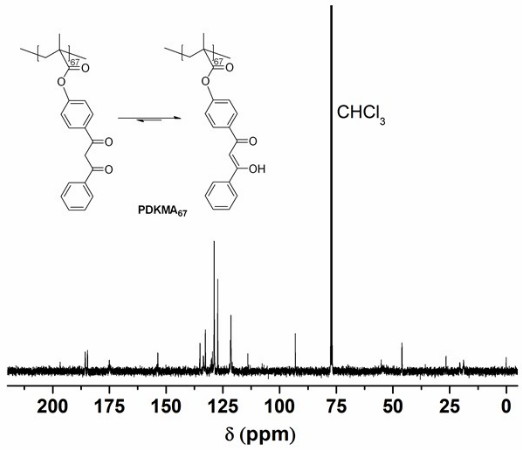


Figure S3. ^{1}H NMR spectra of homo-polymer of PDKMAs (from top to bottom: **1**, **2** and **3** in Table 1) and ^{13}C NMR profile of $PDKMA_{67}$. *: water.

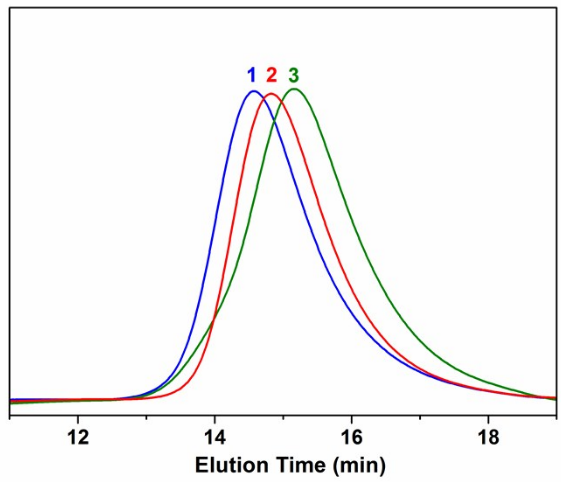


Figure S4. SEC traces of polymers of $PDKMA_{69}$ (**1**), $PDKMA_{67}$ (**2**) and $PDKMA_{50}$ (**3**).

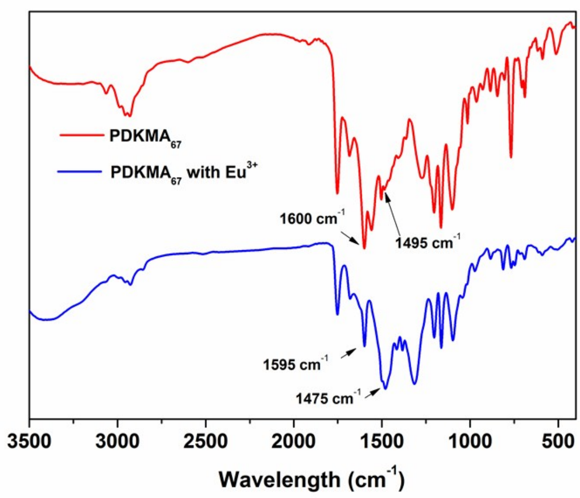


Figure S5. FT-IR spectra (KBr) of $PDKMA_{67}$ and Eu^{3+}-$PDKMA_{67}$ complex.

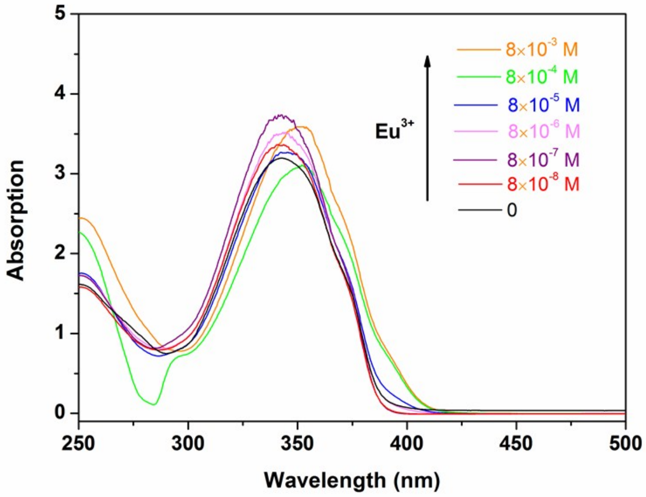


Figure S6. UV-Vis spectra of 0.05 mg/mL $PDKMA_{67}$ and $PDKMA_{67}$ with different concentrations of Eu^{3+} in THF.

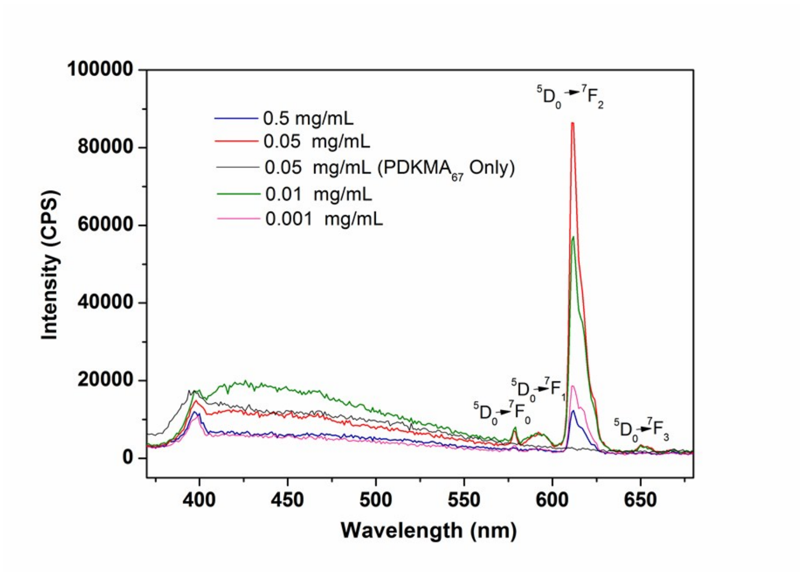


Figure S7. Fluorescent spectra of Eu^{3+} complex in aqueous solution (2 × 10^{-5} mol/L) with different concentrations of $PDKMA_{67}$ under excitation of 350 nm UV light at 25 °C. The molar ratio of PDKMA and C_2H_5ONa is 1:1.

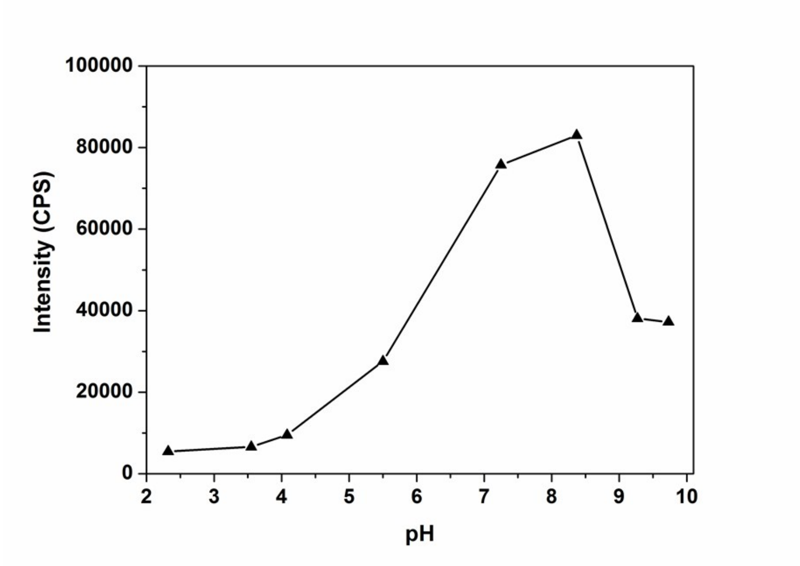


Figure S8. The PL intensityies of Eu^{3+}-PDKMA complex in pH ranges between 2 and 10 at 0.05 mg/mL PDKMA coordinated with Eu^{3+} (2 × 10^{-5} mol/L).

Quantum chemical calculation details of coordination of PDKMA with Eu^{3+}

All the geometries were optimized under gas phase using density functional theory (DFT) without any symmetry restrictions as implemented in Gaussian 03 program.[1] Becke's three-parameter-Lee-Yang-Par hybrid functional B3LYP method was carried out with 6-31G(d,p) basis sets by adding diffuse d functions to C and O atoms and diffuse p functions to H atoms. Eu atom was treated with Stuttgart-Dresden ECP. The analytical frequency calculation confirmed that the geometries had no imaginary frequency and verified the nature of minima. The basis sets 6-311+G(d,p) for C, H and O atoms were used in high-level energy calculation. Time-dependent density functional theory (TD-DFT) was used for the excited state calculations.

References:

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr., T. Vreven, K. N. Kudin, J. C. Burant, N. J. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Aynla, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wrong, C. Gonzalez and J. A. Pople, *Gaussian 03 (Revision E.01)*, Gaussian, Inc., Wallingford, CT, USA, 2004.