Electronic Supplementary Material (ESI) for Materials Advances.

Supporting information

Impact of the isomerism of peptide mimetics on the assembly and properties: quick and onsite gas phase detection of acids and alcohols

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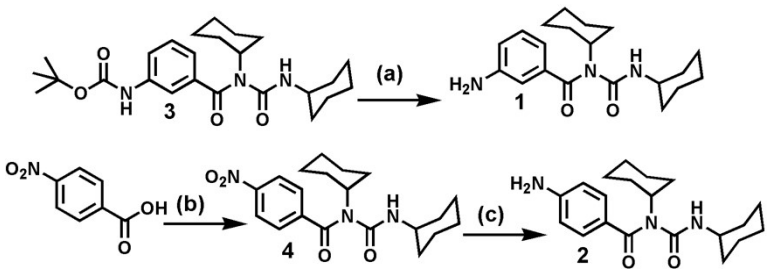
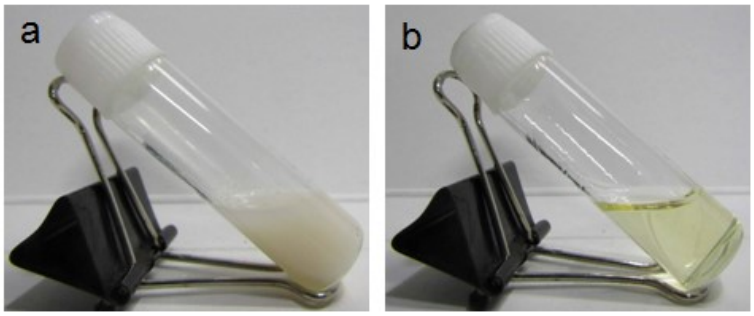
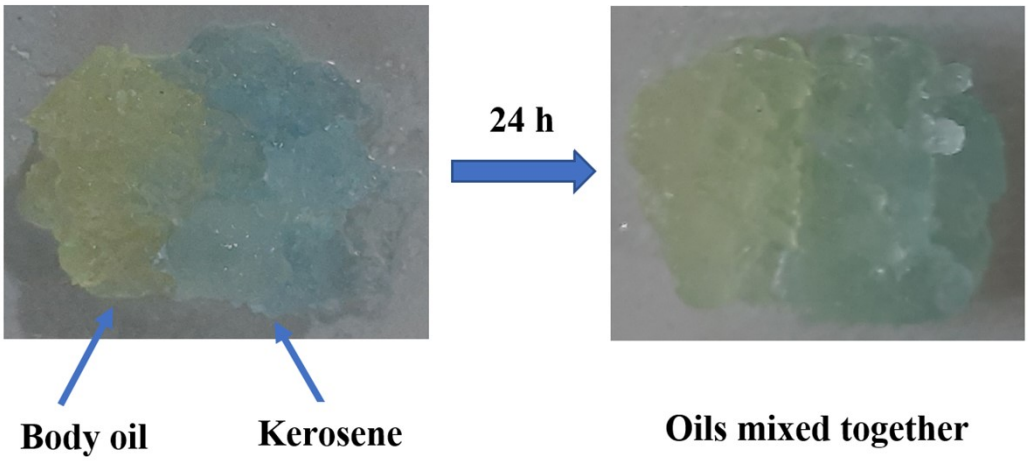


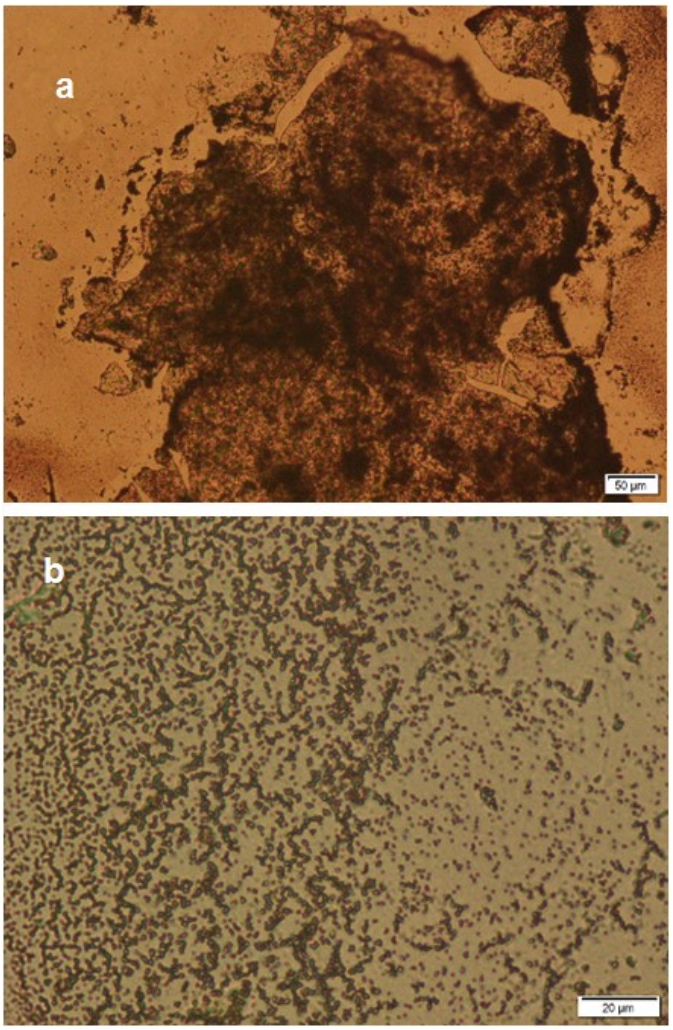
ESI Figure S1. The schematic representation for the synthesis of peptide mimetics **1** and **2**. Reagents and conditions: (a) TFA, DCM, 1h 95% (b) DCC, DCM, reflux, 5h, 75%, (c) (1:1) Fe, AcOH, Acetone-H_2O, reflux 4h, 70%.



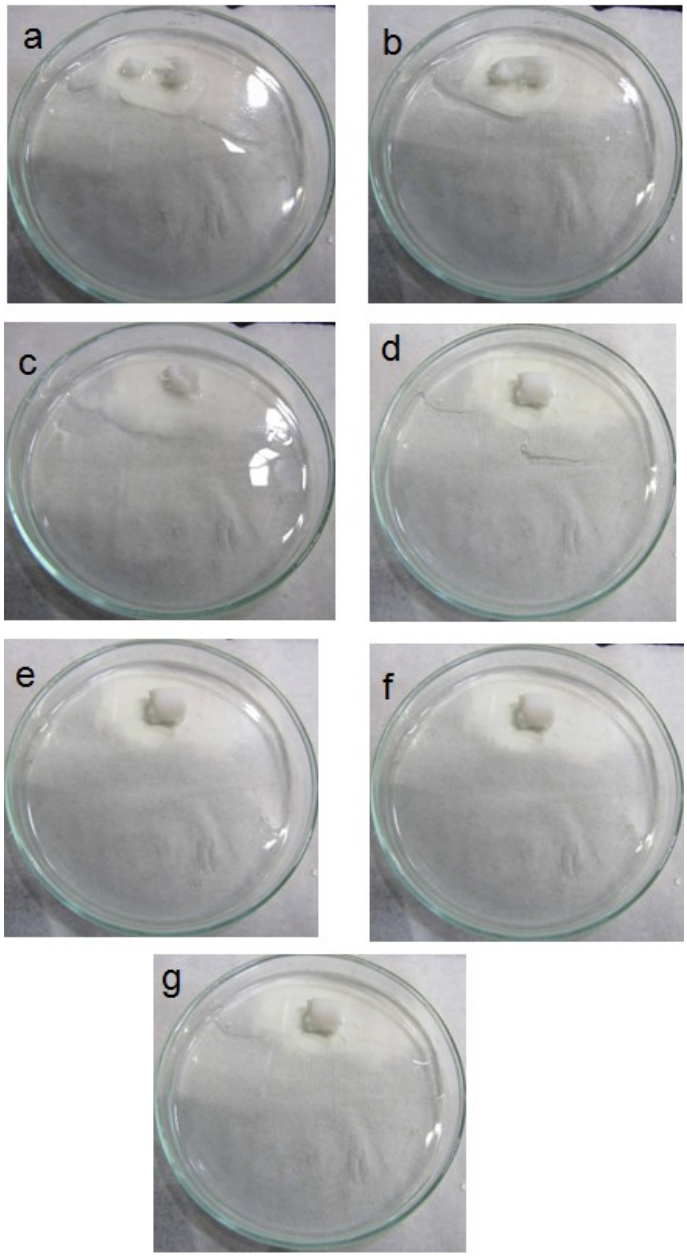
ESI Figure S2. The compound **1** forms white suspension in methylcyclohexane and clear solution in chloroform.



ESI Figure S3. Dynamic and self-healing nature of the organogel of compound **1**.



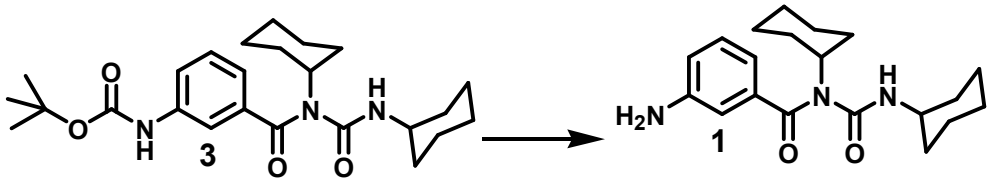
ESI Figure S4. (a) POM image of γ-peptide **1** xerogel from 19:1 hexane/EtOAc (b); POM image of γ-peptide **2** in hexane.



ESI Figure S5. The gel gets deformed towards strong mineral acid such as (a) H_2SO_4 (b) HNO_3. The gel is sensitive to (c) acetic acid but not (d) formic acid. The gel is not responsive to (e) NH_3, (f) methylamine and (g) ethylamine.

Experimental Section

Synthesis of compound 1.



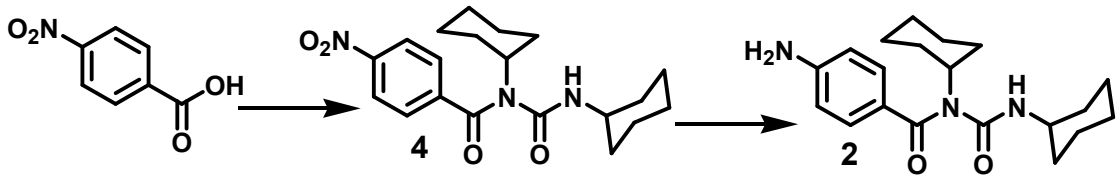
Compound 3 was synthesized as per report by

S. K. Maity, S. Maity, P. Jana and D. Haldar, *Chem. Commun.*, 2012, **48**, 711-713.

Compound 1: To a solution of compound **3** (1.86 g, 5 mmol) in DCM (80 mL), 4 mL of trifluroacetic acid were added. Then the mixture was stirred. After 1 h, the reaction mixture was concentrated under reduced pressure. The residue was dissolved in ethyl acetate and neutralized by sodium carbonate solution. The aqueous phase was extracted with ethyl acetate and this operation was done repeatedly. The ethyl acetate extracts were collected, washed with brine and dried over anhydrous Na_2SO_4 and evaporated in vacuum. The product was purified by silica gel (100-200 mesh) using hexane-ethyl acetate (2:1) as eluent. Yield=95%.

^{1}H NMR (500 MHz, $CDCl_3$, δ in ppm): 7.15 (t, 1H, J=7.8 Hz), 6.87 (d, 1H, J=7.8 Hz), 6.79 (t, 1H, J=1.8 Hz), 6.73 (dd, 1H, J=7.8 Hz, 2.4 Hz), 6.19 (s, 1H, amide NH), 4.12-4.05 (m, 1H, CαH cyh), 3.99-3.56 (b, 2H, Ar NH_2), 3.52-3.45 (m, 1H, CαH cyh), 2.09-2.00 (m, 2H, cyh), 1.82-1.74 (m, 4H, cyh), 1.68-1.48 (m, 6H, cyh), 1.28-1.19 (m, 4H, cyh), 1.17-1.02 (m, 2H, cyh), 0.94-0.85 (m, 2H, cyh); ^{13}C NMR (125 MHz, $CDCl_3$, δ in ppm): 171.5, 154.5, 146.9, 138.1, 129.5, 117.2, 116.5, 113, 57.2, 49.7, 34, 32.3, 30.7, 29.7, 26.3, 25.7, 25.4, 25.3, 25, 24.6. Mass spectral data TOF-MS m/z: $[M + Na]^+$ = 366.55, calculated mol. wt. = 343.47.

Synthesis of compound 2.



Compound 4: p-nitrobenzoic acid (1.67 g, 10 mmol) was dissolved in 60 mL of DCM at room temperature. N,N/ -dicyclohexylcarbodiimide(DCC) (3.1 g, 15 mmol) and Et_3N (2 mL,

15 mmol) was added to the reaction mixture after which it was put under reflux. After 5 hours, the reaction mixture was cooled to room temperature and DCM was evaporated. Solid was mixed with ethyl acetate and dicyclohexylurea(DCU) was filtered out. The organic layer was washed with 1 N sodium carbonate solution (3 X 50 mL) followed by brine (2 X 50 mL), dried over anhydrous sodium sulphate and concentrated under vacuum. The product was purified by silica gel column (60-120 mesh) using 15% ethyl acetate/hexane as eluent. Yield=2.57 g (6.9 mmol, 69%).

^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 8.25 (d, 2H, J=9.2 Hz), 7.70 (d, 2H, J=9.2 Hz), 6.19 (s, 1H, amide NH), 4.11-3.99 (m, 1H, CαH cyh), 3.52-3.41 (m, 1H, CαH cyh), 1.98-1.88 (m, 2H, cyh), 1.87-1.75 (m, 4H, cyh), 1.72-1.53 (m, 6H, cyh), 1.41-1.28 (m, 2H, cyh), 1.18-1.02 (m, 4H, cyh), 0.95-0.83 (m, 2H, cyh); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 168.8, 153.6, 148.9, 142.8, 127.9, 123.9, 57.4, 50, 34, 32.4, 30.9, 29.8, 26.2, 25.7, 25.4, 25.3, 25, 24.6. Mass spectral data TOF-MS m/z: $[M + Na]^+$ = 396.72, calculated mol. wt. = 373.45.

Compound 2: To a solution of compound **4** (1.86 g, 5 mmol) in acetone (80 mL), 4 mL of water, 4 mL of acetic acid and iron powder (3.35 g, 60 mmol) were added. Then the mixture was heated to reflux. After 6 h, the reaction mixture was cooled and filtered through a pad of celite. The filtrate was concentrated under reduced pressure. The residue was dissolved in ethyl acetate and neutralized by sodium carbonate solution. The aqueous phase was extracted with ethyl acetate and this operation was done repeatedly. The ethyl acetate extracts were collected, washed with brine and dried over anhydrous Na_2SO_4 and evaporated in vacuum. The product was purified by silica gel (100-200 mesh) using hexane-ethyl acetate (2:1) as eluent. Yield=1.21g (3.5 mmol, 70%).

^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm): 7.42 (d, 2H, J=8.5 Hz), 6.61 (d, 2H, J=8.5 Hz), 5.92 (d, 1H, J=8.3 Hz, Amide NH), 4.18-4.09 (m, 1H, CαH cyh), 4.07-3.61 (br, 2H, Ar NH_2), 3.54-3.43 (m, 1H, CαH cyh), 2.09-1.98 (2H, m, cyh), 1.95-1.88 (1H, m, cyh), 1.83-1.74 (3H, m, cyh), 1.7-1.51 (6H, m, cyh), 1.34-1.21 (3H, m, cyh), 1.15-1.03 (3H, m, cyh), 0.93-0.85 (2H, m, cyh); ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm): 171.5, 155, 149.4, 129.4, 126.2, 114, 57.5, 49.5, 33.9, 32.4, 30.8, 26.3, 25.6, 25.4, 25.3, 24.9, 24.5. Mass spectral data TOF-MS m/z: $[M + Na]^+$ = 366.85, calculated mol. wt. = 343.47.

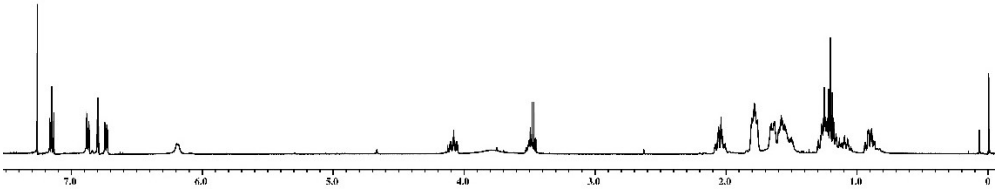


Figure S6: ^{1}H NMR (500 MHz, $CDCl_3$, δ in ppm) spectra of compound **1.**

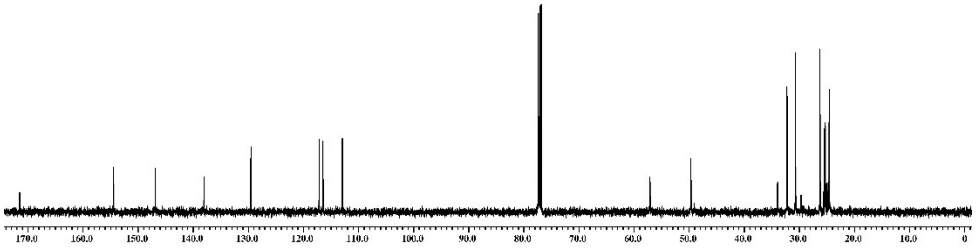


Figure S7: ^{13}C NMR (125 MHz, $CDCl_3$, δ in ppm) spectra of compound **1.**

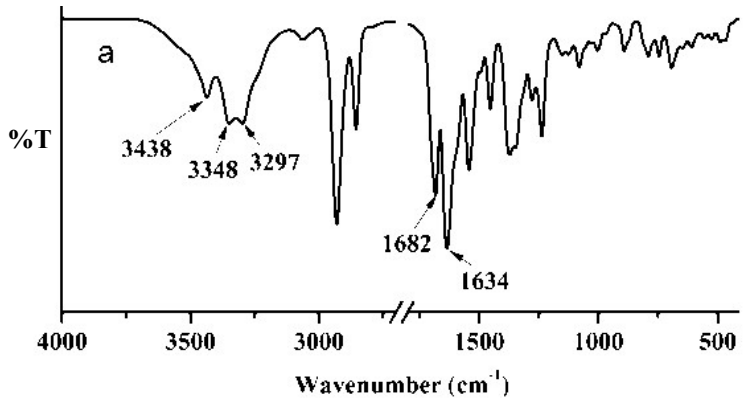


Figure S8: Solid state FT-IR spectra of compound **1.**

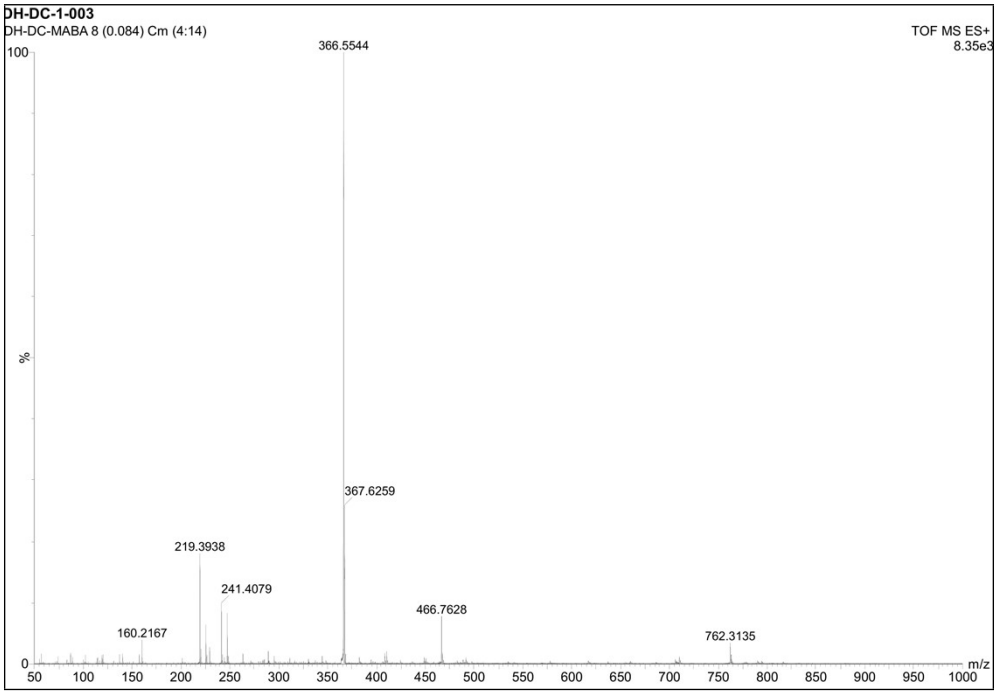


Figure S9: Mass spectra of compound **1.**

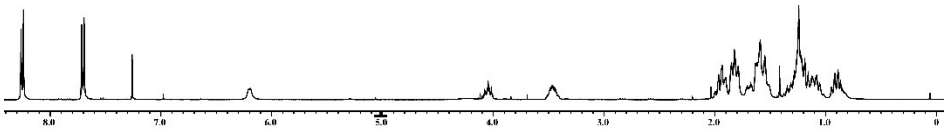


Figure S10: ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm) spectra of compound **4.**

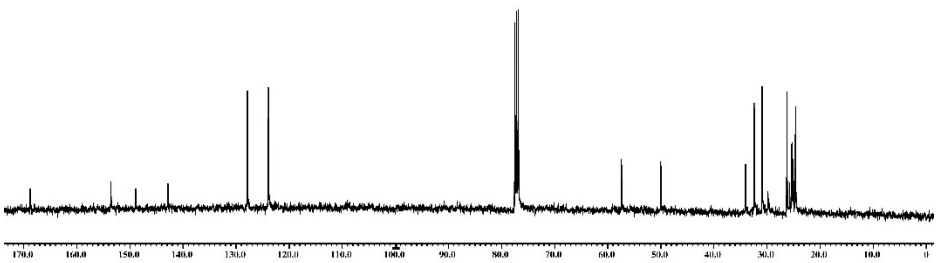


Figure S11: ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm) spectra of compound **4.**

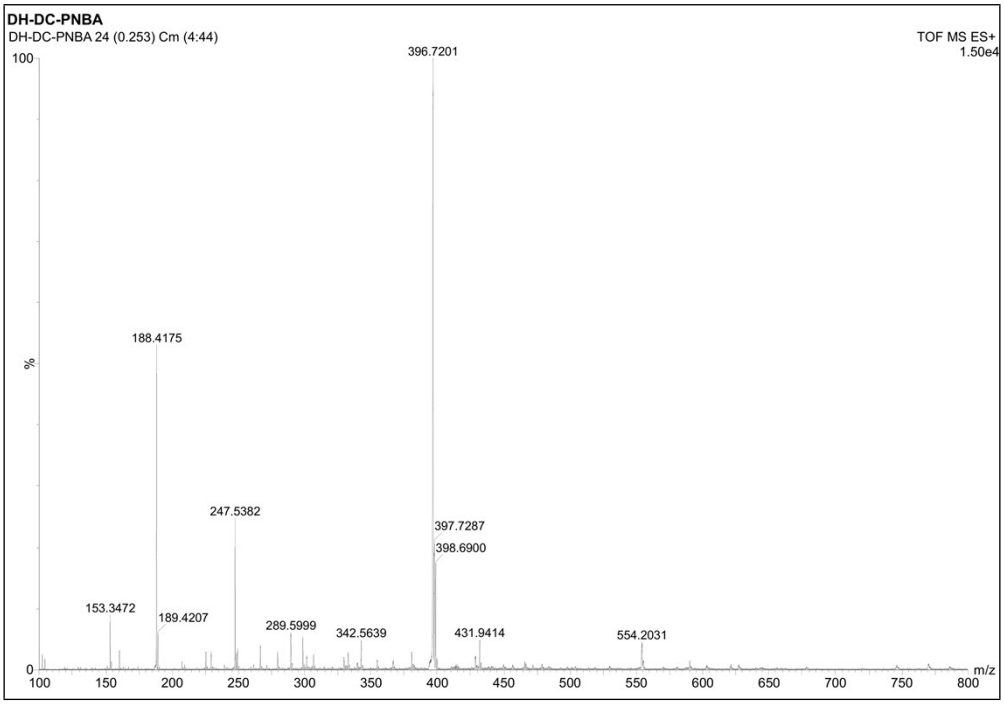


Figure S12: Mass spectrum of compound **4.**

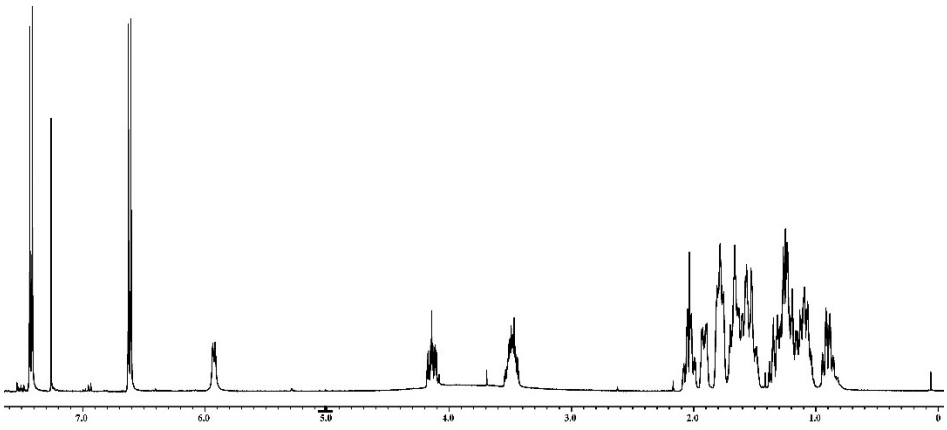


Figure S13: ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm) spectra of compound **2.**

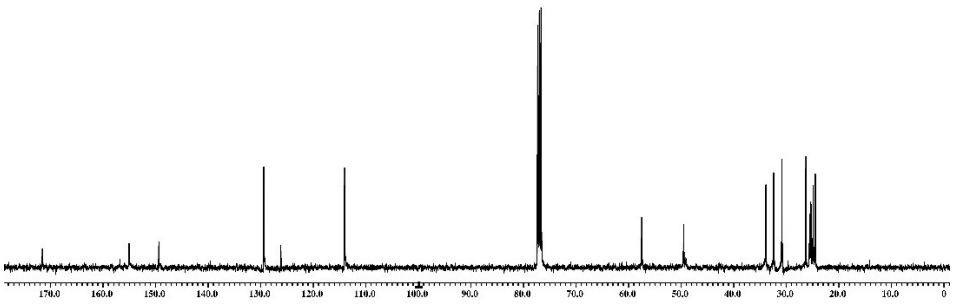


Figure S14: ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm) spectra of compound **2.**

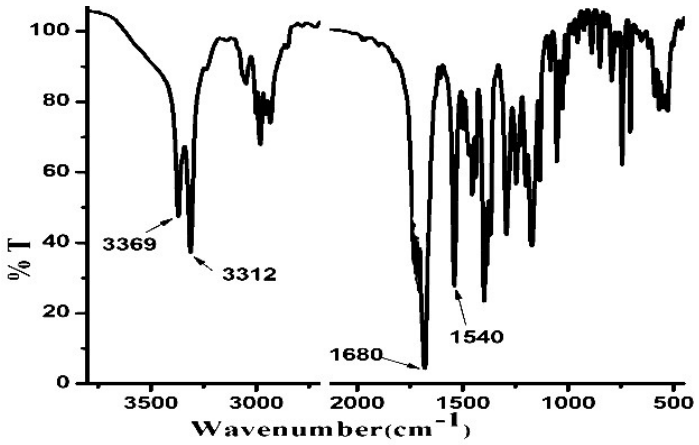


Figure S15: Solid state FT-IR spectra of compound **1.**

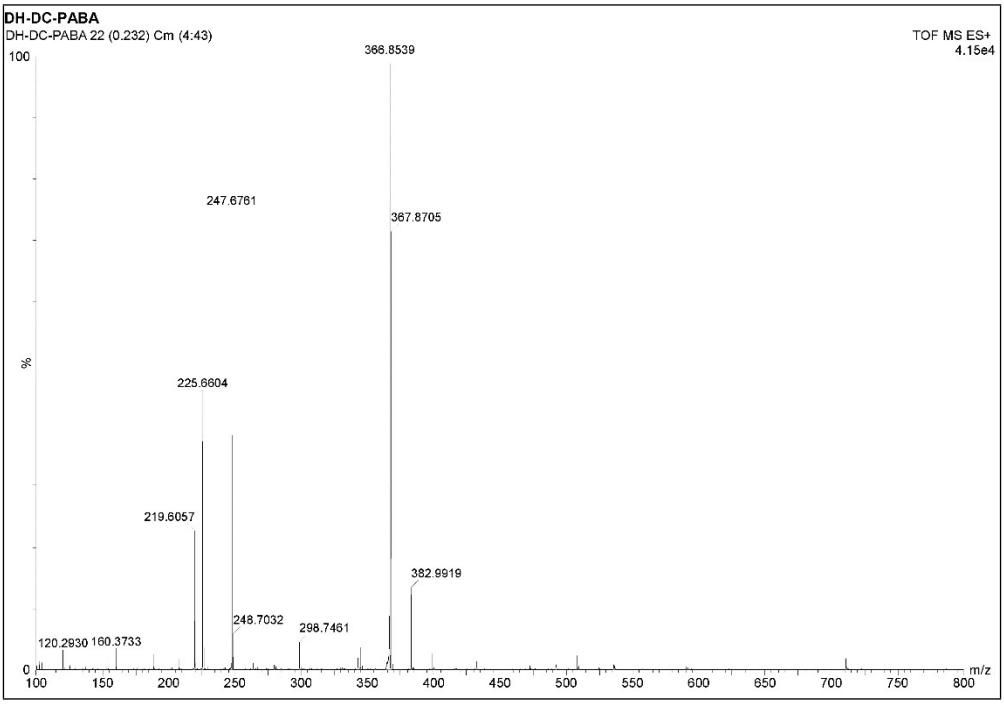


Figure S16: Mass spectrum of compound **2.**