Supplementary Information (SI) for Materials Advances.
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Supporting Information

Facile and Selective Cost-effective Detection of Creatinine from Human Urine by Cyclometalated Dinuclear Iridium(III) Complex Through Creatinine-triggered Emission

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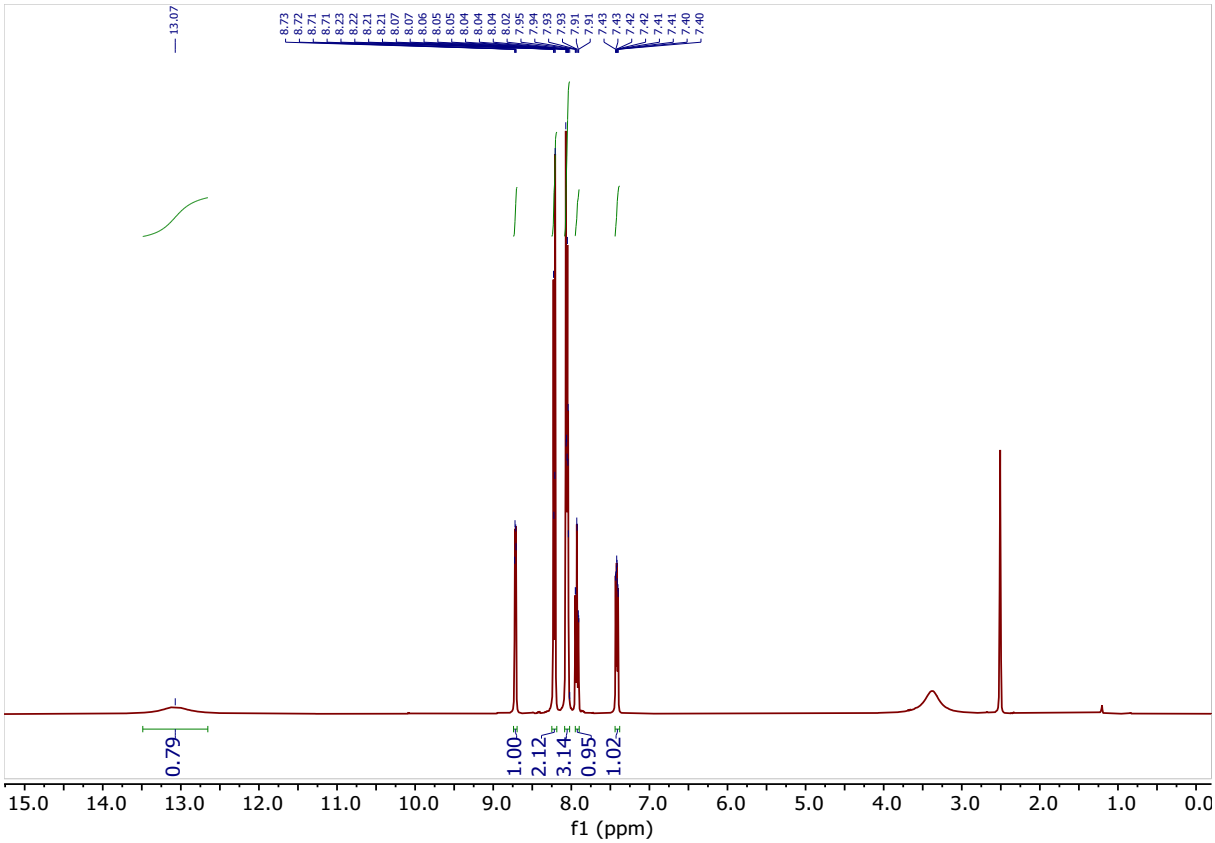


Figure S1. ^{1}H NMR spectrum of L2 in DMSO-d_6 solvent.

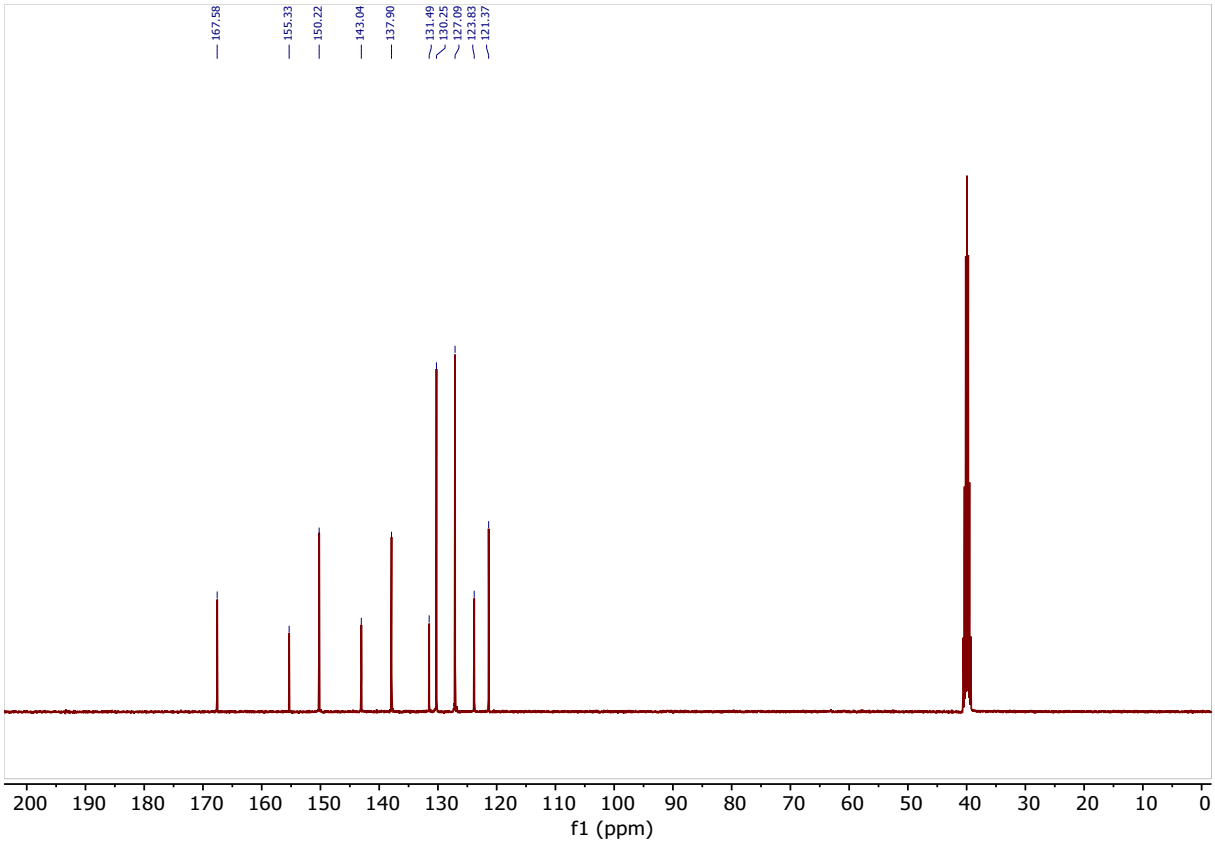


Figure S2. ^{13}C NMR spectrum of L2 in DMSO-d_6 solvent.

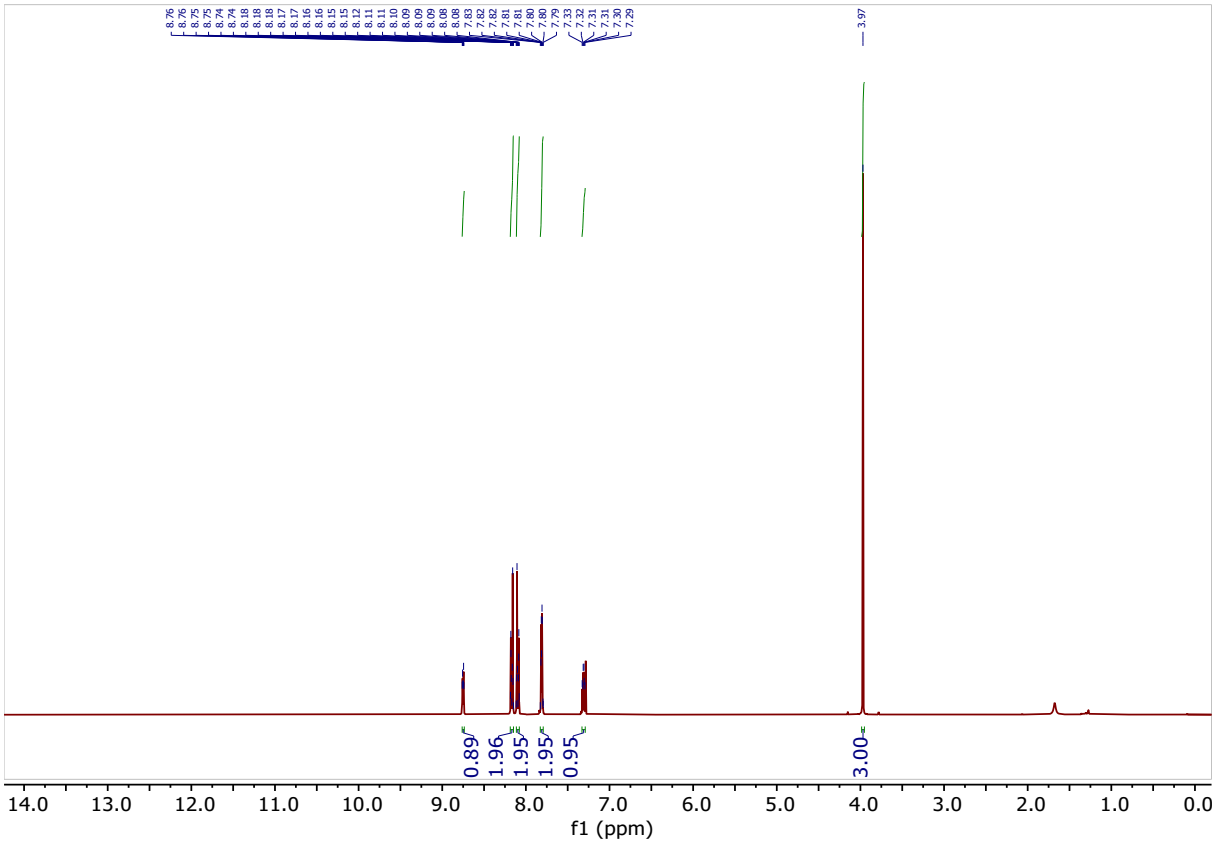


Figure S3. ^{1}H NMR spectrum of L3 in $CDCl_3$ solvent.

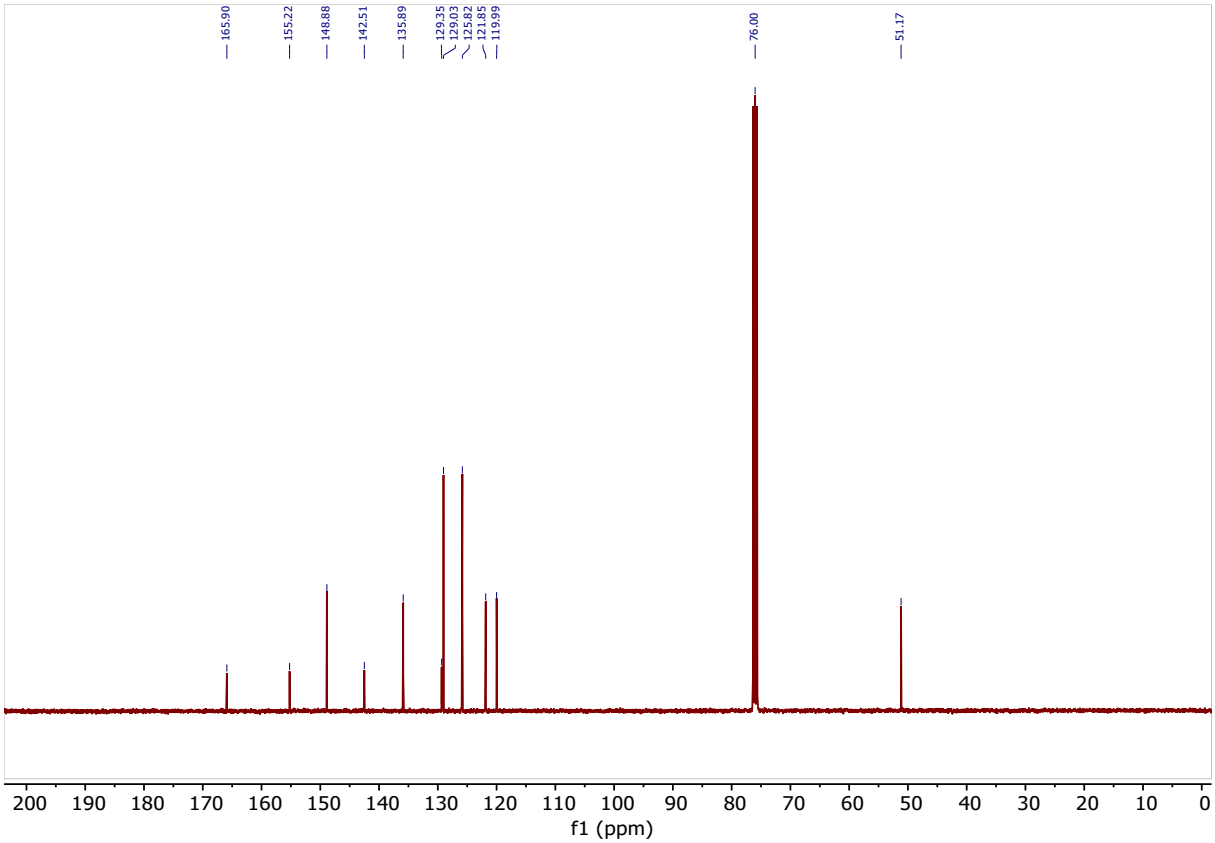


Figure S4. ^{13}C NMR spectrum of L3 in $CDCl_3$ solvent.

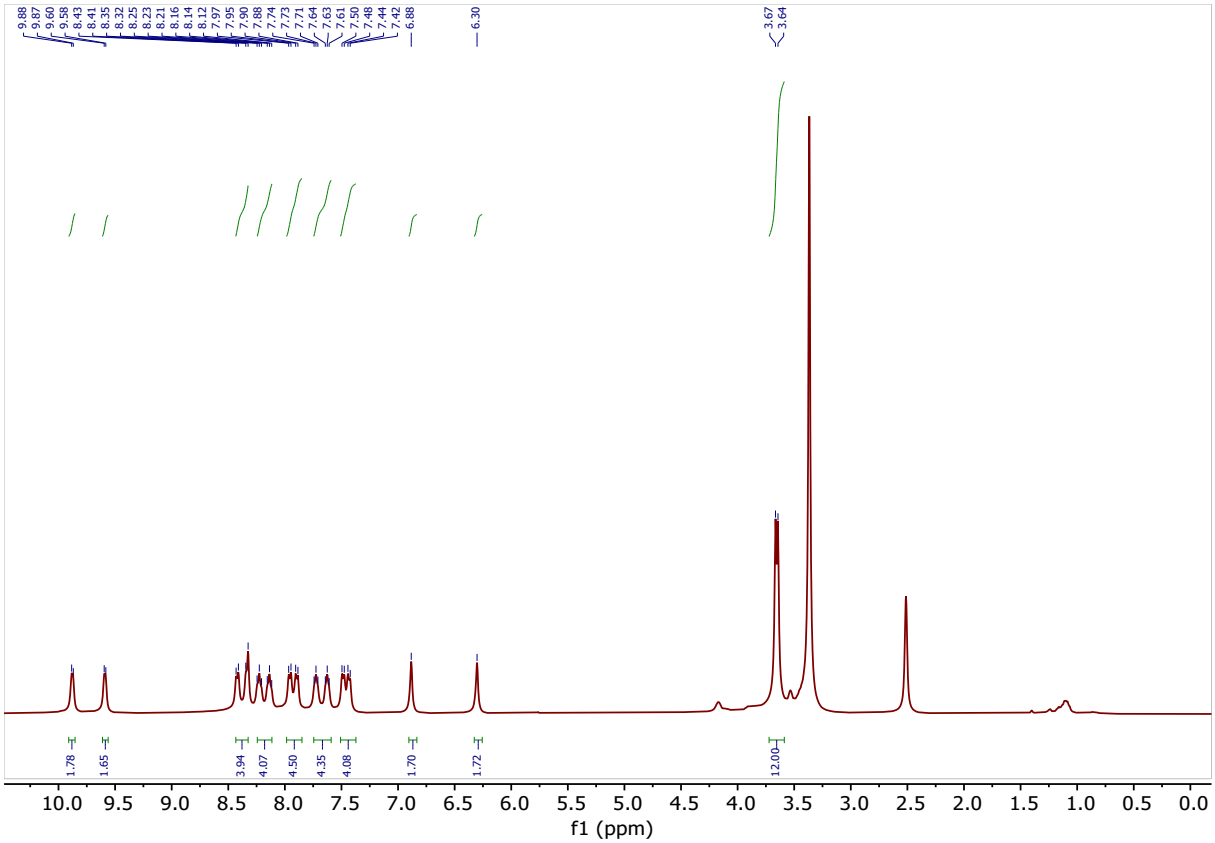


Figure S5. [1]H NMR spectrum of M1 in DMSO-d_6 solvent.

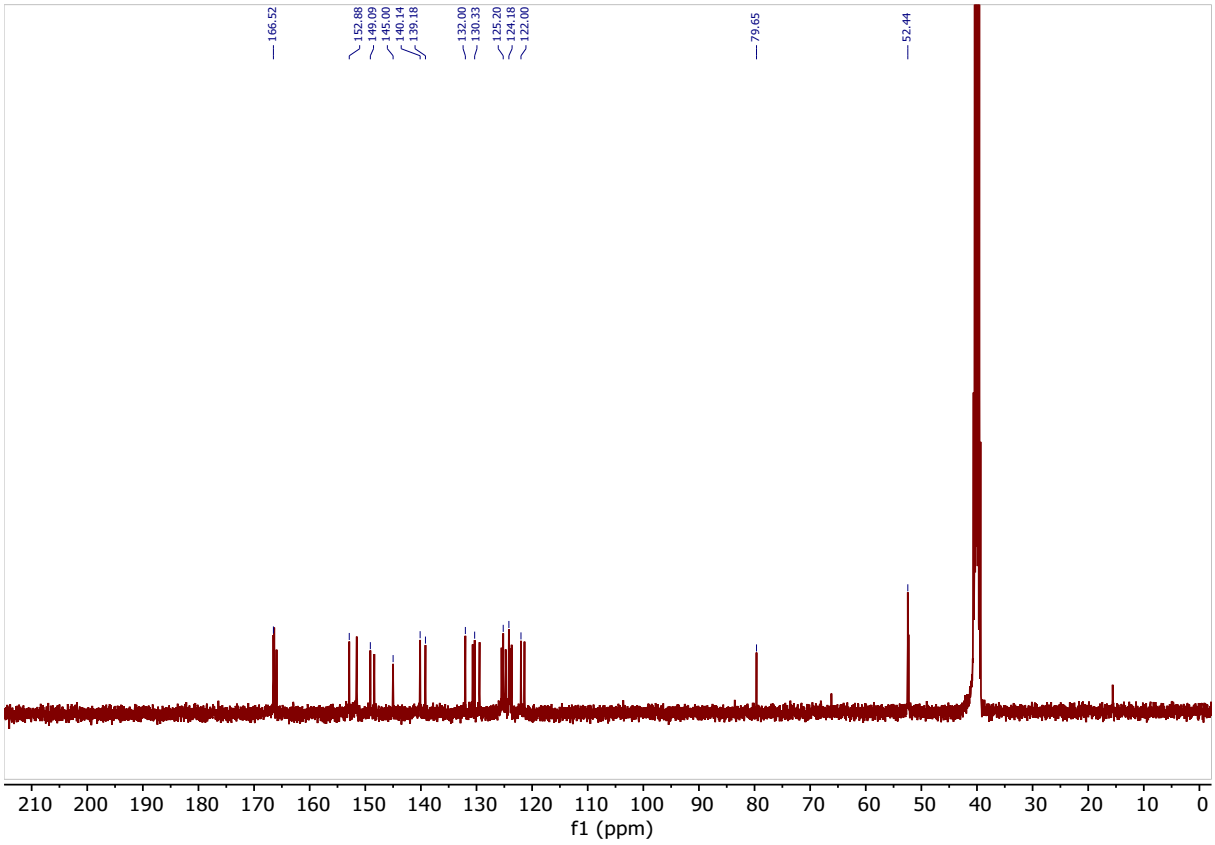


Figure S6. ^{13}C NMR spectrum of M1 in DMSO-d_6 solvent.

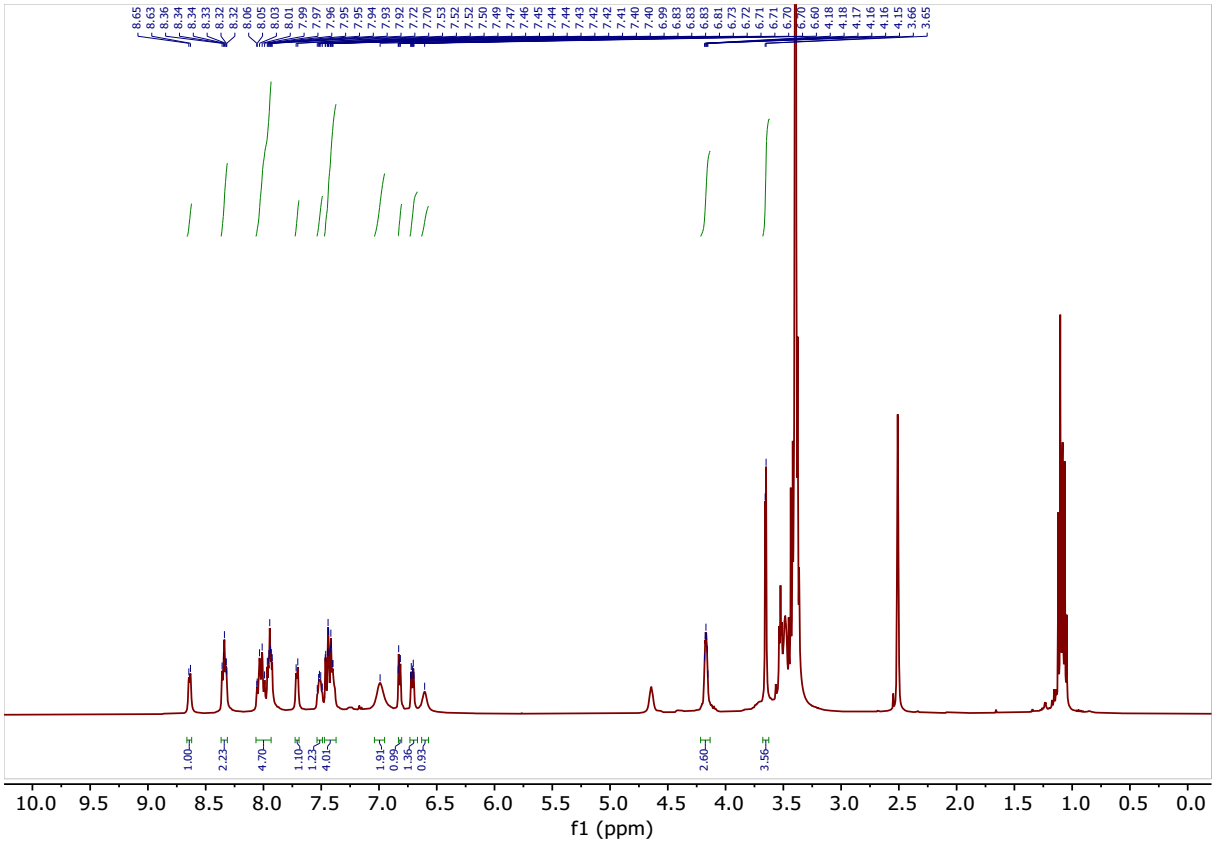


Figure S7. ^{1}H NMR spectrum of M2 in DMSO-d_6 solvent.

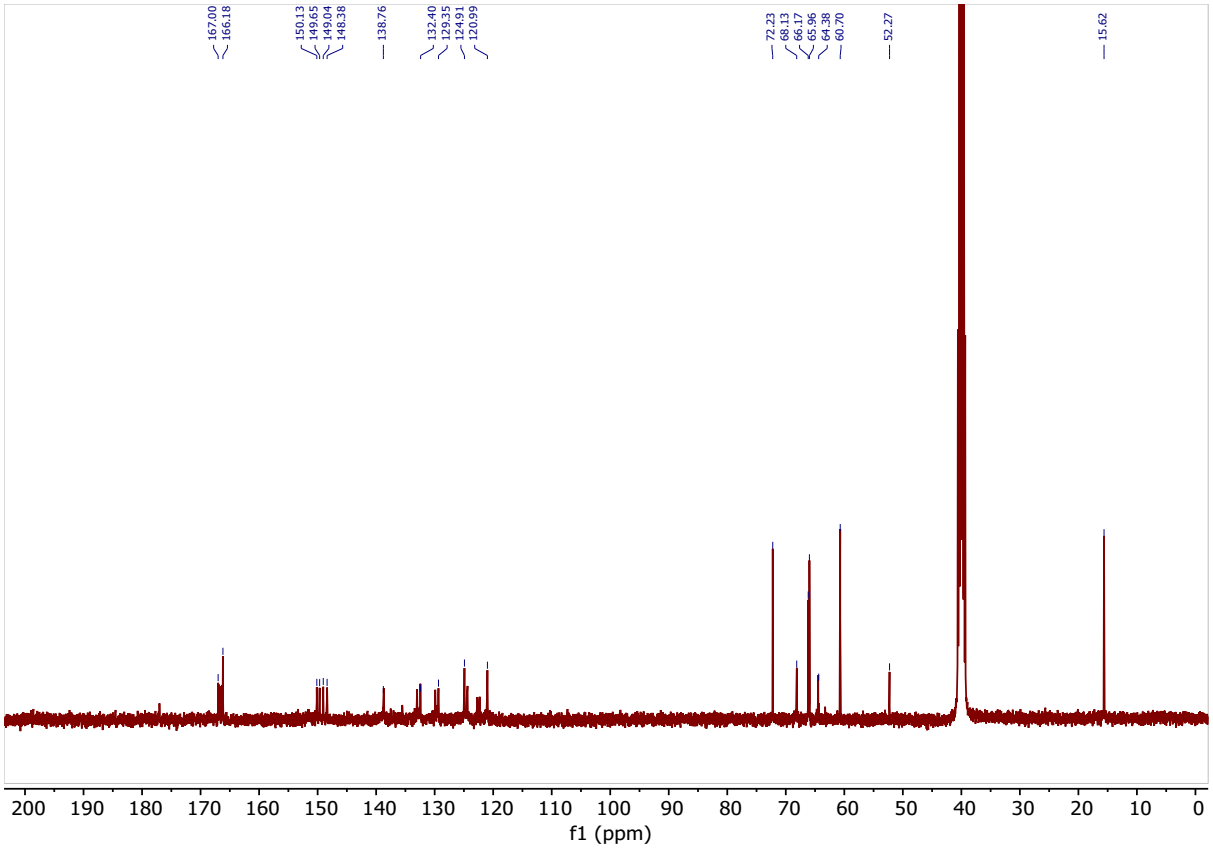


Figure S8. ^{13}C NMR spectrum of M2 in DMSO-d_6 solvent.

MS zoomed spectra:

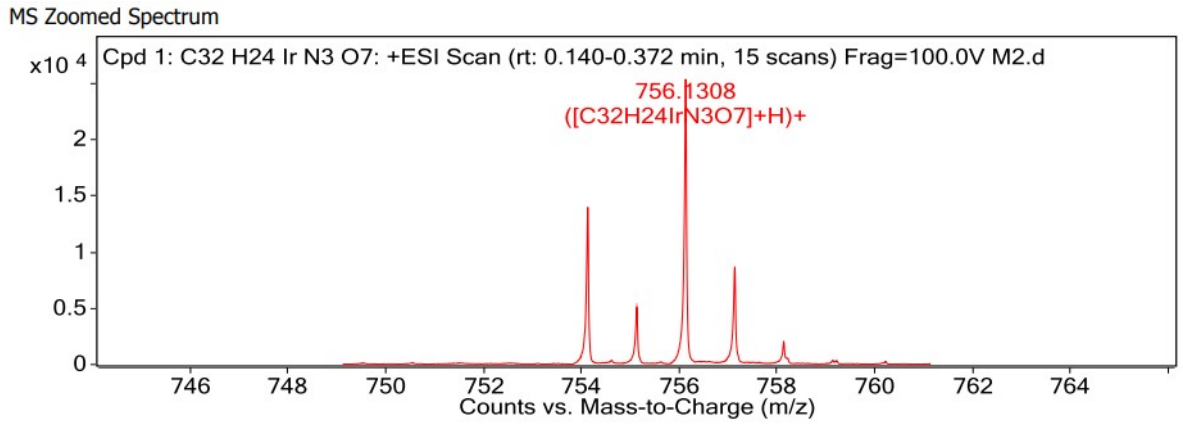


Figure S9. Mass spectrum of compound M2.

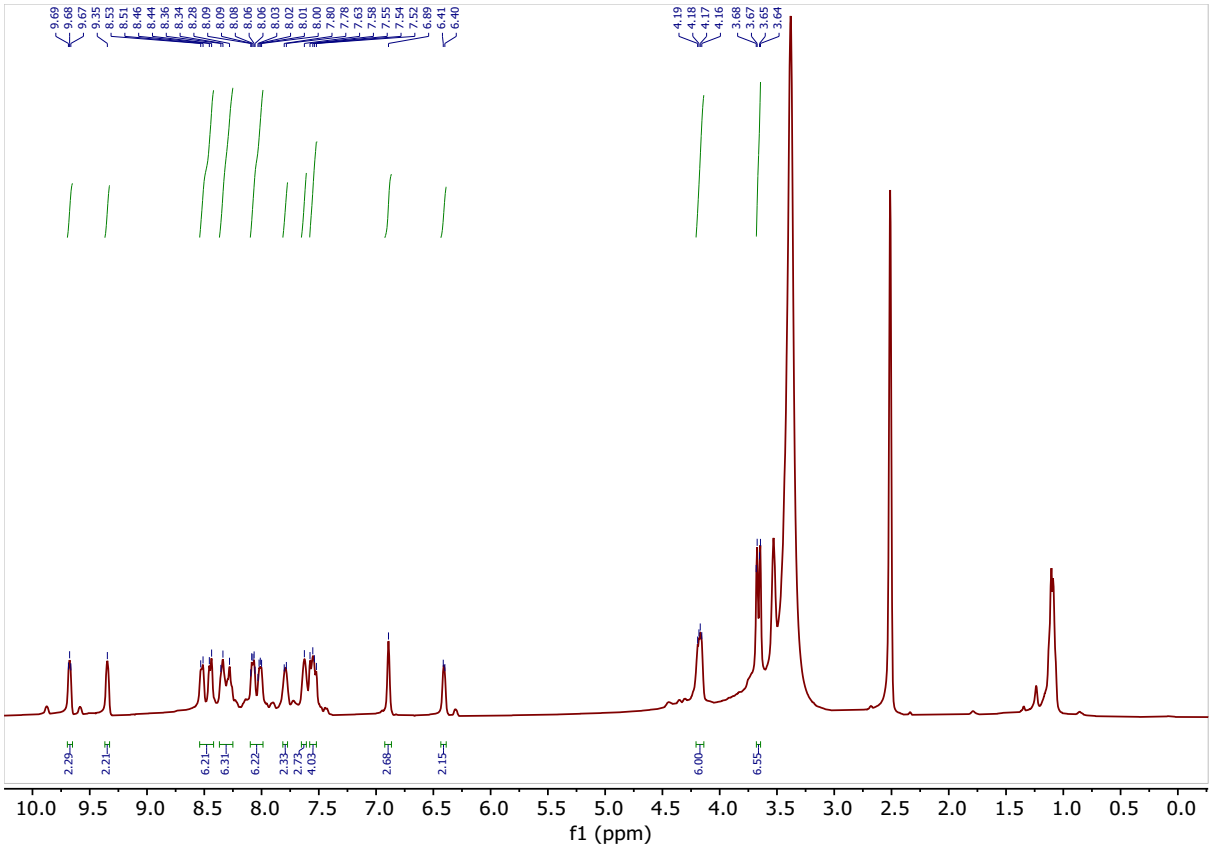


Figure S10. ^{1}H NMR spectrum of M3 in DMSO-d_6 solvent.

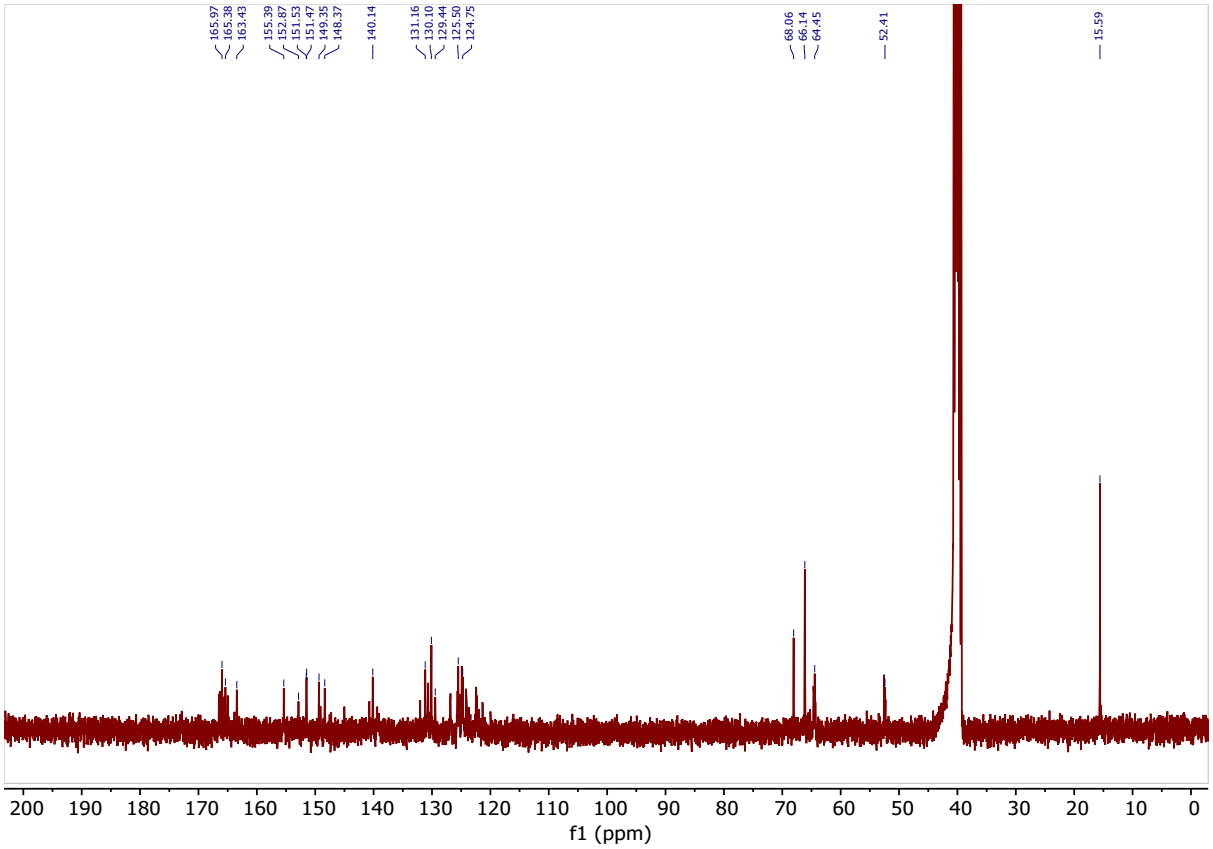


Figure S11. ^{13}C NMR spectrum of M3 in DMSO-d_6 solvent.

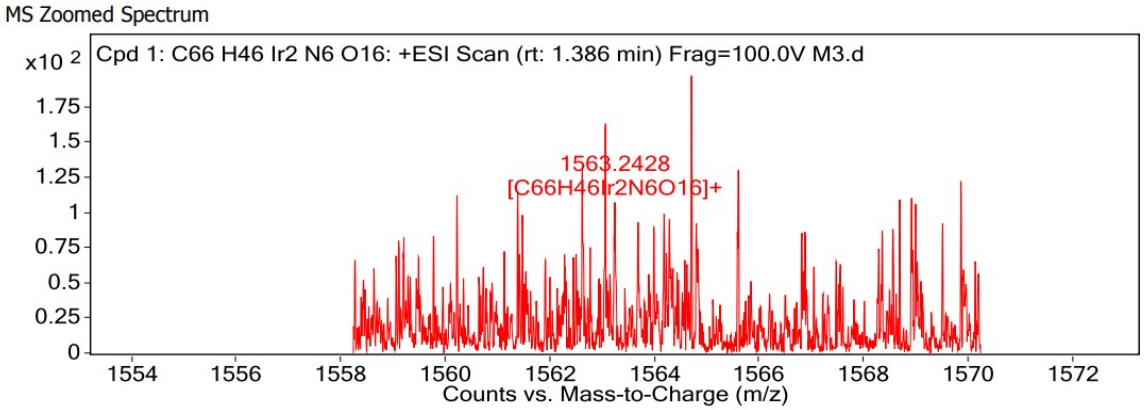


Figure S12. Mass spectrum of compound M3.

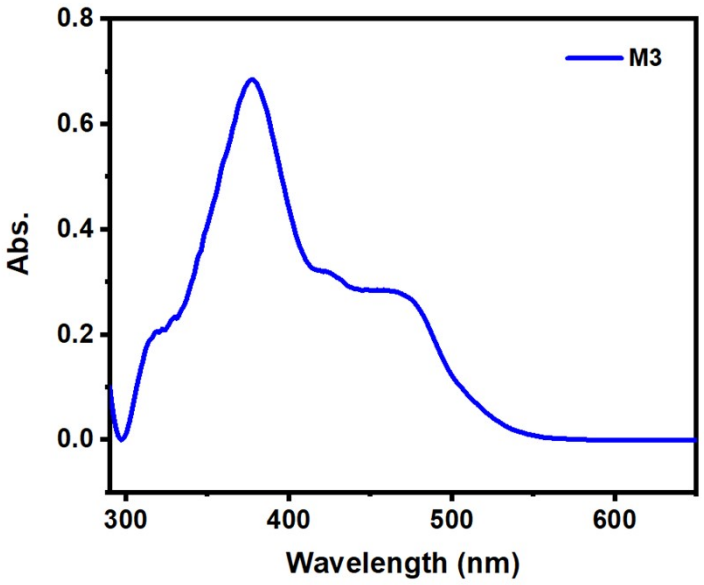


Figure S13. Absorption plot for solid-state M3.

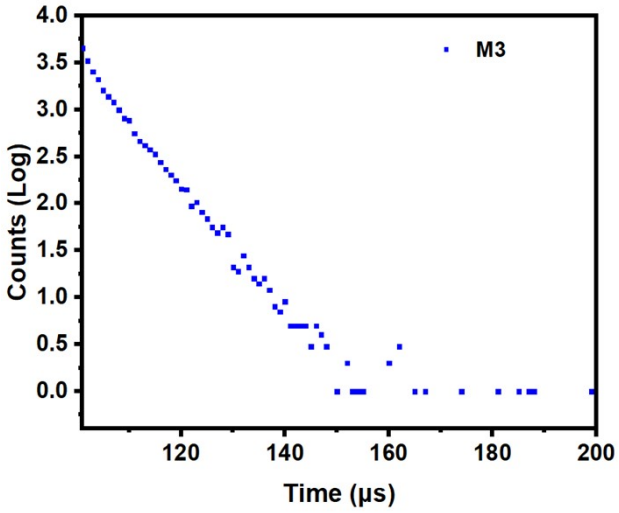


Figure S14. The characteristic fluorescence lifetime decay curve for THF solution of M3 (10^{-5} M) ($\chi^2 = 1.2$).

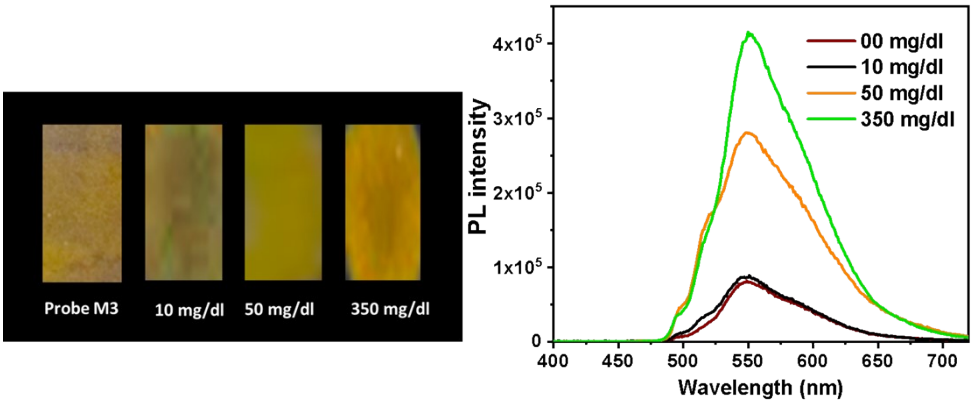


Figure S15. Photograph of paper strip impregnated with M3 probe and after treating with different concentrations of aqueous Crt9 with recorded PL emission plot.

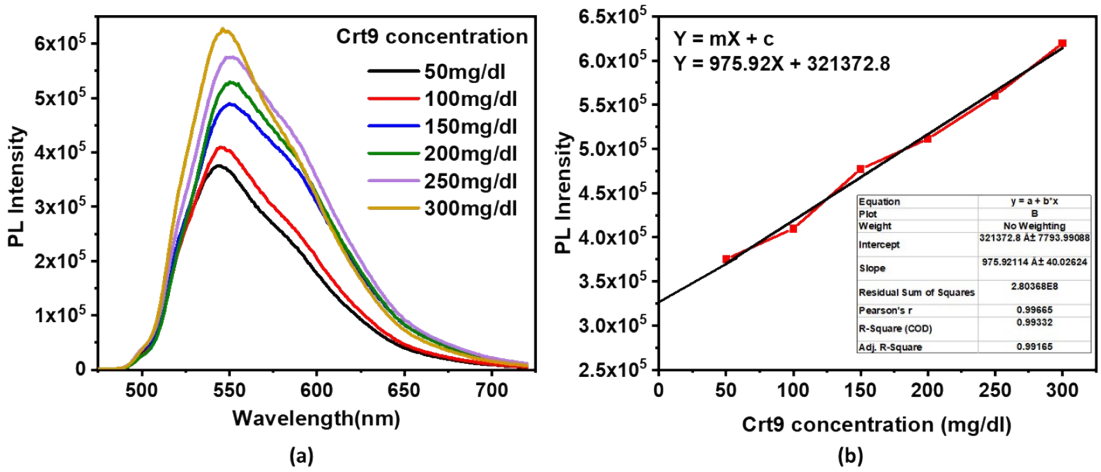


Figure S16. (a) PL spectra recorded for M3-impregnated paper strip after treated with different concentrations of aqueous creatinine solutions; (b) Calibration curve for the same.

Table S1. Different techniques for creatinine detection.

Sr. No.	Methods	Sensitivity	Reference
1.	Computer Screen Photo Assisted Technology (CSPT)	89-111 µmol/L (1.07-1.25 mg/dl)	*1*
2.	High Performance Liquid Crystallography (HPLC)	1.49 mg/dl	*2*
3.	Electrophoretic	2.4 mg/L (0.24 mg/dl)	*3*
4.	Strip Assay Technique	0.04 mg/mL (4 mg/dl)	*4*
5.	Tandem Mass Spectroscopy	303 mol/L (3.42×10^6 mg/dl)	*5*
6.	Portable Raman Spectrometer	1.45 mg/L (0.145 mg/dl)	*6*
7.	Enzymeless Electrochemical	5.0 µM (0.056 mg/dl)	*7*
8.	Differential Pulse Voltammetery	144 nM (0.00128 mg/dl)	*8*
9.	Photochemical Biosensor Connected to the Smartphone	0.03 µmol/L (0.00033 mg/dl)	*9*
10.	Fluorescent Biosensor	5.1×10^{-16} mg/dl	*10*
11.	This work	50 mg/dl	

Samples	Clinical Data (mg/dl)	M3 Data (mg/dl)
S1	50	30.7
S2	200	206
S3	CKD	274

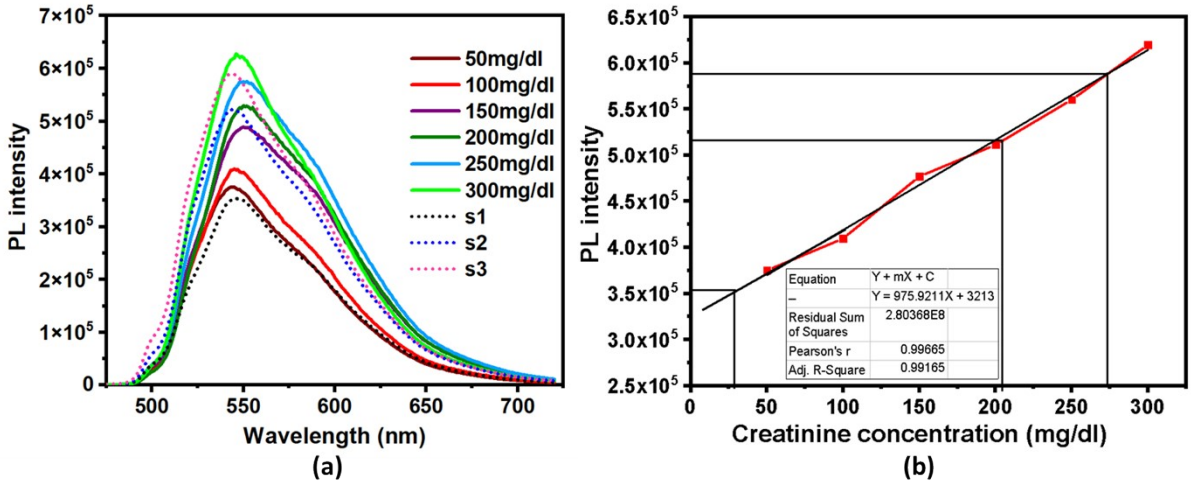


Figure S17. Creatinine detection from the urine samples of non-CKD and the person suffering from CKD, (a) PL emission spectra for different concentrations of aqueous Crt9, non-CKD person's sample (S1, S2), and CKD patient's sample (S3); (b) regression plot for the same.

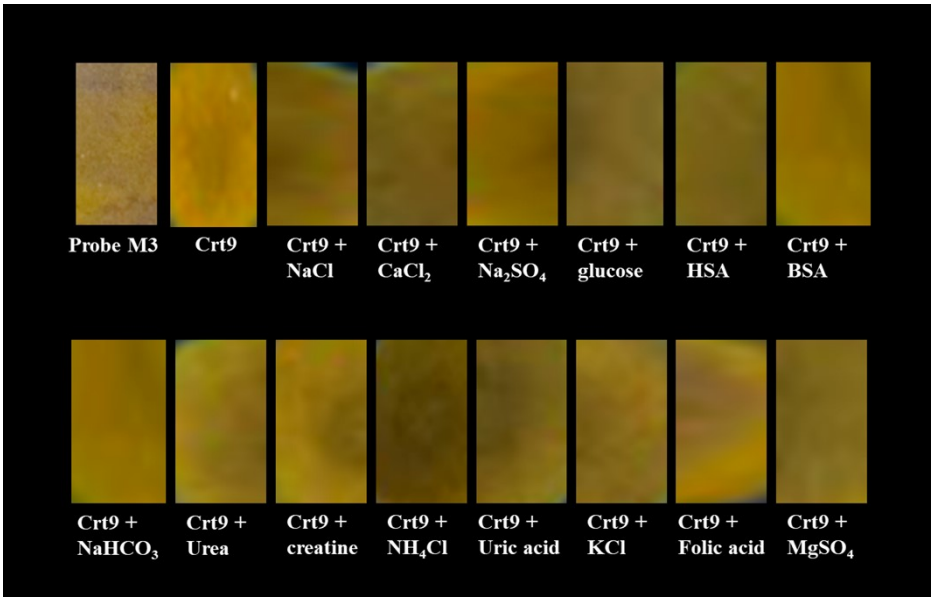


Figure S18. Photograph of probe M3 impregnated filter paper strips under UV lamp (365 nm) after dipping in various aqueous solutions of urine components including metal ions, and biomolecules with creatinine (Crt9).

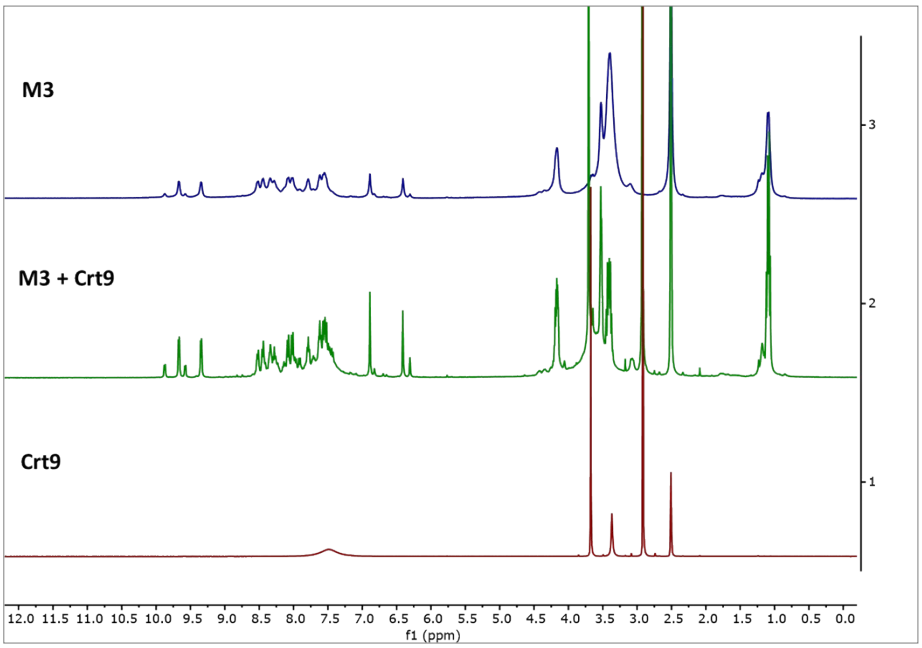


Figure S19. ^{1}H NMR spectrum of M3, M3 + Crt9, and Crt9 in DMSO-d_6 solvent.

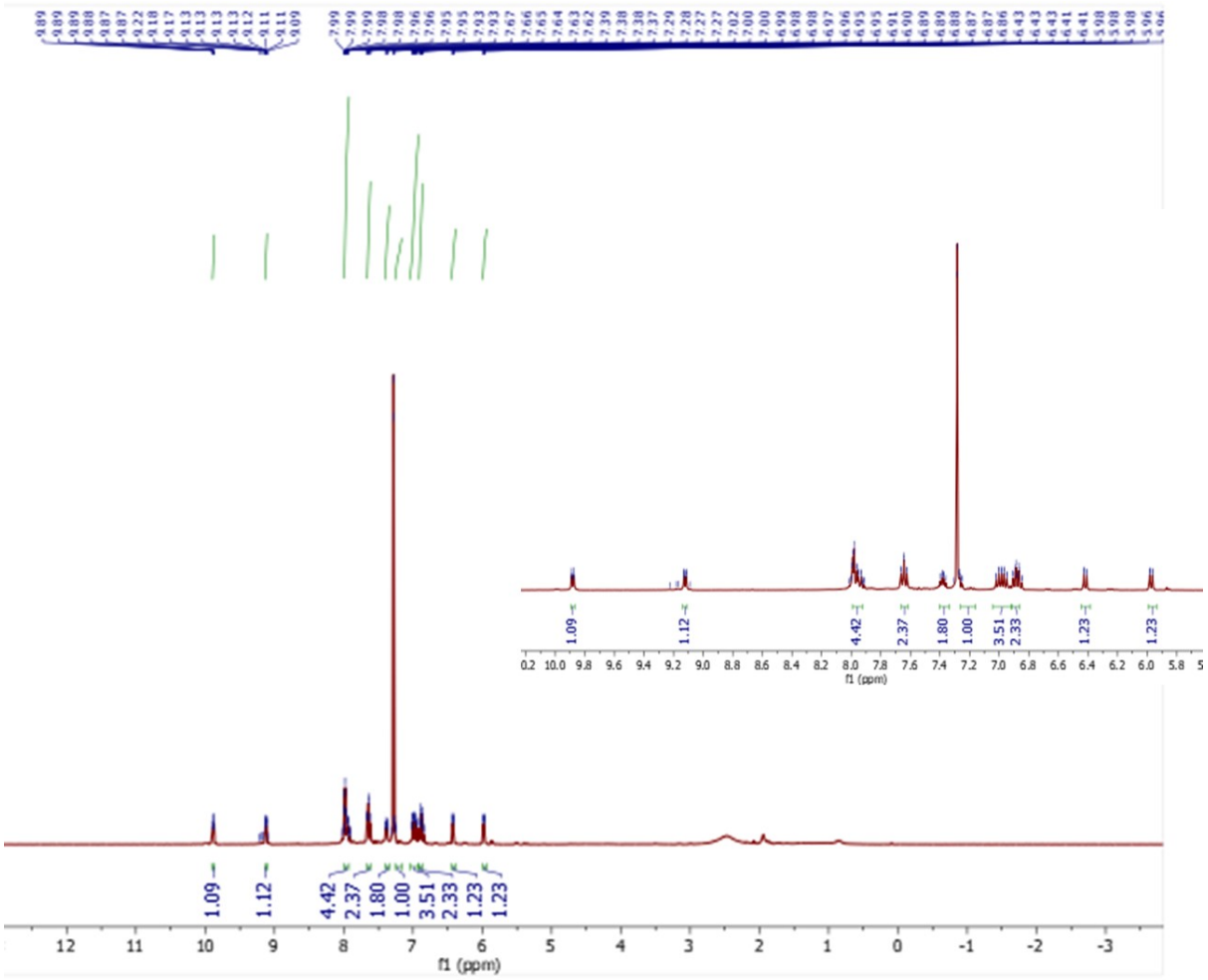


Figure S20. ^{1}H NMR spectrum of M4 in $CDCl_3$ solvent.

^{1}H NMR of M4 (400 MHz, Chloroform-*d*) δ 9.88 (dd, *J* = 5.9, 1.3 Hz, 1H), 9.32 – 9.02 (m, 1H), 8.18 – 7.81 (m, 4H), 7.64 (td, *J* = 8.0, 1.4 Hz, 2H), 7.45 – 7.34 (m, 2H), 7.28 (m, *J* = 0.5 Hz, 1H), 6.98 (dtd, *J* = 14.7, 7.4, 1.2 Hz, 4H), 6.93 – 6.83 (m, 2H), 6.48 – 6.36 (m, 1H), 6.03 – 5.89 (m, 1H).

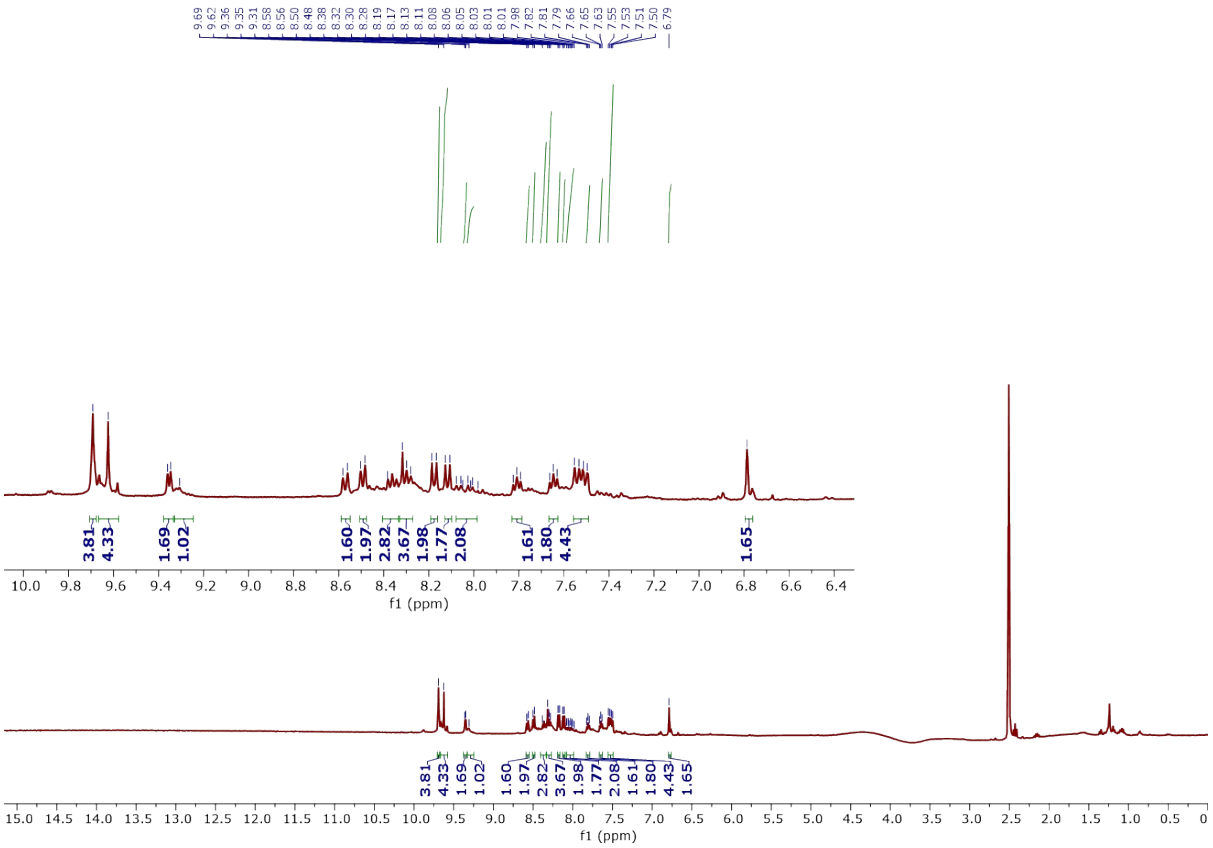


Figure S21. ^{1}H NMR spectrum of M5 in DMSO-d_6 solvent.

^{1}H NMR of M5 (400 MHz, DMSO-d_6) δ 9.69 (s, 4H), 9.62 (d, 4H), 9.35 (d, *J* = 5.7 Hz, 2H), 9.31 (s, 1H), 8.57 (d, *J* = 8.1 Hz, 2H), 8.49 (d, *J* = 8.0 Hz, 2H), 8.38 (s, 3H), 8.33 – 8.28 (m, 4H), 8.17 (s, 2H), 8.12 (d, *J* = 8.1 Hz, 2H), 8.08 – 7.98 (m, 2H), 7.83 – 7.78 (m, 2H), 7.67 – 7.62 (m, 2H), 7.52 (dd, *J* = 15.3, 7.4 Hz, 4H), 6.79 (s, 2H).

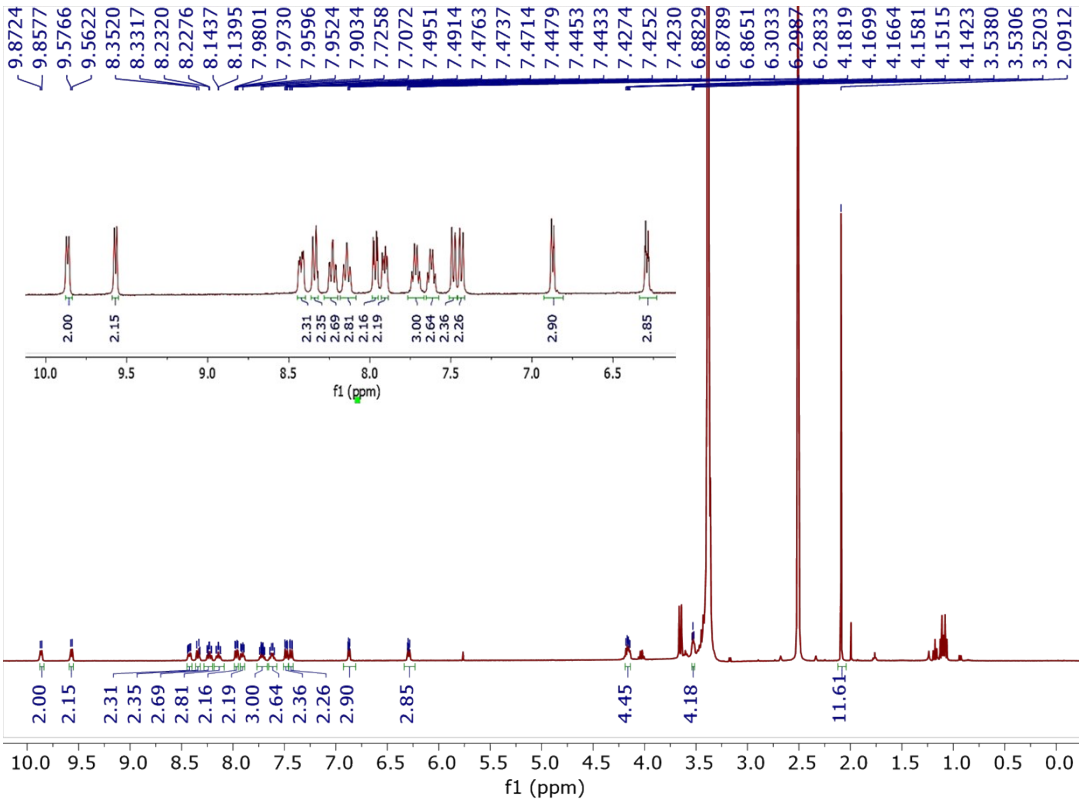
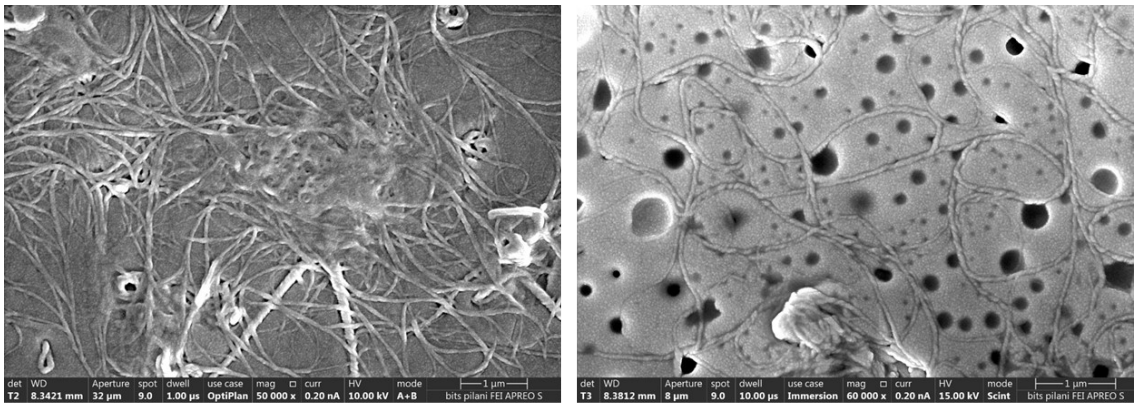


Figure S22. ^{1}H NMR spectrum of M6 in DMSO-d_6 solvent.

^{1}H NMR of M6 (400 MHz, DMSO-d_6) δ 9.87 (d, J = 5.7 Hz, 2H), 9.57 (d, J = 5.7 Hz, 2H), 8.42 (dd, J = 7.9, 3.4 Hz, 2H), 8.34 (d, J = 8.1 Hz, 2H), 8.28 – 8.18 (m, 3H), 8.14 (td, J = 7.8, 1.8 Hz, 3H), 7.97 (dd, J = 8.2, 2.8 Hz, 2H), 7.95 – 7.87 (m, 2H), 7.76 – 7.67 (m, 3H), 7.62 (q, J = 6.1 Hz, 3H), 7.52 – 7.45 (m, 2H), 7.47 – 7.39 (m, 2H), 6.87 (dt, J = 5.5, 1.6 Hz, 3H), 6.29 (dt, J = 6.1, 1.8 Hz, 3H), 4.23 – 4.10 (m, 4H), 3.53 (m, J = 2.7, 2.3 Hz, 4H), 2.09 (s, 12H).



(**a**) (**b**)

Figure S23. FESEM images for; (a) the M3, and (b) Crt9 treated M3.

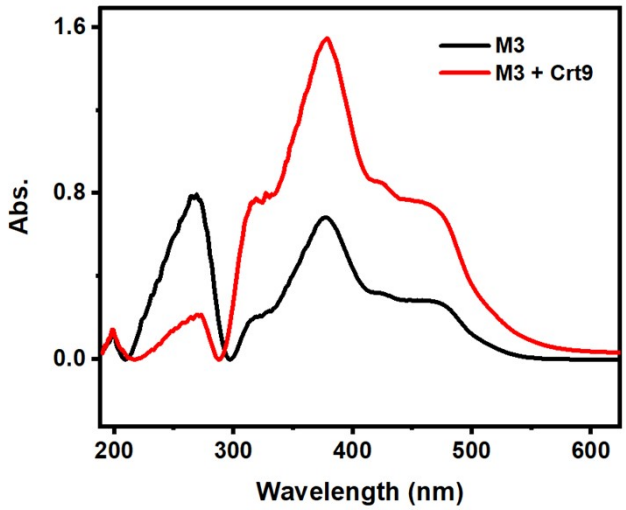


Figure S24. Solid-state absorption spectra for M3 and M3 + Crt9.

References:

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