Electronic Supplementary Information (ESI)

Facile one-pot multicomponent synthesis of peptoid based gelators as novel scaffolds for drug incorporation and pH-sensitive release

Sharol Sebastian,[a] Eqvinshi Yadav,[a] Priya Bhardwaj,[b] Mulaka Maruthi,[b] Deepak Kumar[c] and Manoj K. Gupta [a,*]

[a]*Department of Chemistry, School of Basic Sciences, Central University of Haryana, Mahendergarh 123031, Haryana, India. Email – mkgupta@cuh.ac.in; Phone: +91 9728739075*
[b]*Department of Biochemistry, School of Interdisciplinary and Applied Sciences, Central University of Haryana, Mahendergarh 123031, Haryana, India*
[c]*Department of Pharmaceutical Chemistry, School of Pharmaceutical Sciences, Shoolini University, Solan- 173229, Himachal Pradesh, India*

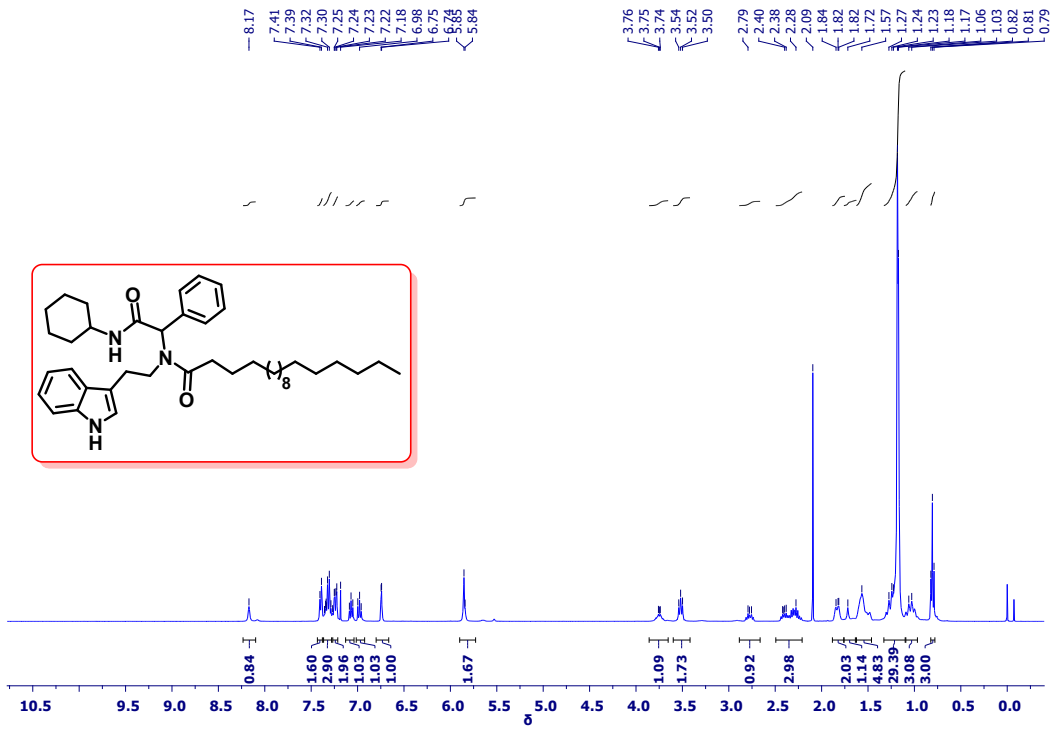

Fig. S1 ^{1}H NMR spectrum of compound **5a**

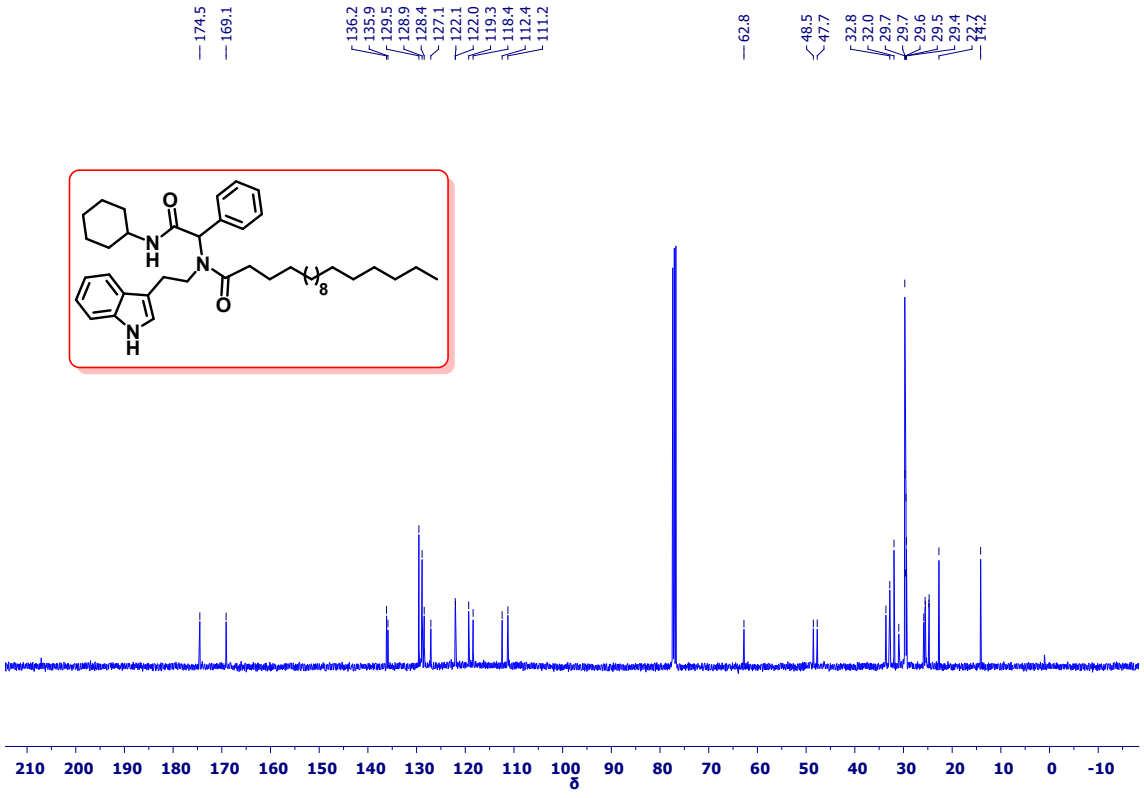

Fig. S2 ^{13}C NMR spectrum of compound **5a**

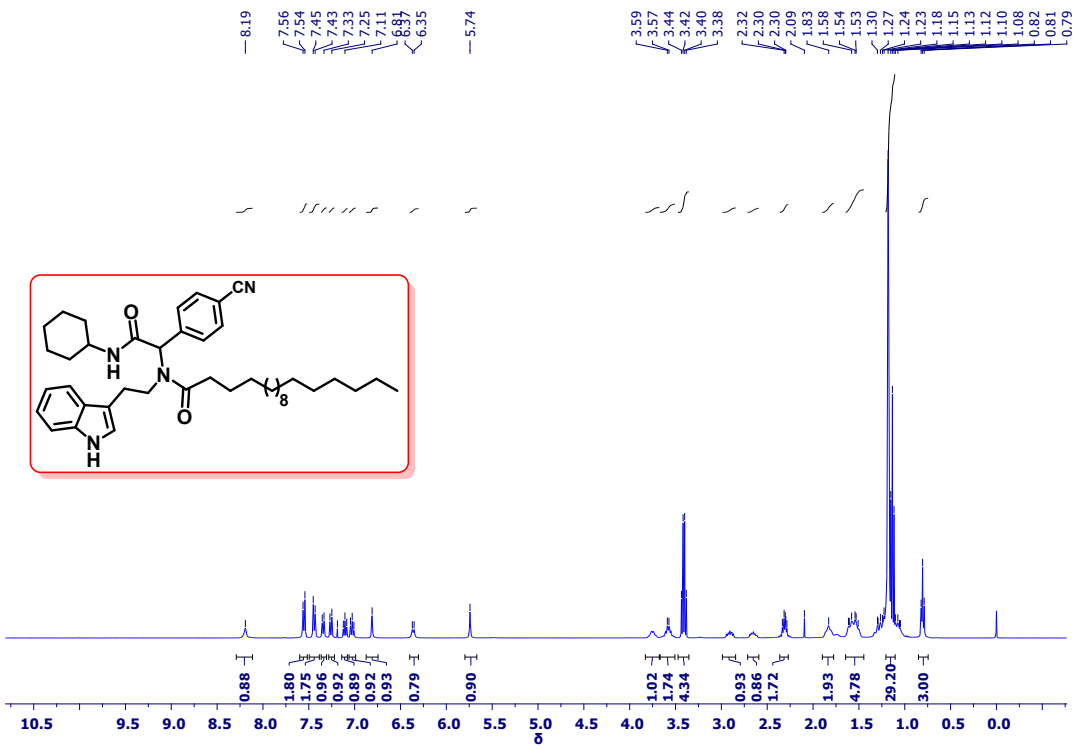

Fig. S3 ^{1}H NMR spectrum of compound **5b**

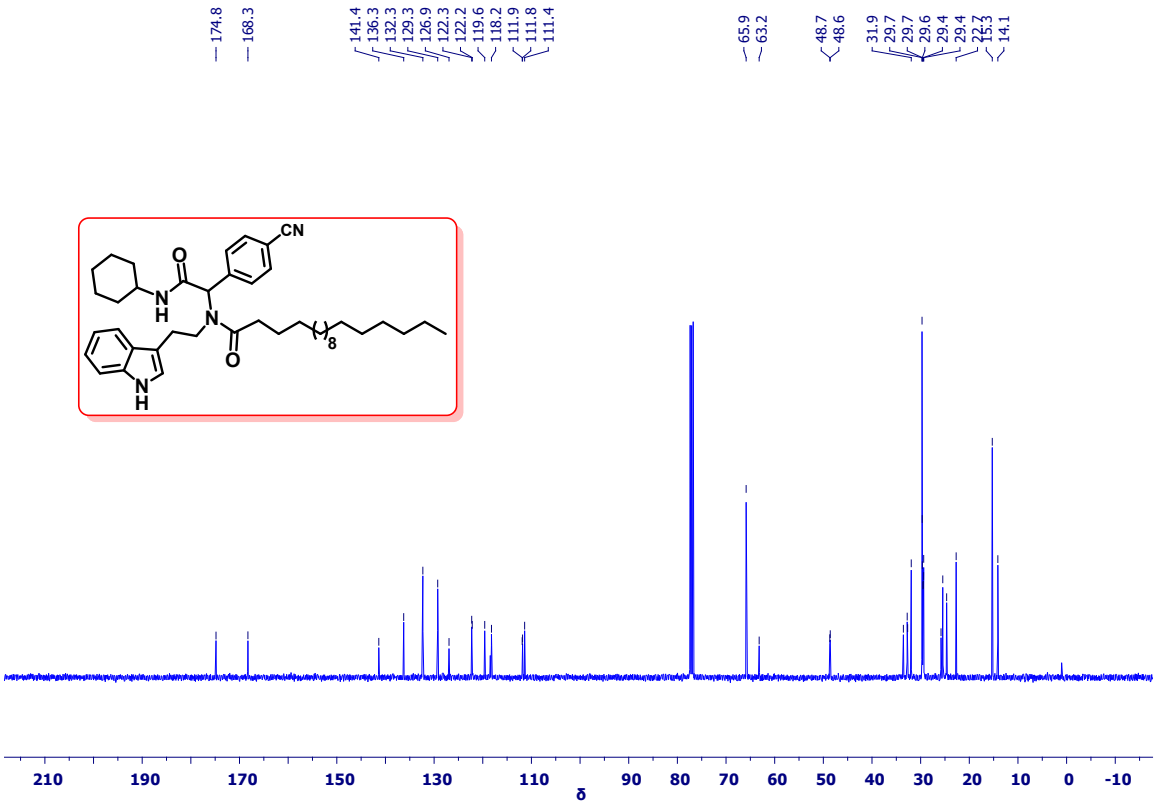

Fig. S4 ^{13}C NMR spectrum of compound **5b**

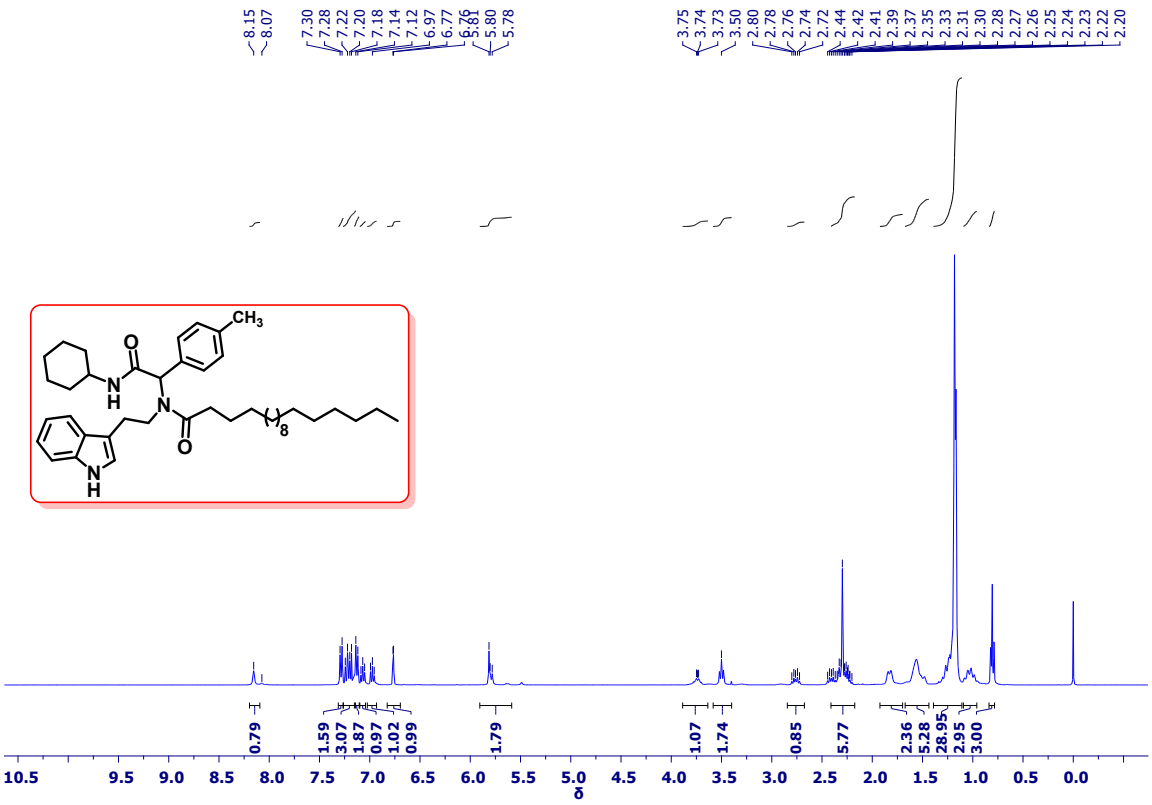

Fig. S5 ^{1}H NMR spectrum of compound **5c**

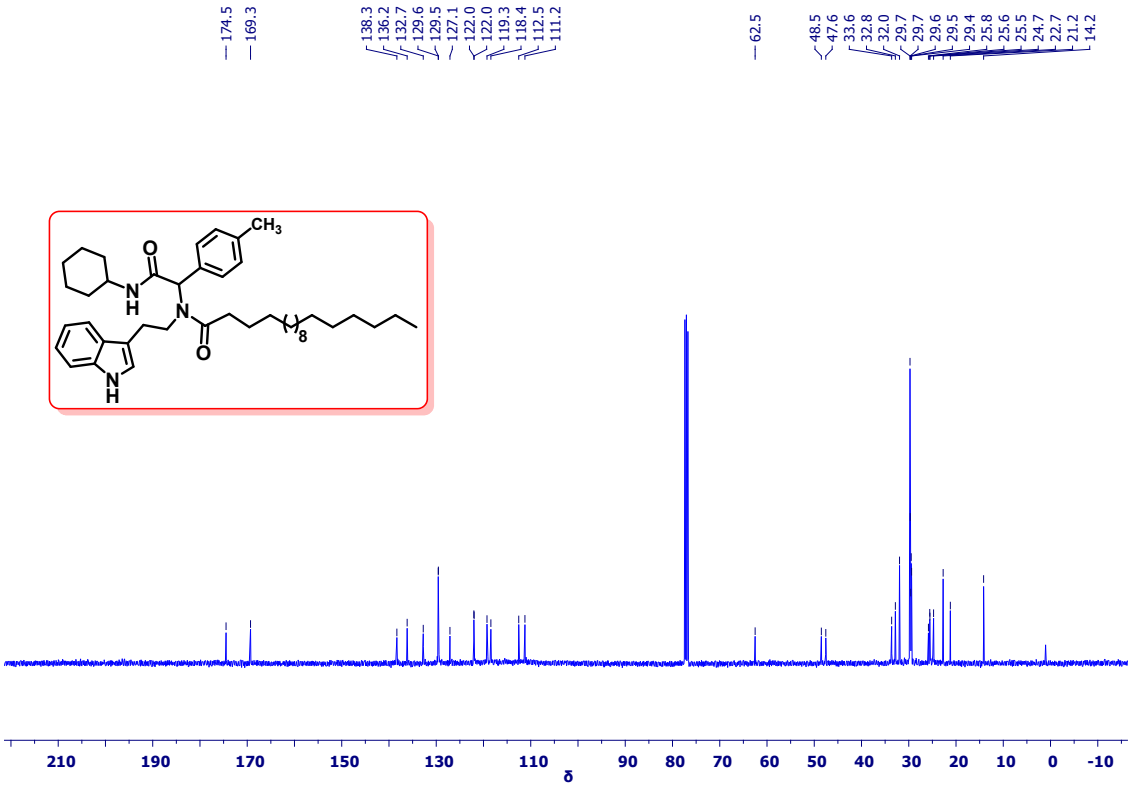

Fig. S6 ^{13}C NMR spectrum of compound **5c**

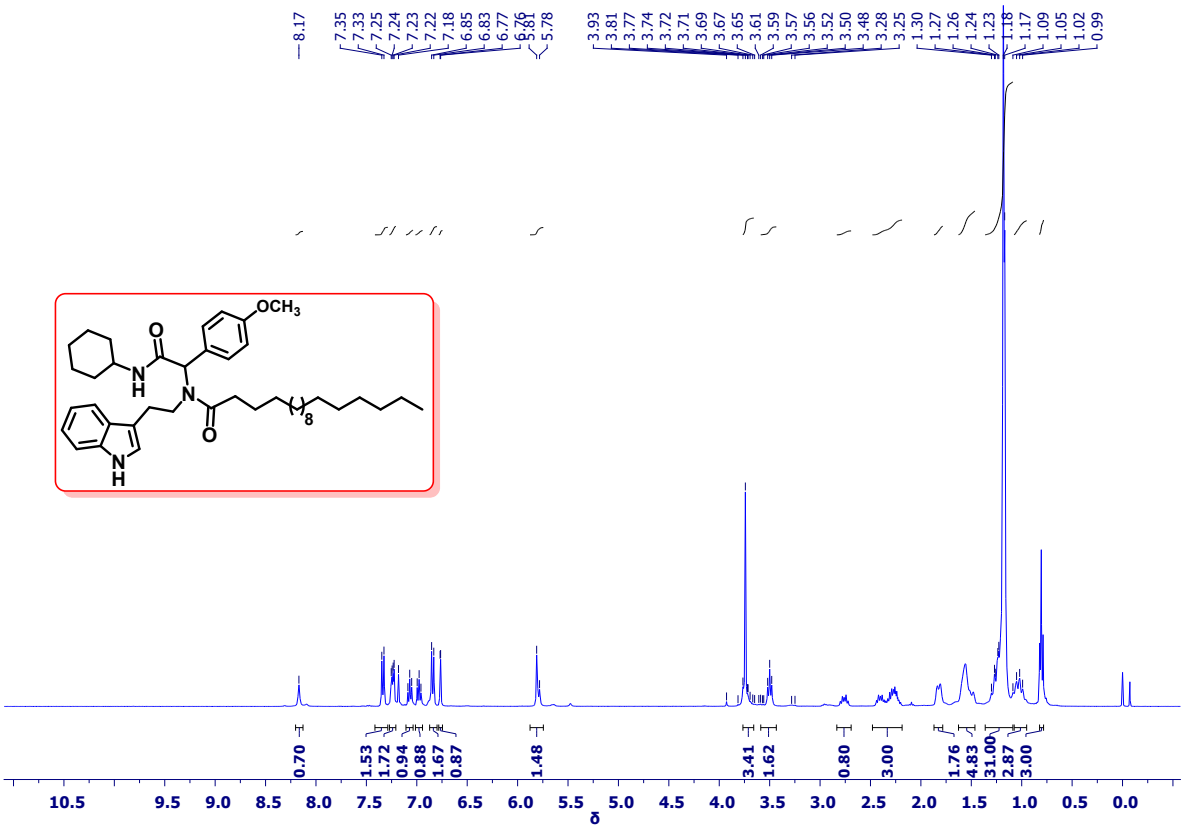

Fig. S7 ^{1}H NMR spectrum of compound **5d**

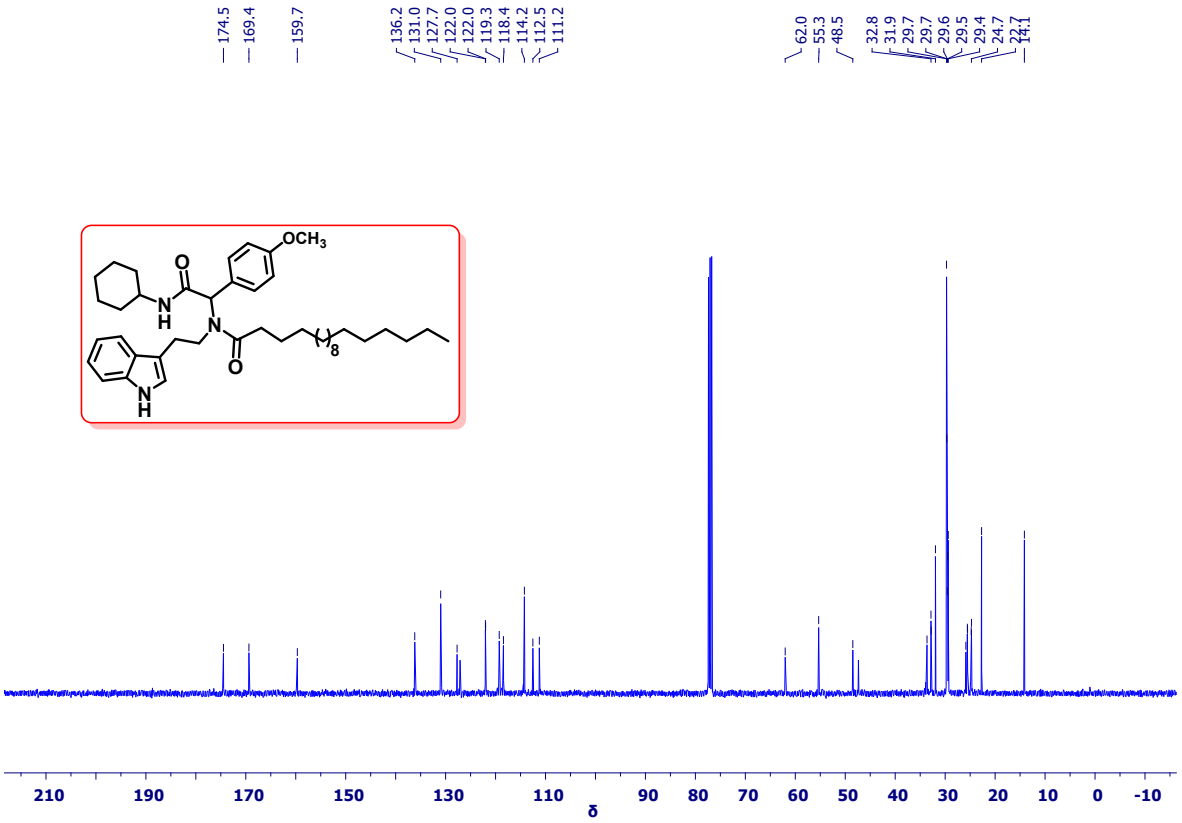

Fig. S8 ^{13}C NMR spectrum of compound **5d**

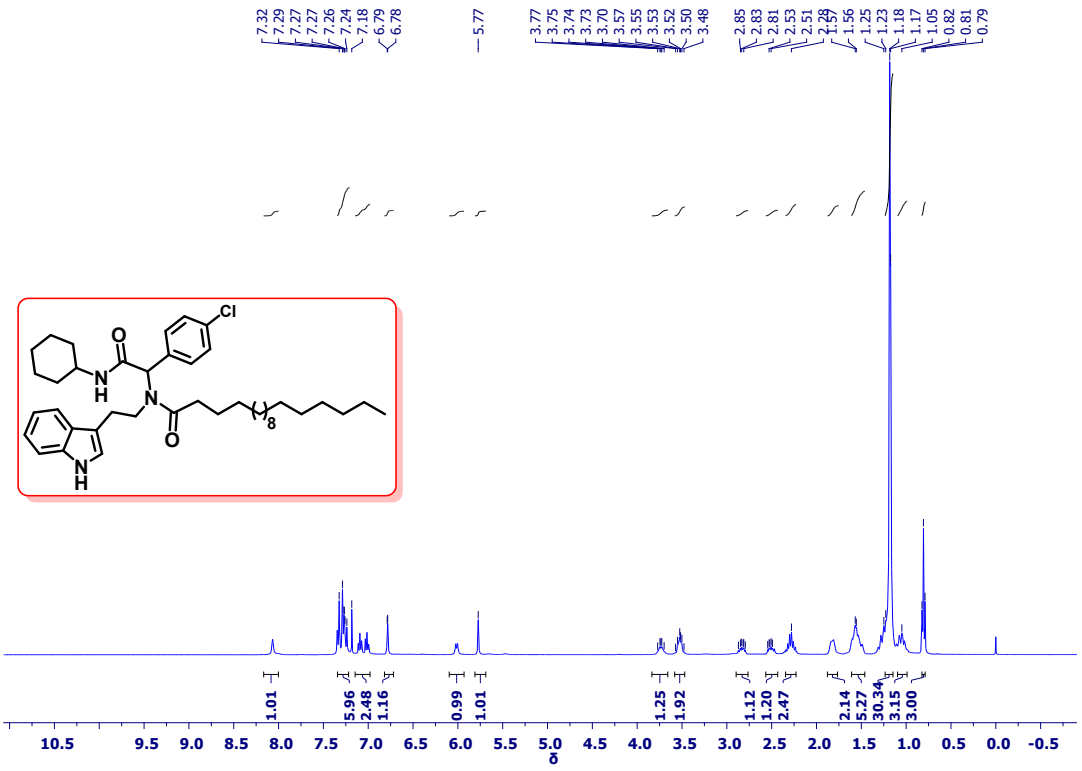

Fig. S9 ^{1}H NMR spectrum of compound **5e**

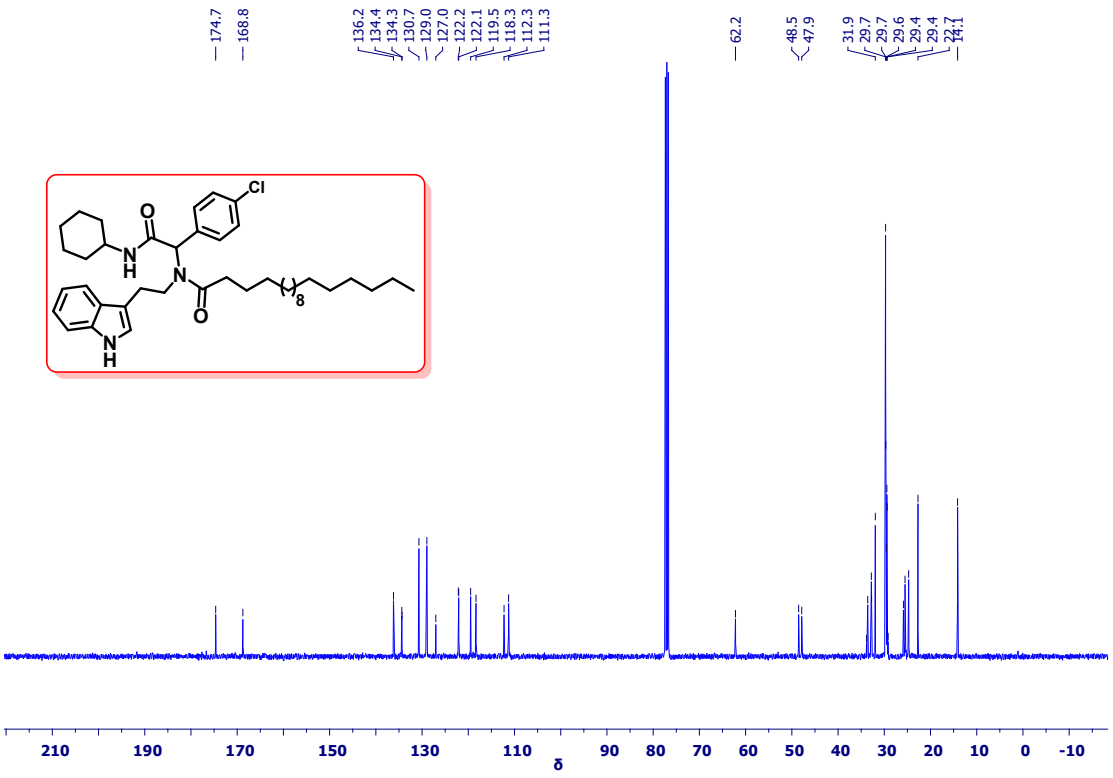

Fig. S10 ^{1}H NMR spectrum of compound **5e**

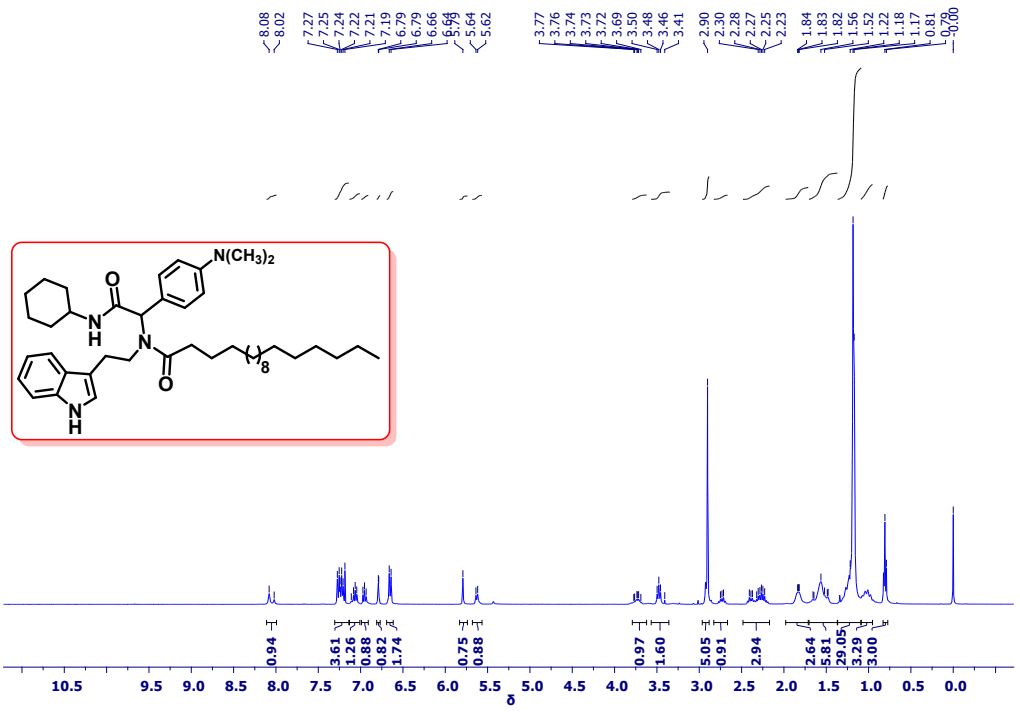

Fig. S11 ^{1}H NMR spectrum of compound **5f**

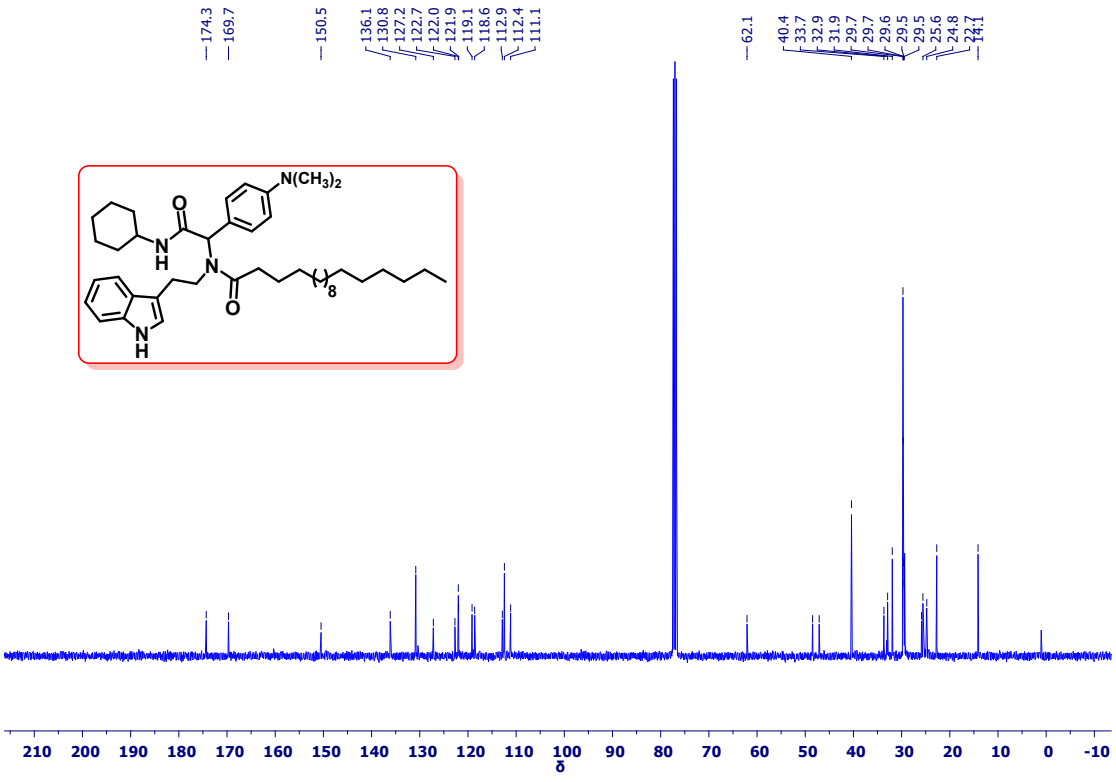

Fig. S12 ^{13}C NMR spectrum of compound **5f**

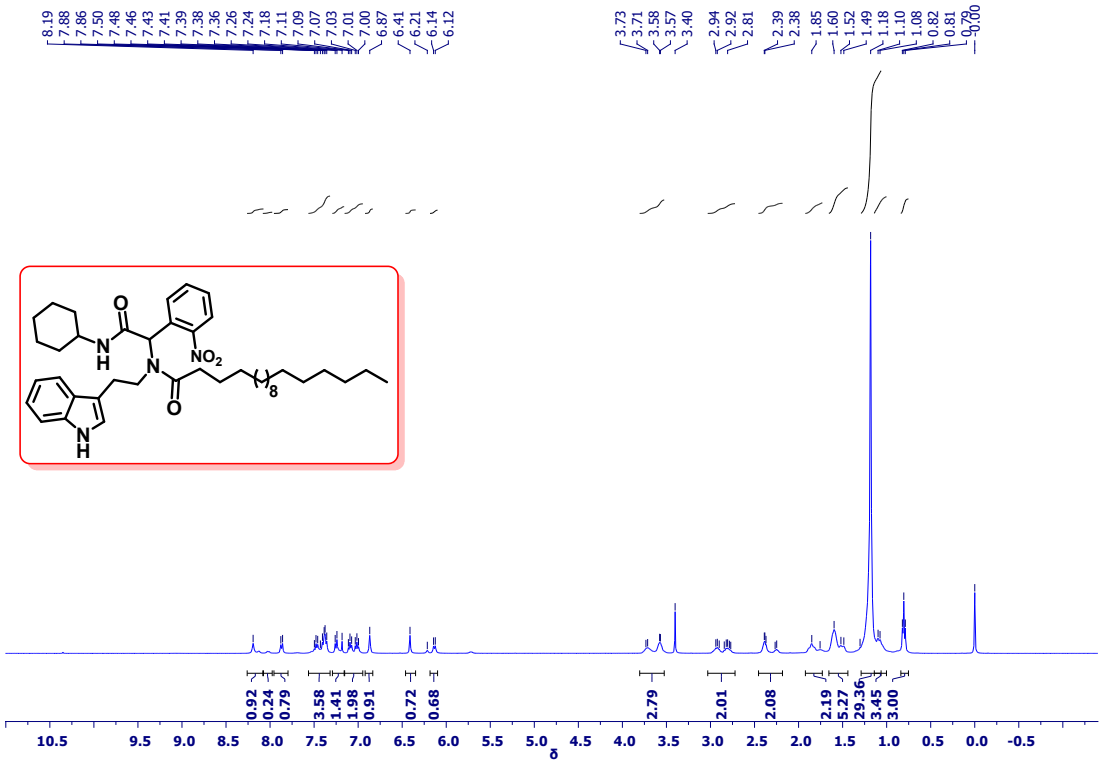

Fig. S13 ^{1}H NMR spectrum of compound **5g**

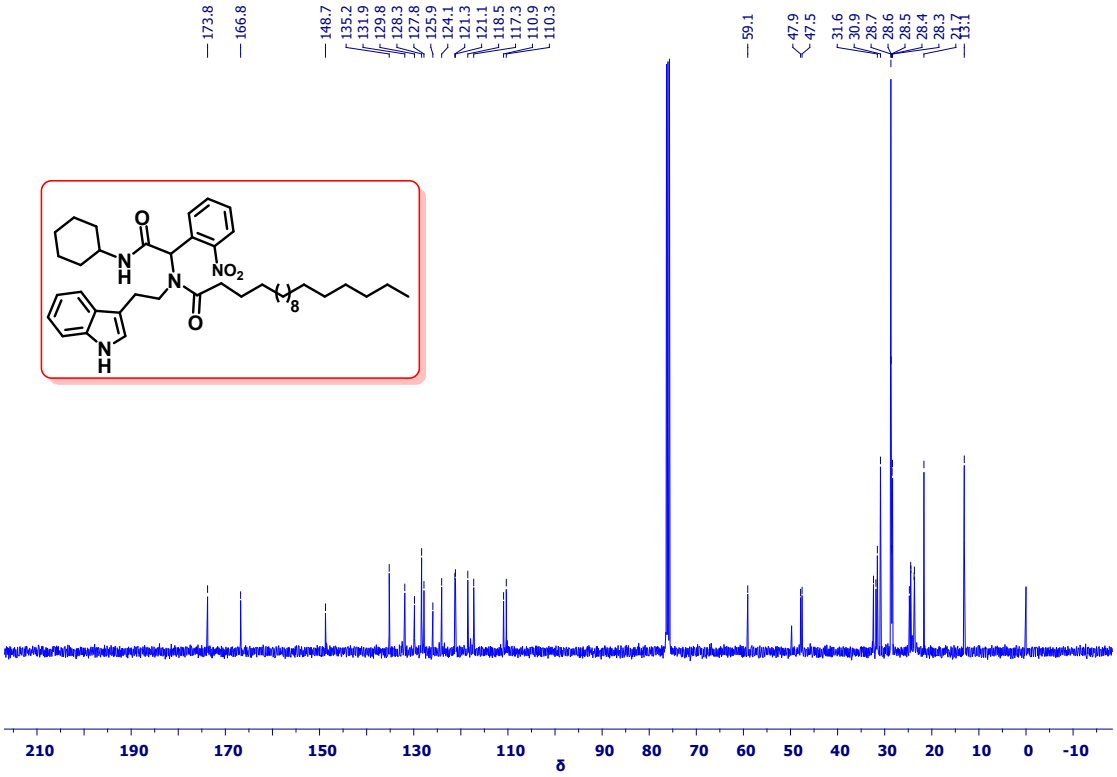

Fig. S14 ^{13}C NMR spectrum of compound **5g**

Fig. S15 ^{1}H NMR spectrum of compound **5h**

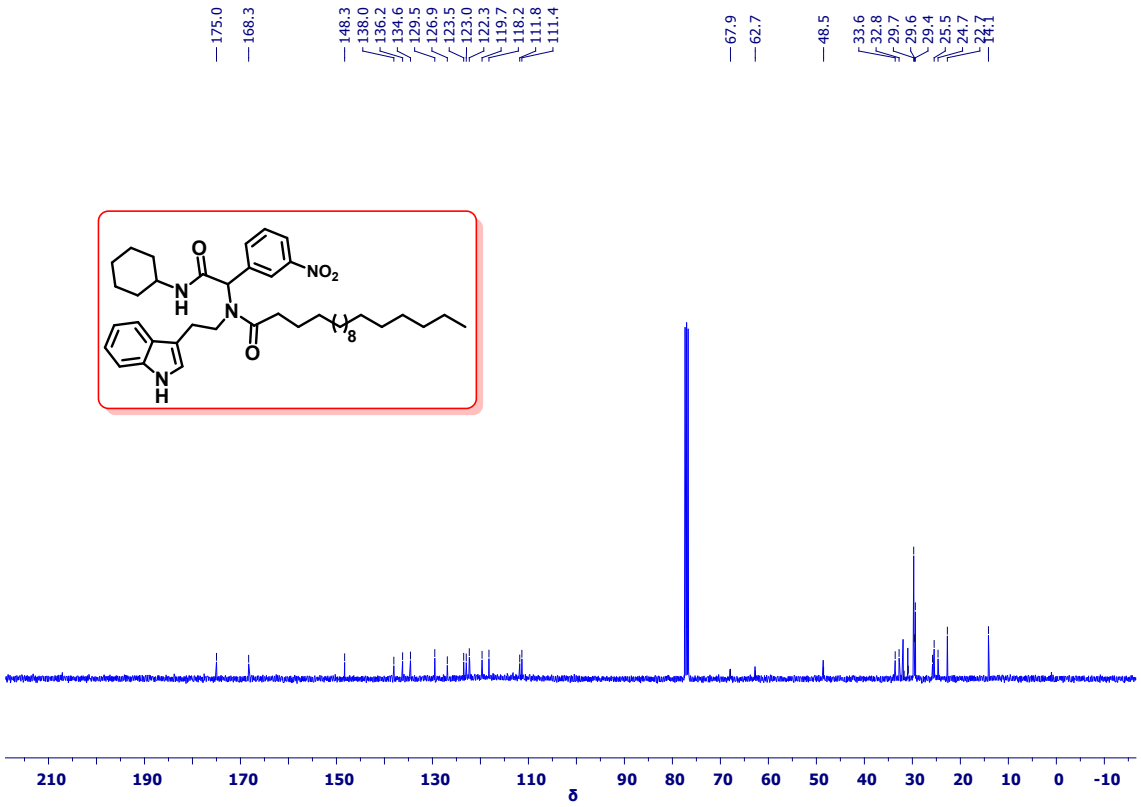

Fig. S16 ^{13}C NMR spectrum of compound **5h**

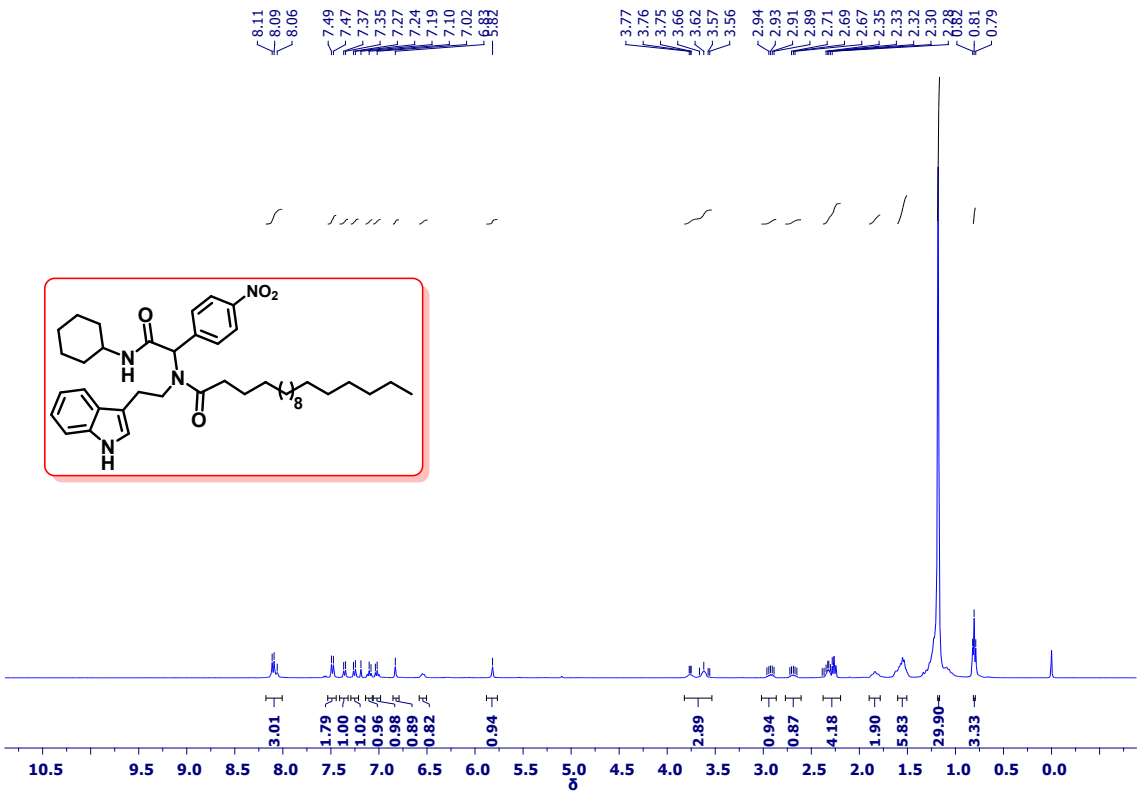

Fig. S17 ^{1}H NMR spectrum of compound **5i**

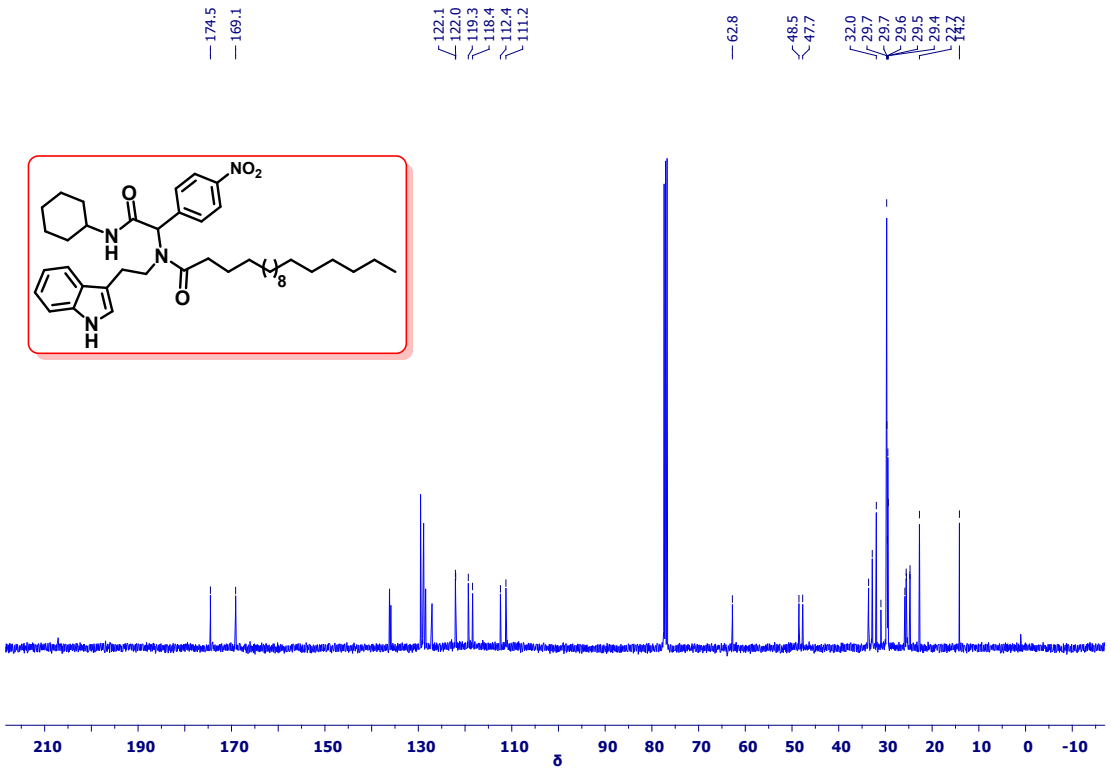

Fig. S18 ^{1}H NMR spectrum of compound **5i**

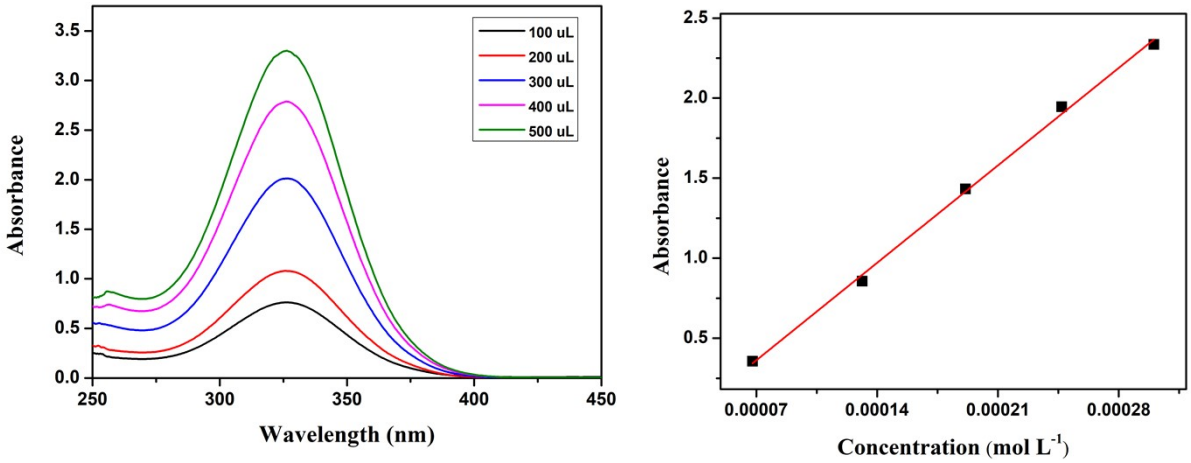

Fig. S19 UV-Vis spectra collected for Metronidazole (**MZ**) solutions at different concentrations (left), highlighting the **MZ** band at 319 nm used to establish the calibration curve (right) for calculating cumulative drug release

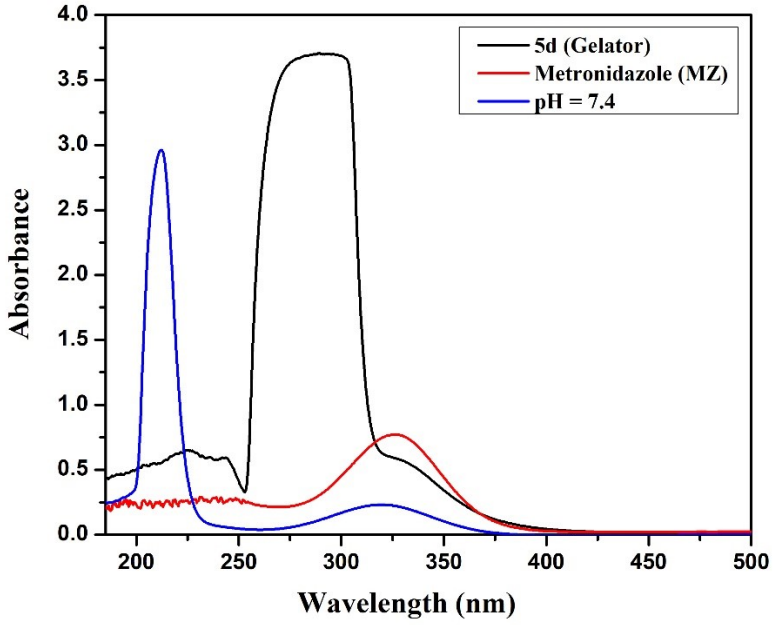

Fig. S20 UV-Vis spectra of gelator (**5d**), drug metronidazole (**MZ**), and release of **MZ** at pH 7.4 from drug loaded gel

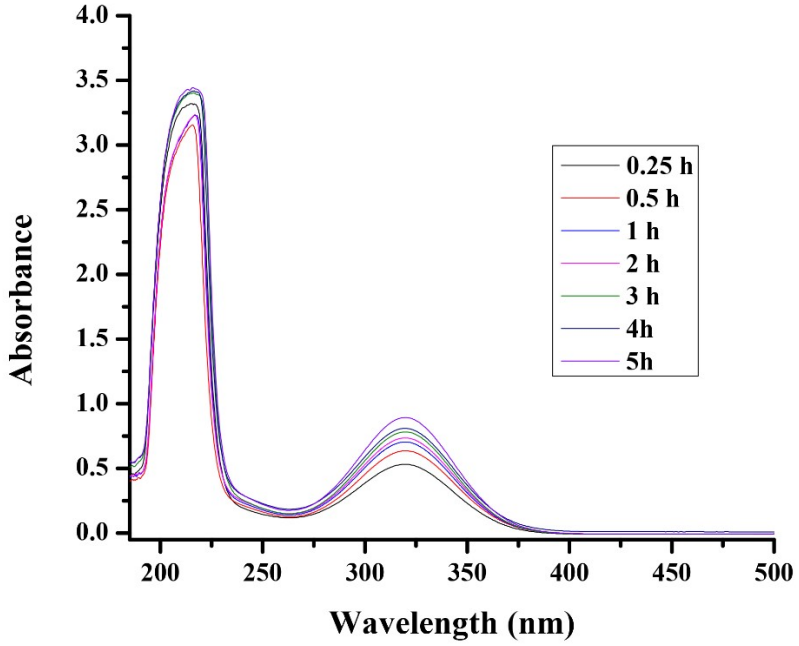

Fig. S21 UV-Vis spectra of kinetic degradation of drug composite organo/hydrogel at pH 5.5

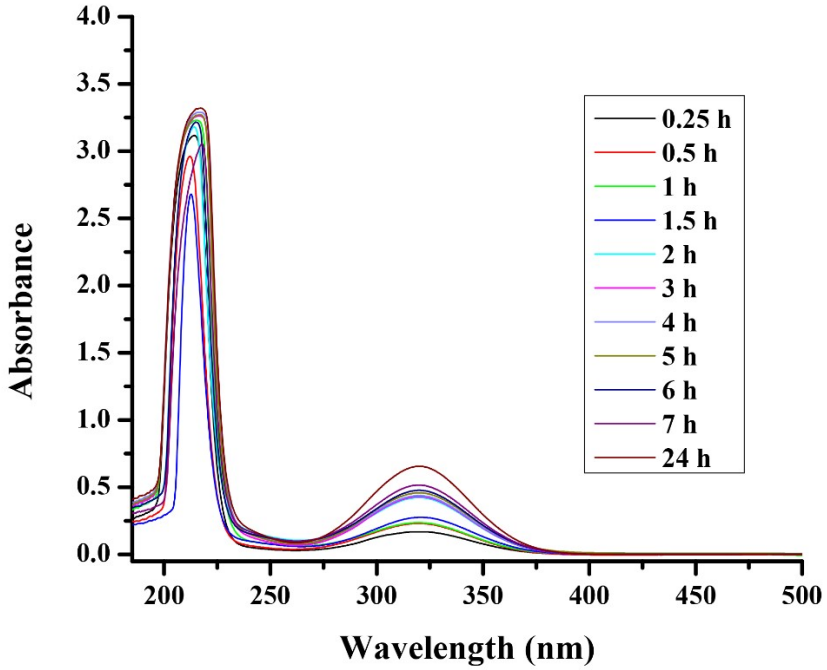

Fig. S22 UV-Vis spectra of kinetic degradation of drug composite organo/hydrogel at pH 7.4

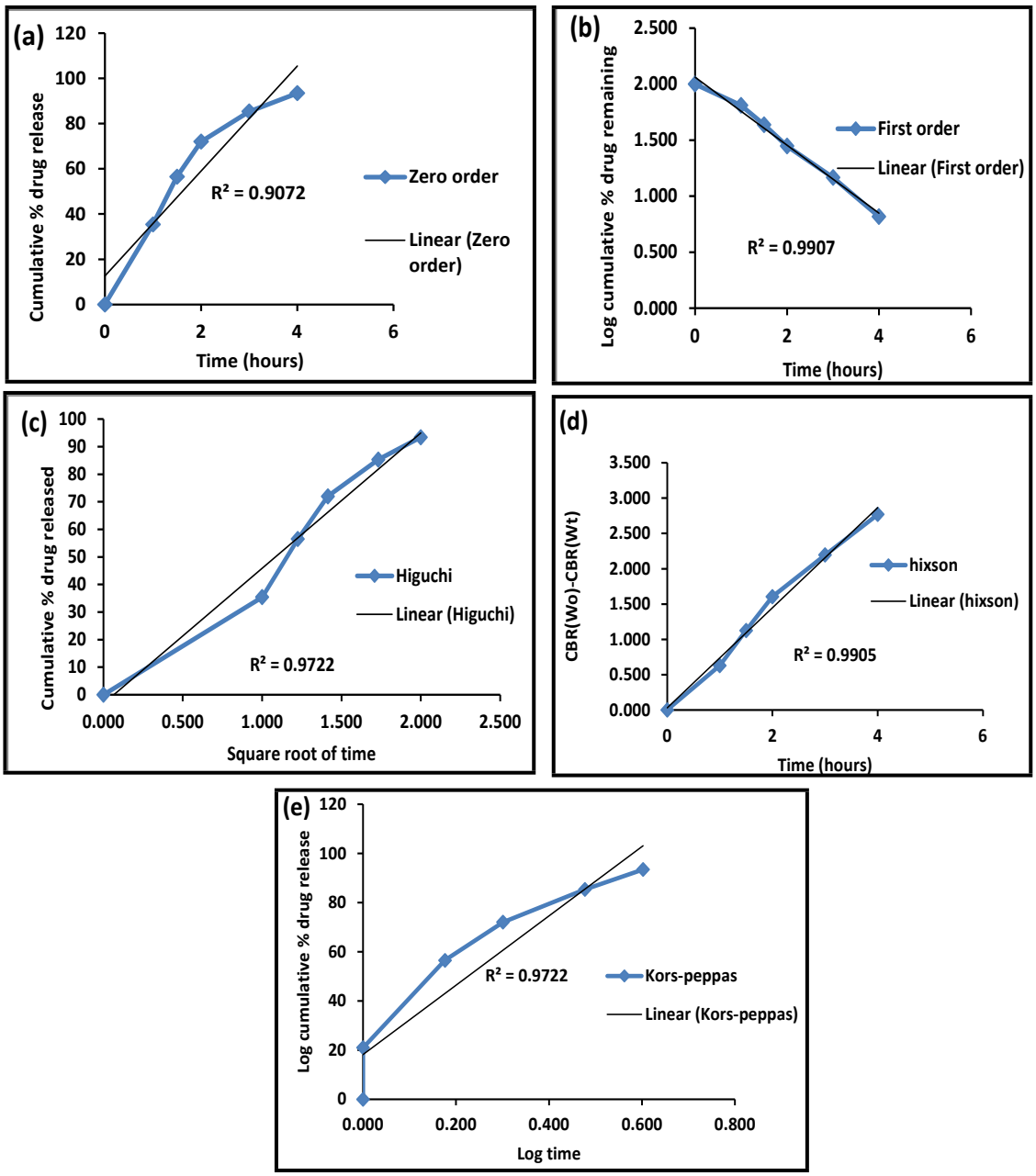

Fig. S23 Drug release kinetics plots for drug loaded organo/hydrogels at pH 5.5 (a): zero-order; (b): first-order; (c): Higuchi; (d): Korsmeyer-Peppas; (e): Hixson-Crowell models

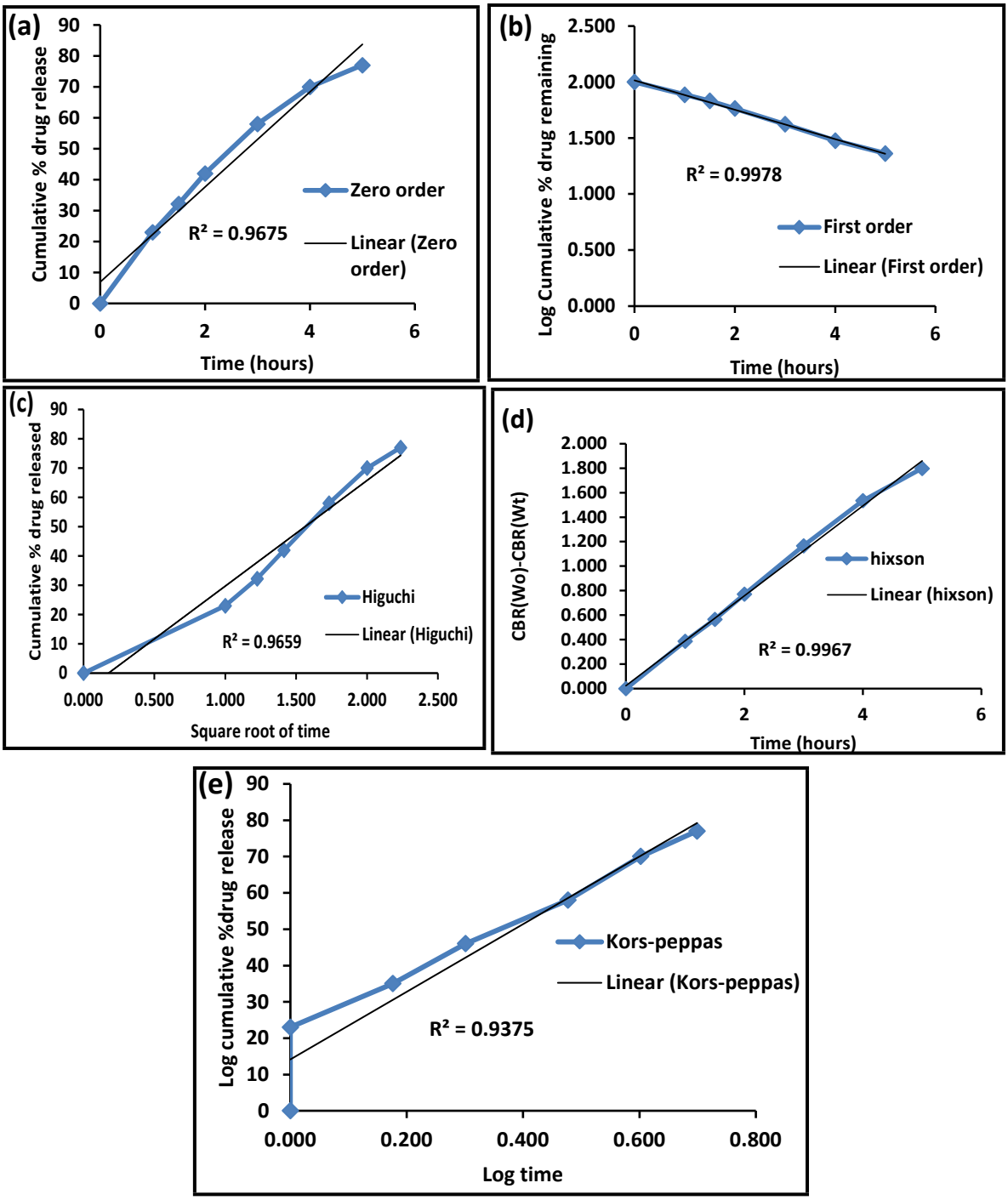

Fig. S24 Drug release kinetics plots for drug loaded organo/hydrogels at pH 7.4 (a); zero-order (b); first-order (c); Higuchi (d); Korsmeyer-Peppas (e); Hixson-Crowell models

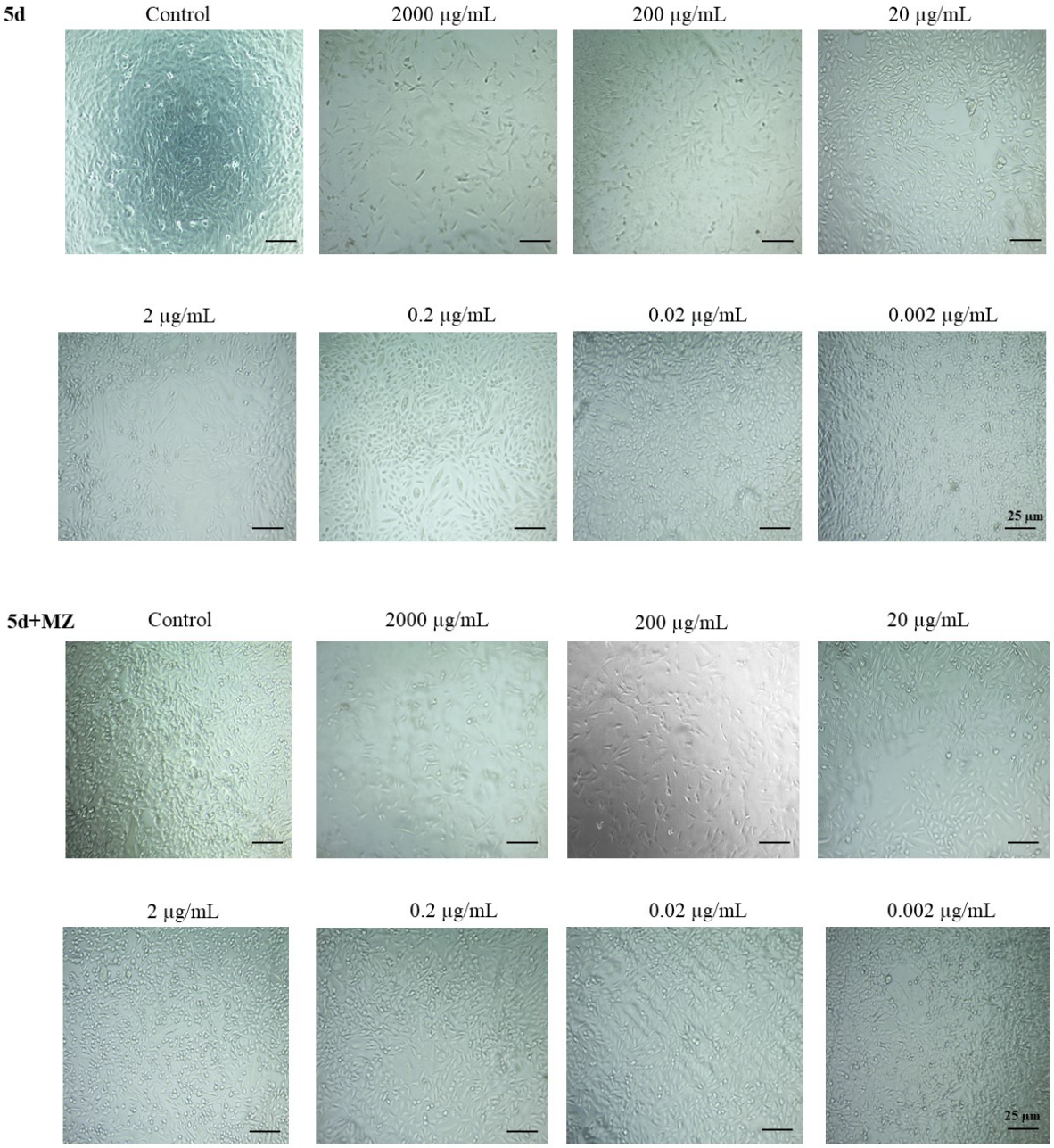

Fig. S25 Cell viability images at different concentrations (2000 µg/mL, 200 µg/ml, 20 µg/mL, 2 µg/mL, 0.2 µg/mL, 0.02 µg/mL, 0.002µg/mL) in comparison with the control (0.000 µg/mL) condition of **5d** and **5d**+**MZ**

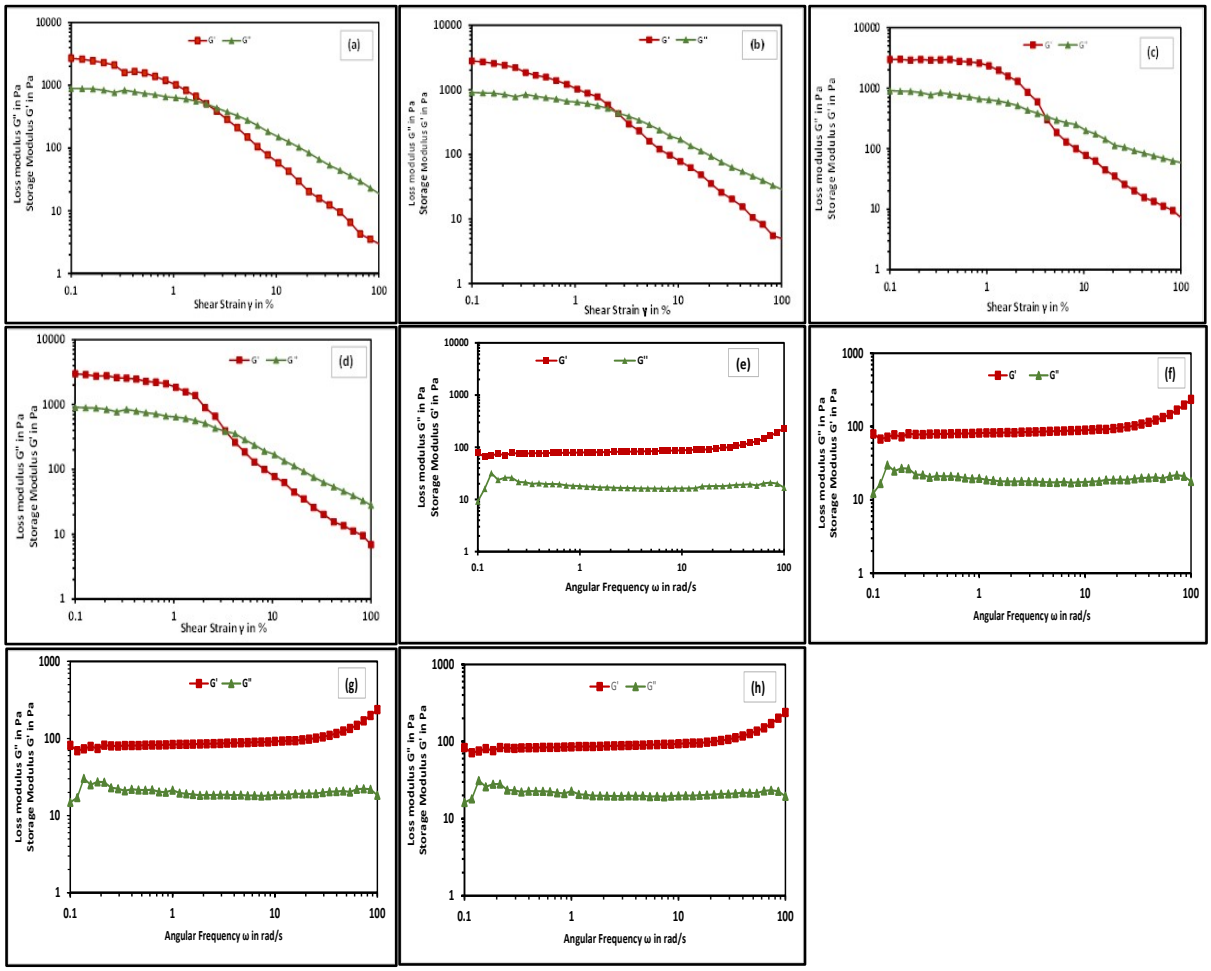

Fig. S26 The strain amplitude rheological experiment for **5d** in DMSO/water at constant frequency 1 Hz; a) 15 mg; (b) 18 mg; (c) 21 mg; (d) 24 mg. The Frequency sweep rheological experiment for **5d** DMSO/water at constant strain of 1%; (e) 15 mg; (f) 18 mg; (g) 21 mg; (h) 24 mg