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Supporting Information

An Easy Access to Self-Assembled Glycolipid derived from Bhilawanol: A Promising Anti-Cancer Drug

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Experimental section:

Materials and general method: All the essential chemicals and solvents for the preparation of the glycolipids were purchased from TCI Chemicals, Alfa Aesar, Sigma-Aldrich, Avra, SRL, and Spectrochem chemicals, and were used as such without further purification and the Bhilawanol was extracted from semecarpus Anacardium seeds. The LR-grade chemicals were purchased and used for column chromatography and for the required purification processes of the compounds. Pre-coated silica gel was used to check the progress of the reaction.

Characterisations: The ^{1}H and ^{13}C NMR spectra for all the compounds were acquired using a Bruker Avance 400MHz instrument at room temperature. The solvents used included $CDCl_3$ or $CDCl_3$ with a few drops of DMSO-d_6 or DMSO-d_6. TMS was employed as an internal standard, and chemical shifts (δ) are reported in parts per million (ppm) relative to TMS. Coupling constants (*J*) are expressed in Hz. Proton multiplicity is determined using the following abbreviations: singlet (s), doublet (d), triplet (t), quartet (q), and multiplet (m). Electrospray ionisation mass spectra (ESI-MS) were conducted in positive mode using a Thermo Fisher LCQ Advantage Max instrument. This was achieved by dissolving the solid sample in either acetonitrile or methanol.

Gelation method: The gelation study is carried out by taking a known amount of compound with an appropriate amount of solvent, heating the mixture at a high temperature of about 110 °C to 120 °C, and letting it cool down to room temperature, upon cooling the gelation molecule tend to assemble in a 3D molecular network which is further confirmed by the stable-to-inversion method. The gelation ability of the compounds was examined in different solvents and vegetable oils. The minimum

concentration where the gel is formed is critical gelation concentration CGC % (wt./v). The compounds show different behaviour upon heating in various solvents, such as soluble (S), gel (G), partial gel (PG), partial insoluble (PI), and insoluble (I).

Gel to sol. Temperature (Tg): The melting temperature of the gel is considered the sol. to gel temperature. Above this temperature, the gel converts to the solution form, and when kept at room temperature, it reverses back to the gel state, as gels are thermally reversible. The gel was prepared in a glass vial, then kept in an oil bath, and slowly heated until it melted, recorded as the gel to sol temperature.

Morphological analysis: The gel's morphological analysis was carried out by scanning electronic microscopy (SEM). The gel was prepared using a sufficient amount of gelator in the required solvent, placed over a glass slide, and scanned under the microscope.

XRD analysis: The xerogel formed by drying the hydrogel is further used to record the small-angle XRD by transferring the sample into the sample holder and coating it like a thin film.

Rheological analysis: The rheological studies were carried out to investigate the gel's viscoelastic nature, as well as its thermal and mechanical strength in response to external forces, heat, or temperature. The analysis was conducted at 23 °C using a stress control rheometer (Anton Paar 302 rheometer) equipped with a steal-coated parallel plate geometry (25mm diameter) instrument. The rheological measurements are carried out in terms of storage modulus (G`), which represents the elastic nature of the gel and loss modulus(G``), which represents the viscous nature of the gel in response to externally applied forces.

Cytotoxic study (Experimental section).

The cytotoxic behaviour of the compound BCG6a was analysed on normal cells, specifically human corneal epithelial cells (HCEC), and was thoroughly studied. Initially, the cells were seeded in 96-well plates containing DMEM/F12 (Lonza, Walkersville, MD) media supplemented with 10% fetal bovine serum (FBS; Lonza, Walkersville, MD), 4 µg/mL insulin (HiMedia Laboratory, Maharashtra, India), and 20 ng/mL EGF. Compound BCG6a (500 µM) was added to the cells and incubated for 6 hours and 24 hours at 37°C in a 5% CO_2 incubator. Following incubation, the culture media was aspirated, and the wells were washed with sterile 1X PBS to remove non-adherent cells. Next, 100 µL of 5 mg/mL MTT solution (Sigma-Aldrich, MO) was added to each well, and the plates were incubated at 37°C in a 5% CO_2 incubator for 2 hours. Afterwards, the media was removed, 200 µL of DMSO was added to dissolve the formazan crystals, and the absorbance was recorded at 595 nm.

Anticancer assay (Experimental section): Hela cells were seeded in a 96-well plate at a density of 10,000 cells per well in DMEM media supplemented with 10% FBS. To promote cell adhesion, the plate was then incubated at 37°C in a CO_2 incubator. Upon reaching the logarithmic phase of growth, the cells were treated with four different concentrations of BCG 5,6(a-b) at 20 µM, 50 µM, 75 µM, 100 µM, 125 µM. The compounds were dissolved in DMSO, and the concentration of DMSO was kept at 0.2% at the highest concentration. These concentrations were standardized prior to the final experiment. Following a 24-hour treatment period, cell viability was assessed using Alamar blue reagent (Thermo #DAL1025). It is a cell-permeable, non-toxic indicator dye called resazurin. Resazurin is a blue colour compound that can be reduced to resorufin by living cells. Resorufin is a pink colour compound that is highly fluorescent. Hence, the intensity of fluorescence produced is proportional to the number of living cells present in the sample. Cells were observed under a phase contrast microscope (Invitrogen EVOS M7000 microscope), and the fluorescent intensity was captured at excitation of 560 nm and emission of 590 nm using (Varioskan, Thermo Scientific) as mentioned by the manufacturer. Fluorescence intensity is used to determine cell cytotoxicity. The percentage of cell cytotoxicity was calculated as follows: fluorescence in the treated sample/fluorescence in the control sample × 100. The experiment was conducted in triplicate.

Cell culture: The cervical adenocarcinoma cell line HeLa was procured from the National Centre for Cell Science, Pune, and it was maintained in Dulbecco's Modified Eagle's medium (DMEM) supplemented with 10% Fetal Bovine Serum and in the presence of antibiotics, Penicillin (50 U/ml)-Streptomycin (50 mg/ml). The cells were grown in a humidified incubator at 5% CO_2 and at 37 °C temperature.

Synthesis: The general procedure for the synthesis of glycolipid is followed by the literature corresponding to Cardanol-based amphiphiles. It involves three steps the first step involves the synthesis of esters 2a from bhilawanol 1a, and the second step involves the conversion of esters to the corresponding hydrazides, 3a−b. The final glycolipid was prepared by treating 1,2(3 alkyl phenoxy) acetohydrazide (3a), (3b) (1mmol) with monosaccharides (1mmol) in ethanol followed by ammonium sulfate. The mixture was stirred at reflux conditions for 24 hours. The final products 5a to 5f (with non-reduced long C_{15} chain) and 6a to 6f (with reduced long C_{15} carbon chain) were obtained as a precipitate further filtered using methanol and recrystallised in ethanol.

Synthesis of 1,2(3 alkyl phenoxy) acetate: To a bhilawanol (1mmol, 1a) in acetone, (2mmol) methyl bromoacetate is added in the presence of anhydrous potassium carbonate (4mmol) and refluxed for 24 hours. After confirming using TLC, the reaction is stopped, cooled to room temperature, and extracted using ethyl acetate. The product (2a), a brown golden viscous liquid, was concentrated and isolated using a rotary evaporator.

Compound 2a. Isolated as a brown golden viscous liquid; yield = 93% ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (t, *J* = 7.9 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 6.58 (d, *J* = 8.1 Hz, 1H), 5.30 – 5.24 (m, 3H), 4.64 (s, 2H), 4.56 (s, 2H), 2.70 – 2.59 (m, 3H), 1.96 – 1.89 (m, 4H), 1.50 (t, *J* = 7.2 Hz, 2H), 1.32 – 1.18 (m, 16H), 0.85 – 0.78 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.35, 172.93, 143.24, 129.99, 129.68, 127.89, 121.82, 119.74, 112.70, 68.96, 62.13, 29.79, 29.72, 29.68, 29.55, 29.34, 29.13, 29.10, 27.23, 27.18, 22.69, 22.66, 14.08.

Synthesis of 1,2(3 alklyphenoxy)acetohydrazide: To a (1mmol) solution of 1,2(3alkyl phenoxy) acetate (2a), (0.5mmol) hydrazine hydrate was added in ethanol and refluxed for 12 hours and 24 hours. Accordingly, we got the non-reduced and reduced products, respectively. After confirming by using TLC, the reaction mixture was cooled to room temperature, and the product was precipitated, filtered using ethanol, and dried. A white amorphous solid came as a final product (3a and 3b).

Compound 3a. Isolated as a white amorphous solid; mp 98-100°C yield = 93%
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.31 (s, 1H), 9.25 (s, 1H), 6.97 (t, *J* = 7.9 Hz, 1H), 6.80 (t, *J* = 7.9 Hz, 2H), 5.65 – 5.12 (m, 1H), 4.51 (s, 2H), 4.37 (s, 2H), 2.62 – 2.55 (m, 2H), 1.99 (dd, *J* = 12.4, 6.6 Hz, 2H), 1.50 (s, 2H), 1.26 (d, *J* = 16.4 Hz, 20H), 0.86 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 169.69, 168.24, 149.67, 145.21, 137.25, 130.03, 129.76, 125.11, 123.68, 111.36, 72.01, 67.69, 31.94, 29.88, 29.77, 29.71, 29.67, 29.64, 29.59, 29.55, 29.44, 29.37, 27.24, 14.13. **HRMS (ESI, m/z):** $[M+H]^+$ calcd. for $C_{25}H_{42}N_4O_4$: 463.3276; found 463.3289.
Compound 3b. Isolated as a white amorphous solid; mp 102-104 °C yield = 90%
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 6.98 (t, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 7.7 Hz, 1H), 6.66 (d, *J* = 7.2 Hz, 1H), 4.47 (d, *J* = 34.5 Hz, 6H), 2.84 (s, 5H), 2.24 (t, *J* = 7.6 Hz, 1H), 1.50 (s, 3H), 1.21 (d, *J* = 17.4 Hz, 37H), 0.81 (t, *J* = 6.7 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 169.66, 168.20, 149.67, 145.21, 137.27, 125.11, 123.69, 111.35, 72.02, 67.71, 31.93, 30.75, 29.89, 29.70, 29.64, 29.55, 29.37, 22.70, 14.13. **HRMS (ESI, m/z):** $[M+H]^+$ calcd. for $C_{25}H_{44}N_4O_4$: 465.3433; found: 465.3448
Synthesis of compound (5a-f): To the compound 3a (1 mmol) in ethanol as solvent, monosaccharides (1mmol) were added, and (0.2 mmol) of ammonium sulfate as catalysts refluxed the reaction for 24h. The completion of the reaction was determined using TLC; the precipitated product was filtered using methanol and water and recrystallised in ethanol. The final pure compound was obtained as a white amorphous solid.

Compound 5a. Isolated as a white amorphous solid; mp 117-119 °C yield = 73%

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.96 (d, J = 64.0 Hz, 1H, NH), 9.21 (d, J = 86.5 Hz, 1H, NH), 7.61 (d, J = 113.9 Hz, 1H, NH), 6.96 (s, 1H, Ar-H), 6.83 (d, J = 20.3 Hz, 2H, Ar-H), 5.39 (s, 1H, NH), 5.43 – 5.27 (m, 2H, alk-H), 5.01 (d, J = 26.7 Hz, 2H, sac-H), 4.69 – 4.57 (m, 2H, sac-H), 4.51 (s, 2H, akl-H), 4.38 (s, 2H, alk-H), 4.24 (d, J = 30.1 Hz, 3H, sac-H), 4.08 – 3.89 (m, 4H, sac-H), 3.76 (t, J = 16.4 Hz, 3H, sac-H), 3.64 – 3.52 (m, 4H, sac-H), 3.52 – 3.43 (m, 3H, sac-H), 3.38 (d, J = 4.9 Hz, 2H, sac-H), 2.66 – 2.60 (m, 2H, CH_2), 2.01 (d, J = 5.9 Hz, 2H, CH_2), 1.55 (s, 2H, CH_2), 1.29 (d, J = 21.3 Hz, 21H, CH_2), 0.90 – 0.84 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO- d_6) δ 167.71, 167.13, 151.04, 146.23, 136.67, 130.09, 124.43, 123.00, 112.57, 91.29, 78.46, 77.40, 72.20, 71.76, 71.16, 67.81, 63.31, 61.84, 31.67, 30.45, 29.75, 29.51, 29.40, 29.36, 29.29, 29.03, 27.08, 22.41, 14.17.

HRMS(ESI) m/z calculated for $C_{37}H_{62}N_4O_{14}$ = 787.4333 $[M+H]^+$; observed 787.4345

Compound 5b. Isolated as a white amorphous solid; mp 113-115 °C yield = 76%

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.92 (s, 1H, NH), 9.05 (d, J = 41.9 Hz, 1H, NH), 7.58 (d, J = 109.8 Hz, 1H, NH), 6.97 (t, J = 7.9 Hz, 1H, Ar-H), 6.82 (t, J = 12.0 Hz, 2H, Ar-H), 5.34 (t, J = 5.0 Hz, 2H, alk-H), 4.95 (s, 3H, sac-H), 4.51 (s, 2H, alk-H), 4.40 (s, 2H, alk-H), 4.23 (s, 3H, sac-H), 4.11 (s, 4H, sac-H), 3.75 (d, J = 16.6 Hz, 2H, sac-H), 3.68 – 3.60 (m, 2H, sac-H), 3.58 – 3.41 (m, 3H, sac-H), 3.34 (s, 1H, sac-H), 3.10 (s, 3H, sac-H), 2.68 – 2.59 (m, 2H, CH_2, CH_2), 2.01 (q, J = 6.5 Hz, 3H, CH_2), 1.56 (d, J = 7.5 Hz, 2H, CH_2), 1.29 (d, J = 20.1 Hz, 21H, CH_2), 0.88 (d, J = 6.5 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.70, 167.10, 150.90, 145.75, 136.63, 130.09, 124.51, 122.80, 91.18, 78.53, 77.83, 77.09, 71.43, 70.77, 70.63, 67.25, 61.80, 56.50, 31.77, 30.67, 29.53, 29.48, 29.43, 29.18, 27.07, 22.57, 14.42.

HRMS(ESI) m/z calculated for $C_{37}H_{62}N_4O_{14}$ = 809.4163 $[M+Na]^+$; observed 809.4163

Compound 5c. Isolated as a white amorphous solid; mp 116-118 °C yield = 75%

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.14 (s, 1H, NH), 9.45 (d, *J* = 160.4 Hz, 1H, NH), 7.53 (d, *J* = 120.2 Hz, 1H, NH), 7.01 – 6.92 (m, 1H, Ar-H), 6.79 (d, *J* = 7.7 Hz, 2H, Ar-H), 5.69 (s, 1H, NH), 5.45 – 5.27 (m, 2H, alk-H), 5.07 (d, *J* = 29.6 Hz, 2H, sac-H), 4.91 (s, 3H,sac-H), 4.62 (s, 1H, sac-H), 4.57 (d, *J* = 5.4 Hz, 1H, sac-H), 4.54 – 4.50 (m, 1H, sac-H), 4.45 (s, 2H, alk-H), 4.39 (s, 2H, alk-H), 4.11 (d, *J* = 44.9 Hz, 1H, sac-H), 3.86 – 3.63 (m, 2H, sac-H), 3.57 (s, 1H, sac-H), 3.51 – 3.31 (m, 8H, sac-H), 3.10 (dd, *J* = 53.5, 6.9 Hz, 3H, sac-H), 2.61 (d, *J* = 8.7 Hz, 2H, CH_2), 2.02 – 1.92 (m, 2H, CH_2), 1.51 (s, 2H, CH_2), 1.32 – 1.21 (m, 25H, CH_2), 0.88 – 0.84 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.69, 167.05, 151.05, 146.18, 136.68, 130.08, 124.41, 122.93, 112.58, 78.59, 74.83, 72.04, 71.83, 71.24, 70.52, 70.35, 67.83, 64.26, 31.68, 31.53, 30.46, 29.75, 29.58, 29.52, 29.42, 29.38, 29.30, 29.18, 29.04, 28.67, 27.09, 22.41, 14.18.

HRMS(ESI) m/z calculated for $C_{37}H_{62}N_4O_{14}$ = 809.4163 $[M+Na]^+$; observed 809.4169

Compound 5d. Isolated as a white amorphous solid; mp 108-110 °C yield = 73%

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.96 (d, J = 66.8 Hz, 1H, NH), 9.21 (d, J = 87.5 Hz, 1H, NH), 7.61 (d, J = 113.2 Hz, 1H, NH), 6.96 (d, J = 8.0 Hz, 1H, Ar-H), 6.83 (m, 2H, Ar-H), 5.58 (s, 1H, NH), 5.42 – 5.30 (m, 2H, alk-H), 5.01 (d, J = 26.8 Hz, 1H, sac-H), 4.64 (d, J = 26.2 Hz, 2H, sac-H), 4.48 (s, 2H, alk-H), 4.37 (s, 2H, alk-H), 4.28 (s, 1H, sac-H), 4.20 (s, 2H, sac-H), 4.03 (d, J = 6.2 Hz, 3H, sac-H), 3.76 (t, J = 15.5 Hz, 2H, sac-H), 3.58 (d, J = 9.7 Hz, 3H, sac-H), 3.49 – 3.35 (m, 4H, sac-H), 2.67 – 2.57 (m, 2H, CH_2), 2.06 – 1.95 (m, 3H, CH_2), 1.55 (s, 3H, CH_2), 1.29 (d, J = 19.5 Hz, 22H, CH_2), 0.88 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.79, 167.15, 150.86, 145.75, 136.63, 130.10, 124.57, 122.79, 112.00, 91.88,76.99, 72.64, 72.17, 71.79, 71.57, 70.12, 69.95, 67.23, 62.96, 56.53, 31.75, 31.58, 30.65, 29.49, 29.46, 29.16, 28.72, 27.05, 22.55, 18.95, 14.39.

HRMS(ESI) m/z calculated for $C_{35}H_{58}N_4O_{12}$ = 749.3951 $[M+Na]^+$; observed 749.3963

Compound 5e. Isolated as a white amorphous solid; mp 105-107 °C yield = 71%

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.00 (s, 1H, NH), 7.56 (d, *J* = 113.0 Hz, 1H, NH), 7.65 (d, *J* = 112.0 Hz, 1H, NH), 6.97 (t, *J* = 7.8 Hz, 1H, Ar-H), 6.88 – 6.72 (m, 2H, Ar-H), 5.35 (dd, *J* = 5.7, 4.2 Hz, 2H, alk-H), 4.48 (m, 2H, sac-H), 4.62 – 4.48 (m, 2H, sac-H), 4.42 (s, 2H, alk -H), 4.20 (s, 2H, alk-H), 3.91 – 3.65 (m, 2H, sac-H), 3.61 – 3.53 (m, 1H, sac-H), 3.47 (dq, *J* = 22.8, 5.7 Hz, 2H, sac-H), 3.34 – 2.88 (m, 8H, sac-H), 2.68 – 2.56 (m, 2H, CH_2), 2.03 – 1.96 (m, 1H, CH_2), 1.55 (s, 2H, CH_2), 1.29 (d, *J* = 19.4 Hz, 22H, CH_2), 0.88 (td, *J* = 7.2, 4.7 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.70, 167.11, 150.89, 145.76, 136.62, 124.51, 122.77, 112.02, 91.91, 76.99, 71.83, 71.58, 70.15, 67.26, 62.97, 31.77, 30.67, 29.52, 29.48, 29.41, 29.18, 27.07, 22.57.

HRMS(ESI) m/z calculated for $C_{35}H_{58}N_4O_{12}$ = 727.4121 $[M+H]^+$; observed 727.4117

Compound 5f. Isolated as a white amorphous solid; mp 109-111°C yield = 71%

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.06 (s, 1H, NH), 9.05 (d, *J* = 41.4 Hz, 1H, NH), 7.58 (d, *J* = 111.1 Hz, 1H, NH), 6.96 (d, *J* = 7.8 Hz, 1H, Ar-H), 6.87 – 6.72 (m, 2H, Ar-H), 5.34 (t, *J* = 4.9 Hz, 2H, alk-H), 4.95 (s, 1H, sac-H), 4.51 (s, 2H, alk-H), 4.40 (s, 2H, alk-H), 4.18 (d, *J* = 47.3 Hz, 5H, sac-H), 3.75 (d, *J* = 16.1 Hz, 2H, sac-H), 3.68 – 3.59 (m, 2H, sac-H), 3.59 – 3.44 (m, 2H, sac-H), 3.34 (s, 1H, sac-H), 3.11 (s, 4H, sac-H), 2.75 – 2.59 (m, 3H, CH_2), 2.05 – 1.97 (m, 3H, CH_2), 1.63 – 1.51 (m, 3H, CH_2), 1.35 – 1.23 (m, 21H, CH_2), 0.91 – 0.80 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.67, 150.88, 149.61, 130.12, 130.08, 124.47, 122.79, 112.02, 91.91, 77.00, 77.58, 72.58, 72.21, 71.85, 71.40, 71.19, 70.17, 67.43, 63.00, 31.77, 30.65, 29.53, 29.48, 29.18, 27.08, 22.56, 14.40.

HRMS (ESI) m/z calculated for $C_{35}H_{58}N_4O_{12}$ = 727.4121 $[M+H]^+$; observed 727.4121

Synthesis of compound (6a-f): To the compound 3b (1 mmol) in ethanol as solvent, monosaccharides (1mmol) were added, and (0.2 mmol) of ammonium sulfate as catalysts refluxed the reaction for 24h. The completion of the reaction was determined using TLC, the precipitated product was filtered using methanol, water and recrystallised in ethanol. The final pure compound was obtained as a white amorphous solid.

Compound 6a. Isolated as a white amorphous solid; mp 126-128°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) 10.94 (s, 1H, NH), 9.01 (s, 1H, NH) , 7.75 (d, *J* = 4 Hz, 1H, NH), 6.97 (t, *J* = 4 Hz, 3H, Ar-H), 6.87-6.80(m, 3H, Ar-H), 5.59 (d, *J* = 56 Hz, 1H, NH), 4.98 (s, 1H, Sac-H), 4.52 (m, 2H, Sac-H), 4.45 (s, 2H, alk-H), 4.40 (S, 2H, alk-H), 4.37 (s, 2H, Sac-H), 4.20 (s, 1H, Sac-H), 4.03 (d, *J* = 40 Hz, 2H, Sac-H), 3.80 (t, *J* = 16 Hz, 2H, Sac-H), 3.57 (s, 2H, Sac-H), 3.49-3.38 (m, 3H, Sac-H), 3.09 (s, 6H, Sac-H), 2.67-2.62 (m, 2H, CH_2), 1.55 (s, 2H, CH_2), 1.32-1.27 (m, 25H, CH_2), 0.88(t, *J* = 6 Hz2H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.72, 167.13, 151.04, 136.68, 130.08, 124.42, 122.98, 112.59, 91.29, 78.47, 77.40, 72.21, 71.75, 71.15, 67.80, 64.01, 62.10, 31.67, 31.52, 30.45, 29.74, 29.40, 29.36, 29.03, 28.66, 27.08, 22.41, 14.18.

HRMS(ESI) m/z calculated for $C_{37}H_{64}N_4O_{14}$ = 789.4489 $[M+H]^+$; observed 789.4437

Compound 6b. Isolated as a white amorphous solid; mp 122-124°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.98 (d, J = 67.9 Hz, 1H, NH), 9.05 (d, J = 41.3 Hz, 1H, NH), 7.70 (s, 1H, NH), 6.97 (t, J = 7.9 Hz, 1H, Ar-H), 6.85 – 6.75 (m, 2H, Ar-H), 4.94 (s, 2H), 5.36 (S, J = 4 Hz, 1H, NH) 4.51 (s, 2H, alk-H), 4.40 (s, 2H, alk-H), 4.22 (s, 1H), 4.10 (d, J = 8.7 Hz, 4H, Sac-H), 3.74 (t, J = 7.3 Hz, 2H, Sac-H), 3.63 (s, 2H, Sac-H), 3.51 (d, J = 24.2 Hz, 2H, Sac-H), 3.34 (s, 1H, Sac-H), 3.08 (s, 7H, Sac-H), 2.69 – 2.58 (m, 2H, CH_2), 2.07 – 1.97 (m, 1H, CH_2), 1.56 (d, J = 7.7 Hz, 2H, CH_2), 1.27 (s, 26H, CH_2), 0.91 – 0.84 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.71, 167.12, 151.04, 136.68, 130.09, 124.43, 122.98, 112.62, 91.30, 78.48, 77.40, 72.21, 71.75, 71.16, 67.82, 64.02, 62.10, 31.67, 31.52, 30.46, 29.75, 29.52, 29.41, 29.36, 29.19, 29.03, 28.66, 27.09, 22.41, 14.18.

HRMS(ESI) m/z calculated for $C_{37}H_{64}N_4O_{14}$ = 789.4489 $[M+H]^+$; observed 789.4462

Compound 6c. Isolated as a white amorphous solid; mp 129-131°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.07 (s, 1H, NH), 7.55 (s, 1H, NH), 6.97 (t, J = 7.9 Hz, 1H, Ar-H), 6.82 (dd, J = 13.6, 8.0 Hz, 2H, Ar-H), 5.56 (d, J = 50.2 Hz, 1H, NH), 5.35 (dd, J = 5.5, 4.1 Hz, 1H, Sac-H), 4.95 (d, J = 3.7 Hz, 3H, Sac-H), 4.51 (s, 2H, alk-H), 4.46 (s, 2H, alk-H), 4.40 (s, 1H, Sac-H), 4.21 (s, 1H, Sac-H), 3.85 (s, 2H, Sac-H), 3.72 (s, 1H, Sac-H), 3.70 (d, J = 2.4 Hz, 1H, Sac-H), 3.62 (d, J = 10.9 Hz, 1H, Sac-H), 3.52 (s, 1H, Sac-H), 3.51 – 3.38 (m, 3H, Sac-H), 3.31 – 3.04 (m, 7H, Sac-H), 2.68 – 2.59 (m, 2H, CH_2), 2.01 (d, J = 6.1 Hz, 2H, CH_2), 1.59 – 1.51 (m, 2H, CH_2), 1.29 (d, J = 19.3 Hz, 21H, CH_2), 0.87 (t, J = 6.7 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.69, 167.04, 151.05, 146.21, 136.69, 130.09, 124.42, 122.95, 112.58, 72.04, 71.82, 71.24, 70.52, 70.35, 67.83, 64.26, 31.68, 30.48, 29.76, 29.41, 29.37, 29.30, 29.04, 27.09, 22.42, 14.19.

HRMS(ESI) m/z calculated for $C_{37}H_{64}N_4O_{14}$ = 789.4489 $[M+H]^+$; observed 789.4479

Compound 6d. Isolated as a white amorphous solid; mp 118-120°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.02 (s, 1H, NH), 7.70 (d, J = 92 Hz, 1H, NH), 5.61 (s, 1H, NH), 6.96 (t, J = 7.8 Hz, 1H, Ar-H), 6.87 – 6.74 (m, 2H, Ar-H), 5.35 (t, J = 4.8 Hz, 2H, Sac-H), 4.65 (s, 1H, Sac-H), 4.51 (s, 2H, alk-H), 4.40 (s, 2H, alk-H), 4.19 (d, J = 5.3 Hz, 1H, Sac-H), 4.04 (d, J = 28.2 Hz, 1H, Sac-H), 3.79 (d, J = 40.5 Hz, 2H, Sac-H), 3.60 (q, J = 3.4 Hz, 2H, Sac-H), 3.54 – 3.48 (m, 2H, Sac-H), 3.47 – 3.41 (m, 2H, Sac-H), 3.31 (s, 1H, Sac-H), 3.23 – 3.15 (m, 1H, Sac-H), 3.06 (q, J = 9.2 Hz, 2H, Sac-H), 2.68 – 2.58 (m, 3H, CH_2), 2.00 (s, 2H, CH_2), 1.55 (s, 2H, CH_2), 1.37 – 1.23 (m, 25H, CH_2), 0.90 – 0.84 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.68, 167.09, 150.91, 145.80, 136.63, 124.50, 122.78, 112.05, 91.95, 77.01, 72.67, 71.85, 71.41, 70.18, 67.31, 63.01, 31.77, 30.67, 29.52, 29.18, 22.57, 14.40.

HRMS(ESI) m/z calculated for $C_{35}H_{60}N_4O_{12}$ = 729.4278 $[M+H]^+$; observed 729.4268

Compound 6e. Isolated as a white amorphous solid; mp 121-123°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.02 (s, 1H, NH), 7.56 (d, J = 111.5 Hz, 1H, NH), 6.97 (t, J = 7.9 Hz, 1H, Ar-H), 6.86 – 6.74 (m, 2H, Ar-H), 5.34 (t, J = 4.8 Hz, 1H, Sac- H), 5.00 (s, 4H, Sac- H), 4.52 (d, J = 3.2 Hz, 2H, alk-H), 4.42 (d, J = 18.3 Hz, 2H, alk-H), 4.37 – 4.12 (m, 3H, Sac- H), 4.12 – 3.88 (m, 3H, Sac- H), 3.69 (d, J = 36.0 Hz, 1H, Sac- H), 3.62 – 3.51 (m, 3H, Sac- H), 3.50 (d, J = 3.3 Hz, 1H, Sac- H), 3.49 – 3.48 (m, 1H, Sac- H), 3.47 (s, 1H, Sac- H), 2.68 – 2.55 (m, 3H, CH_2), 2.01 (s, 2H, CH_2), 1.54 (d, J = 9.0 Hz, 2H, CH_2), 1.29 (m, 25H, CH_2), 1.09 (t, J = 7.0 Hz, 2H, CH_2), 0.90 – 0.85 (m, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.70, 167.05, 151.05, 146.19, 136.68, 124.40, 122.94, 112.57, 92.14, 72.90, 71.76, 70.94, 70.73, 70.29, 67.82, 63.83, 31.68, 30.47, 29.41, 29.37, 29.30, 29.04, 22.42, 14.18.

HRMS(ESI) m/z calculated for $C_{35}H_{60}N_4O_{12}$ = 729.4278 $[M+H]^+$; observed 729.4240

Compound 6f. Isolated as a white amorphous solid; mp 115-117°C yield = 84%

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.2 (d, *J* = 69.0 Hz, 1H, NH), 9.21 (d, *J* = 69.0 Hz, 1H, NH), 9.18 (d, *J* = 69.0 Hz, 1H, NH), 7.01 – 6.93 (m, 1H, Ar-H), 6.83 – 6.69 (m, 2H, Ar-H), 5.34 (s, 1H, sac-H), 5.04 – 4.82 (m, 2H, sac-H), 4.61 (s, 1H, sac-H), 4.55 (s, 2H, alk-H), 4.44 (s, 2H, alk-H), 4.39 – 4.32 (m, 2H, sac-H), 4.19 (d, *J* = 15.4 Hz, 1H, sac-H), 4.10 (s, 2H, sac-H), 3.88 (d, *J* = 15.5 Hz, 1H, sac-H), 3.79 – 3.65 (m, 2H, sac-H), 3.54 (s, 1H, sac-H), 3.43 – 3.40 (m, 1H, sac-H), 3.18 (s, 5H, sac-H), 2.60 (d, *J* = 8.2 Hz, 2H, CH_2), 1.99 (d, *J* = 6.1 Hz, 1H, CH_2), 1.52 (d, *J* = 7.4 Hz, 2H, CH_2), 1.24 (s, 22H,CH_2), 0.85 (d, *J* = 1.3 Hz, 3H, CH_3).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.68, 167,09, 150.91, 145.80, 136.63, 124.50, 122.78, 112.05, 91.95, 77.01, 71.41, 70.18, 67.31, 6301, 31.77, 30.67, 29.52, 29.18, 22.57, 14.40.

HRMS(ESI) m/z calculated for $C_{35}H_{60}N_4O_{12}$ = 729.4278 $[M+H]^+$; observed 729.4278

Table S1. Gelation studies of compounds 5,6a-f in various solvents and vegetable oils

S.No	Solvents	5a	5b	5c	5d	5e	5f	6a	6b	6c	6d	6e	6f
1	chloroform	I	I	I	I	I	I	I	I	I	I	I	I
2	DMSO	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**
3	water	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS
4	toluene	I	I	I	I	I	I	I	I	I	I	I	I
5	Olive oil	S	S	S	S	S	S	S	S	S	S	S	S
6	Hexane	I	I	I	I	I	I	I	I	I	I	I	I
7	xylene	I	I	I	I	I	I	I	I	I	I	I	I
8	cyclohexane	I	I	I	I	I	I	I	I	I	I	I	I
9	diesel	S	S	S	S	S	S	S	S	S	S	S	S
10	DMSO + water	**G (1.5)**	PG	PG	S	S	S	**G (1)**	PG	PG	S	S	S
11	Linseed oil	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**	**G (1)**
12	N-methyl pyrrolidine	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS
13	paraffin	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS
14	THF	I	I	I	I	I	I	I	I	I	I	I	I
15	Acetone	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS	PS
16	PEG	I	I	I	I	I	I	I	I	I	I	I	I
17	1 ,4 Dioxane	S	S	S	S	S	S	S	S	S	S	S	S
18	Ethylene glycol	I	I	I	I	I	I	I	I	I	I	I	I

CGC, Critical gelation concentration, is given in %wt/v (parentheses); S, soluble; G, gel; PS, partially soluble; PG, partial gel; I, insoluble.

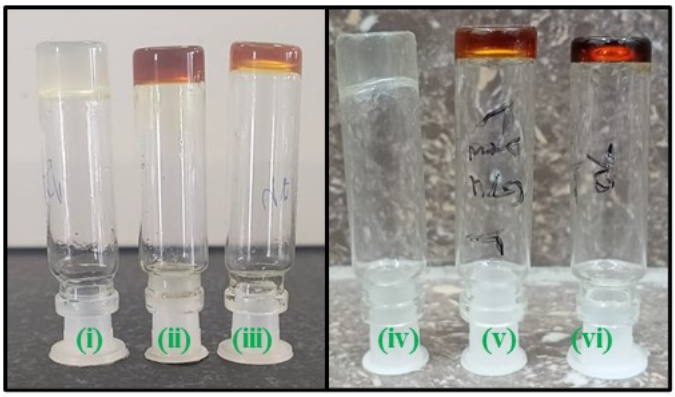

Figure S1. The gel formed by (i) and (ii) compound 5a in DMSO+Water, and Linseed oil respectively. (iii) 5b in linseed oil. (iv) and (v) compound 6a in DMSO+Water and Linseed oil respectively (vi) 6b in linseed oil.

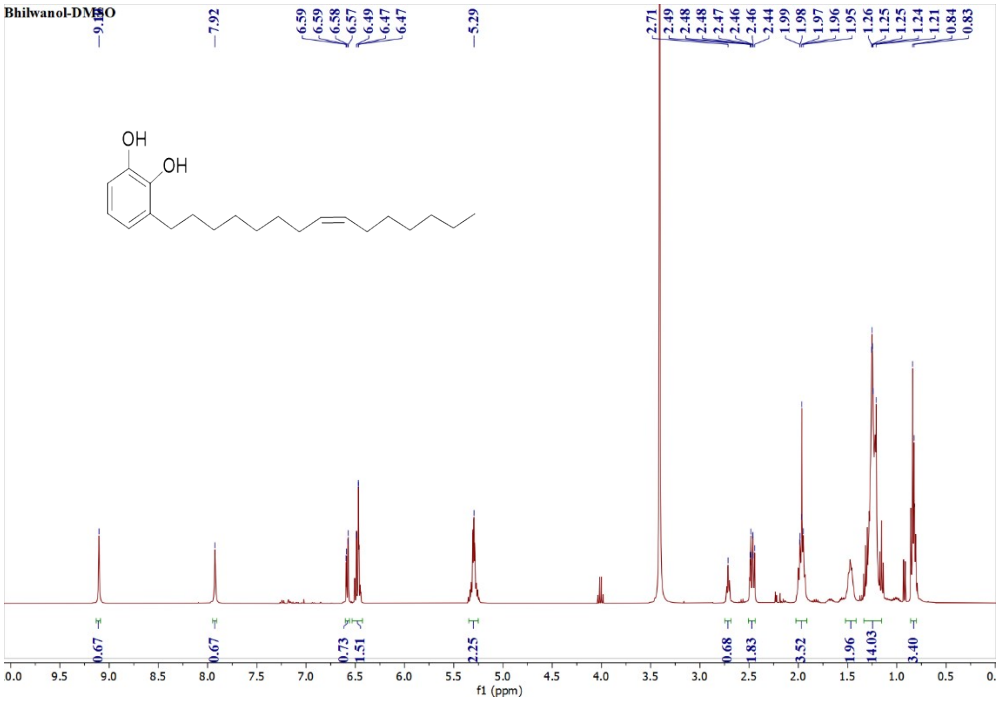

Figure S2. ^{1}H NMR spectra of compound 1a (DMSO-d_6 400MHz)

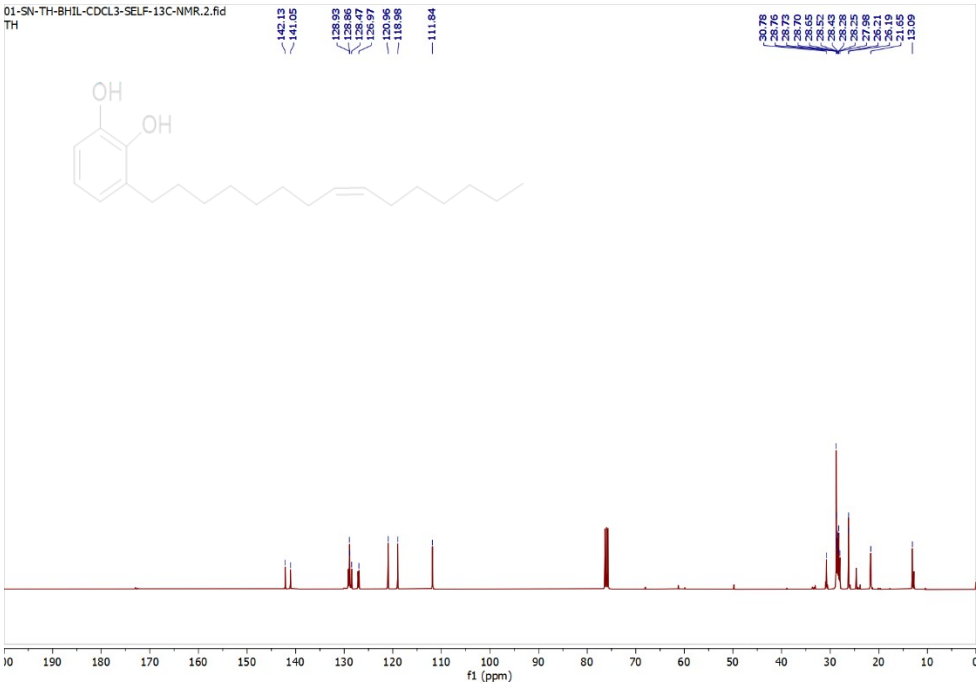

Figure S3. ^{13}C NMR spectra of compound 1a ($CDCl_3$ 100MHz)

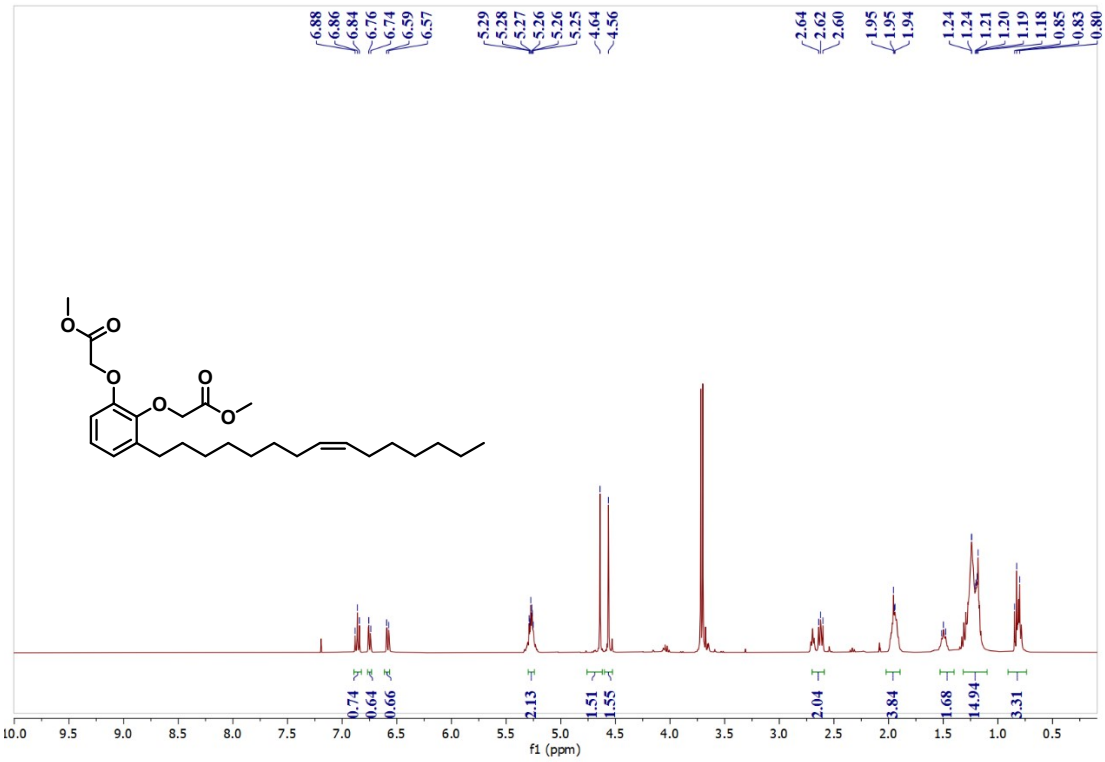

Figure S4. ^{1}H NMR spectra of compound 2a (DMSO-d_6 400MHz)

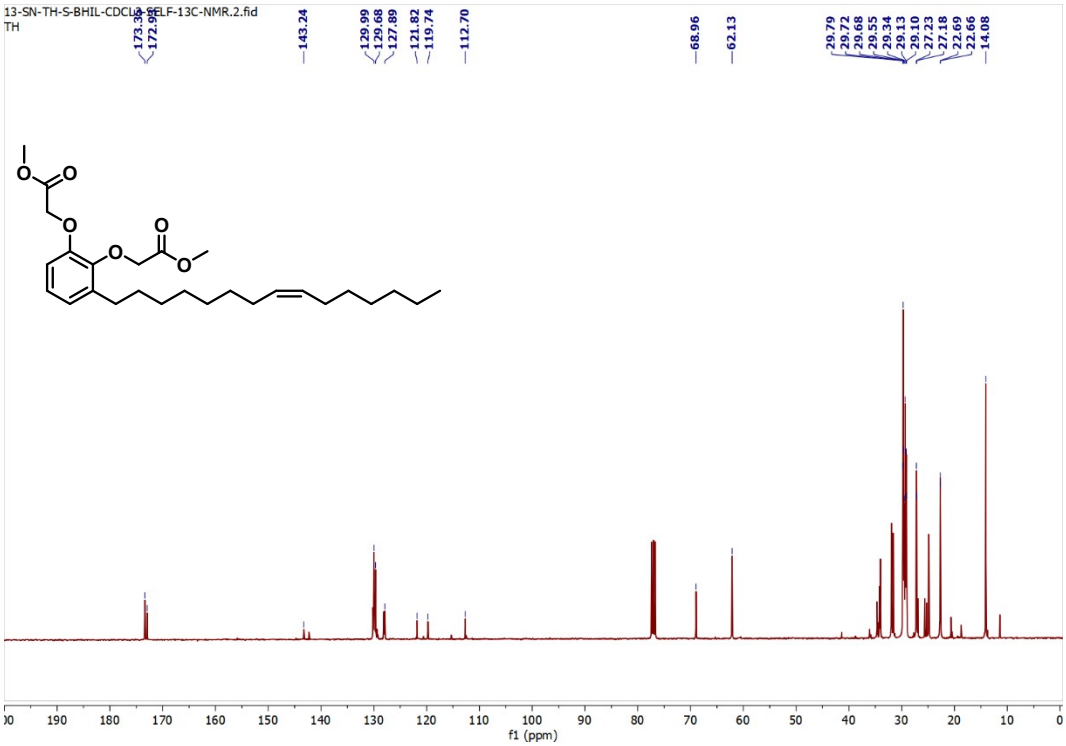

Figure S5. ^{13}C NMR spectra of compound 2a ($CDCl_3$ 100MHz)

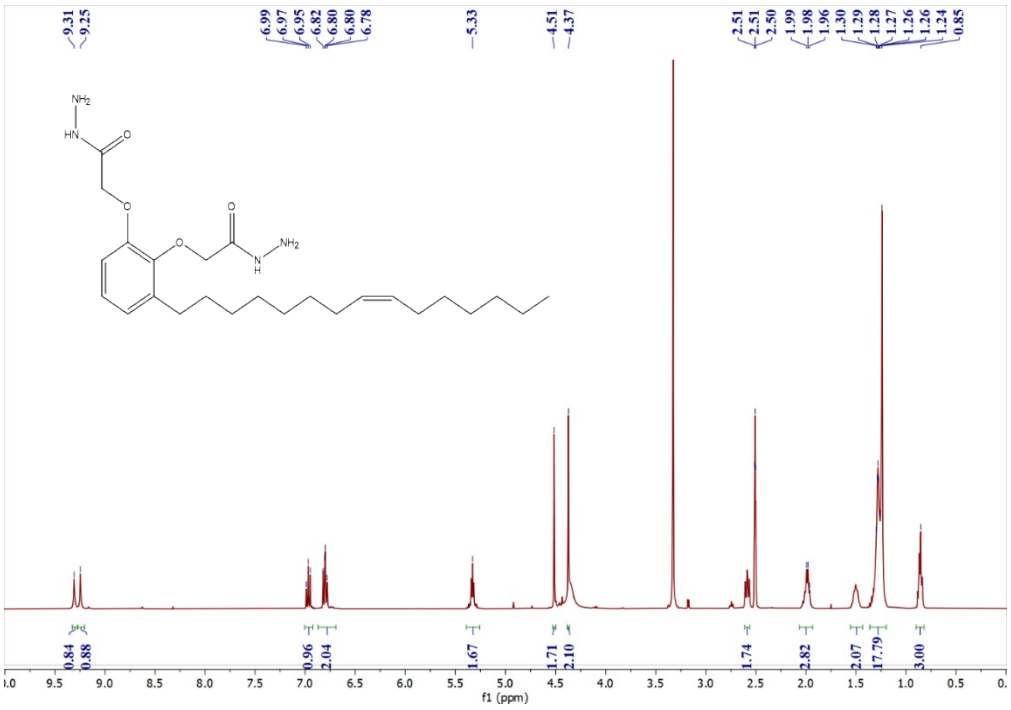

Figure S6. ^{1}H NMR spectra of compound 3a (DMSO-d_6 400MHz)

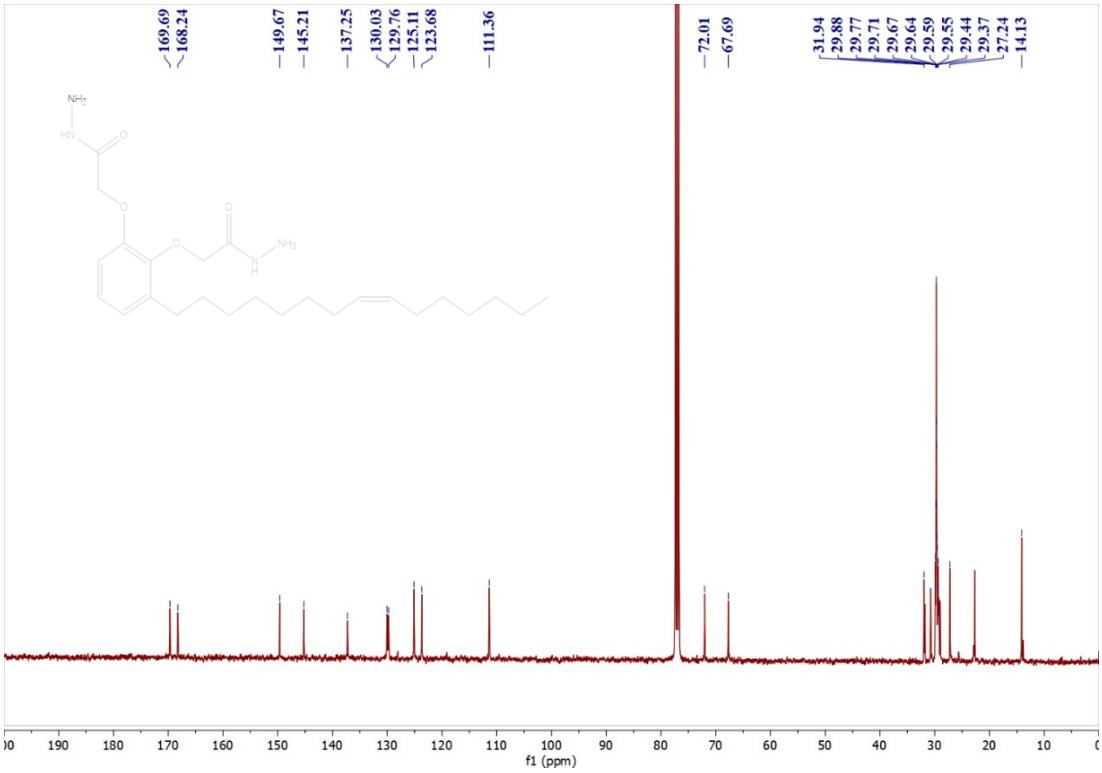

Figure S7. ^{13}C NMR spectra of compound 3a ($CDCl_3$ 100MHz)

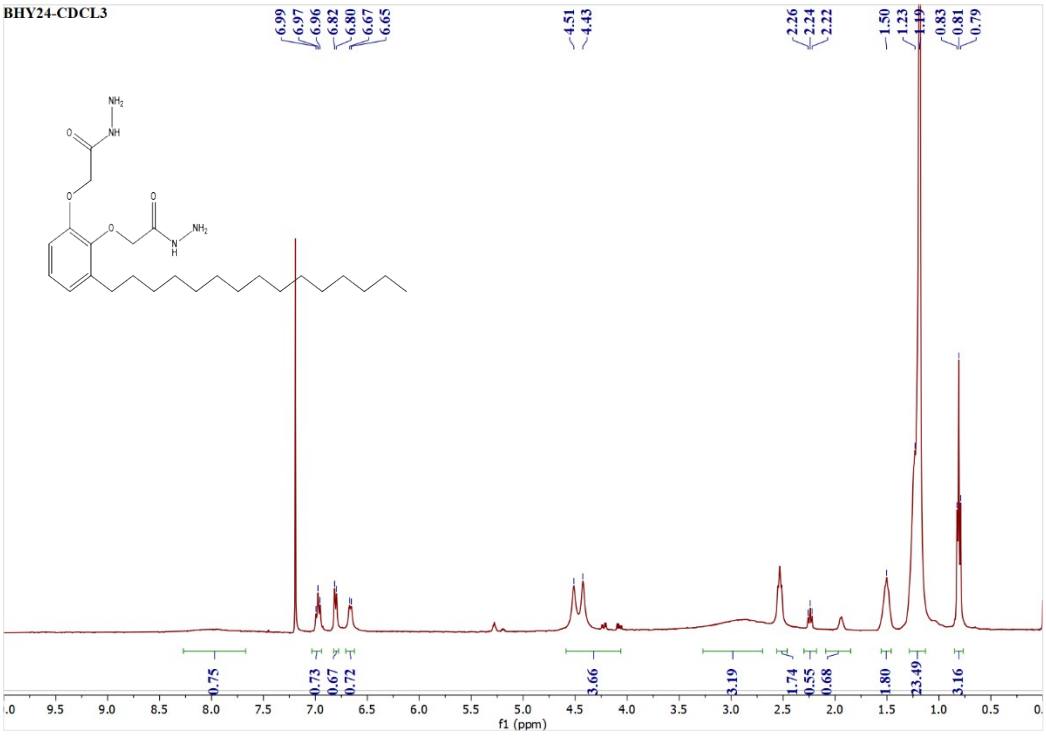

Figure S8. ^{1}H NMR spectra of compound 3b ($CDCl_3$ 400MHz)

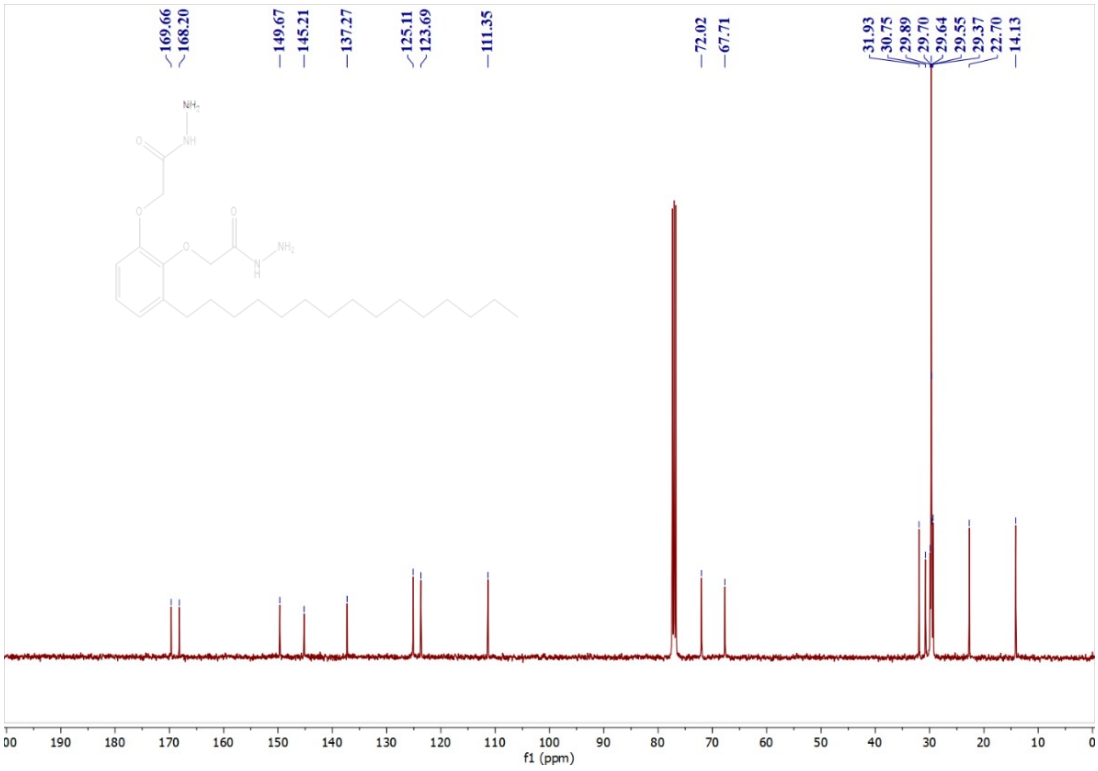

Figure S9. ^{13}C NMR spectra of compound 3b ($CDCl_3$ 100MHz)

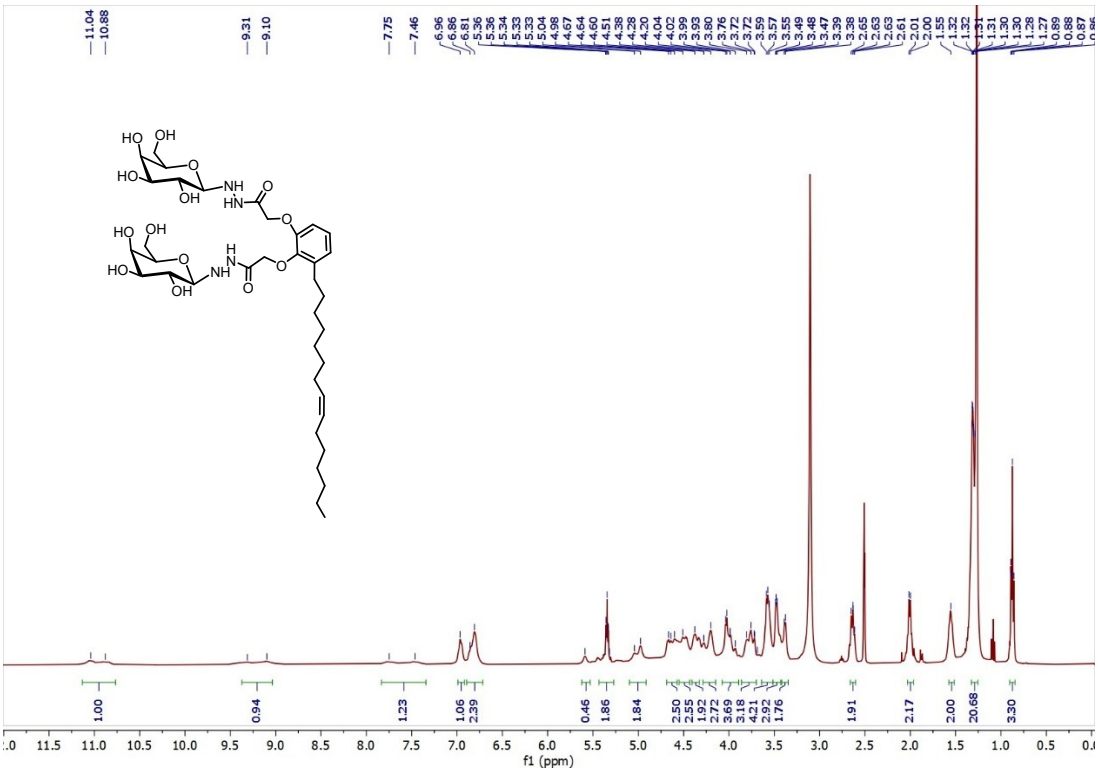

Figure S10. ^{1}H NMR spectrum of compound 5a (DMSO-d_6 400MHz) at 80 °C

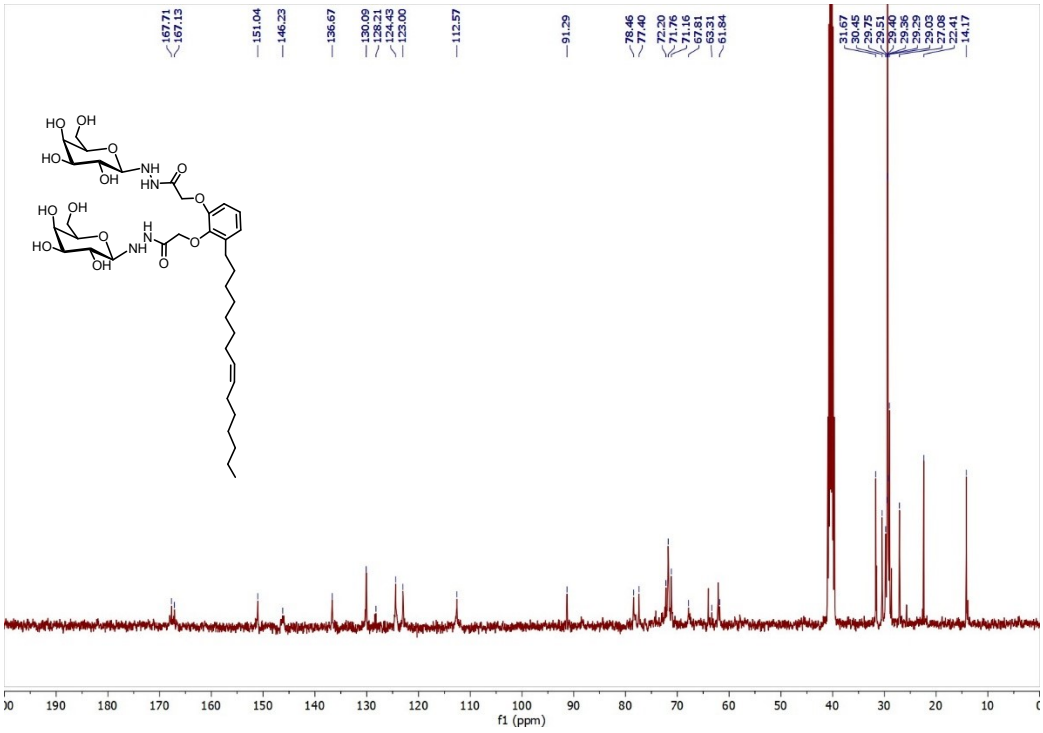

Figure S11. ^{13}C NMR spectrum of compound 5a (DMSO-d_6 100MHz) at 80 ^{o}C

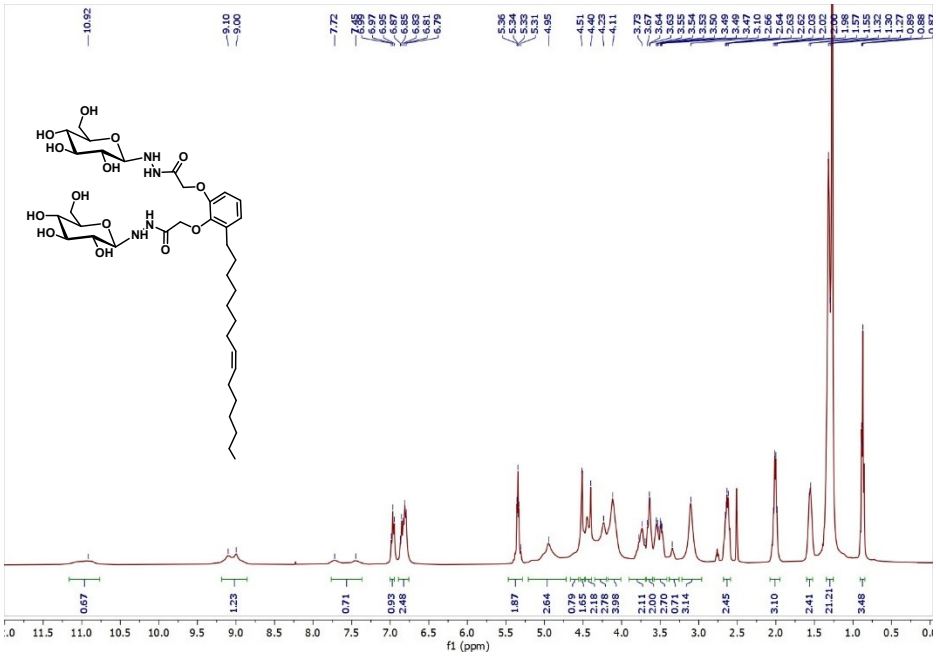

Figure S12. ^{1}H NMR spectrum of compound 5b (DMSO-d_6 400MHz) at 80 ^{o}C

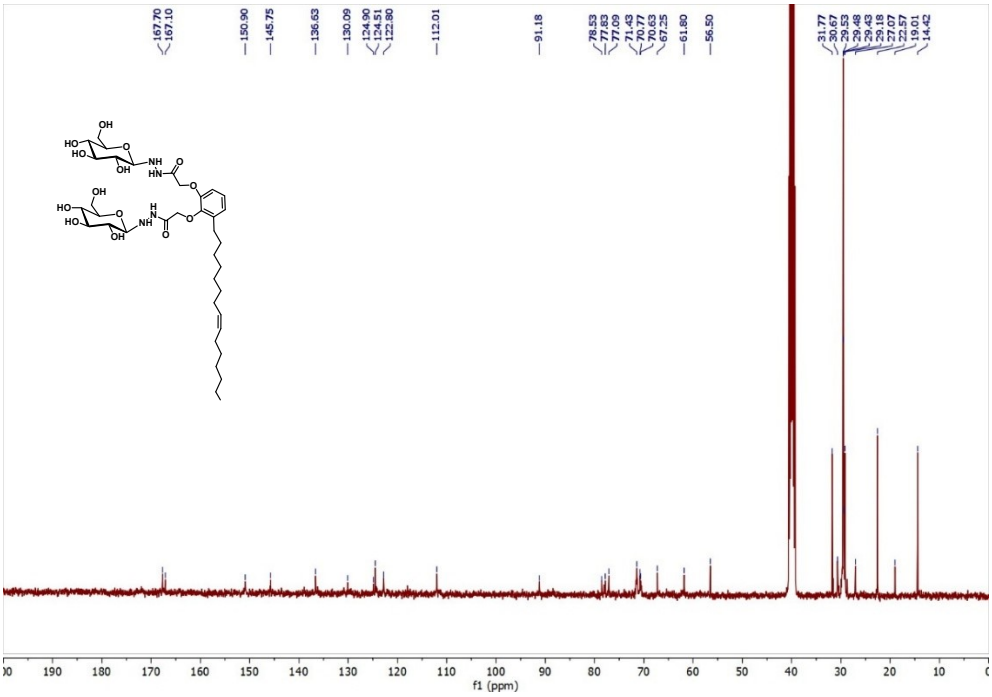

Figure S13. ^{13}C NMR spectrum of compound 5b (DMSO-d_6 100MHz) at 80 °C

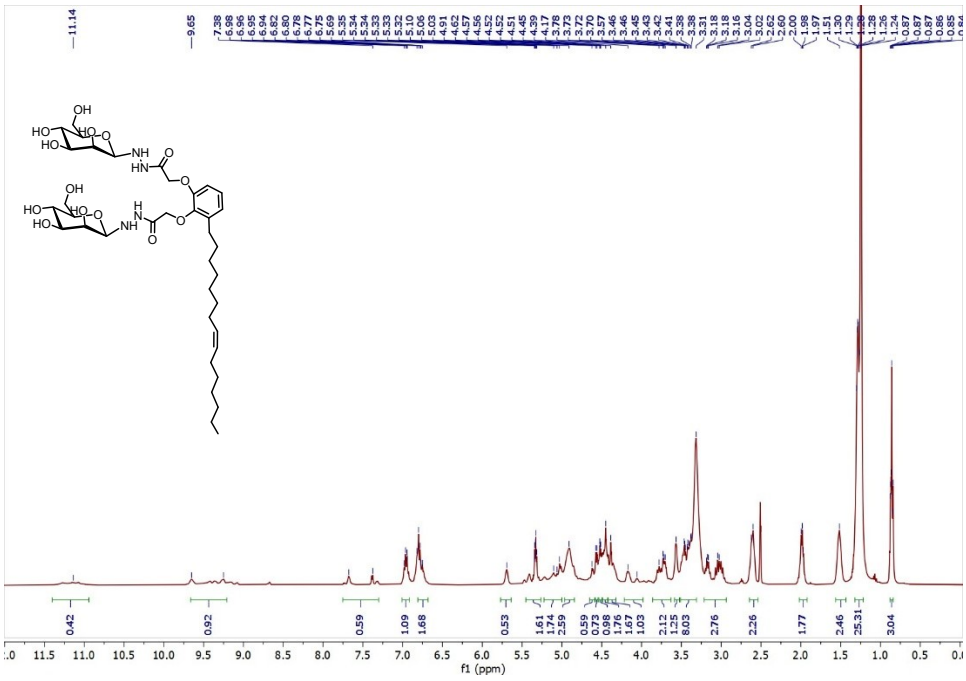

Figure S14. ^{1}H NMR spectrum of compound 5c (DMSO-d_6 400MHz) at 80 °C

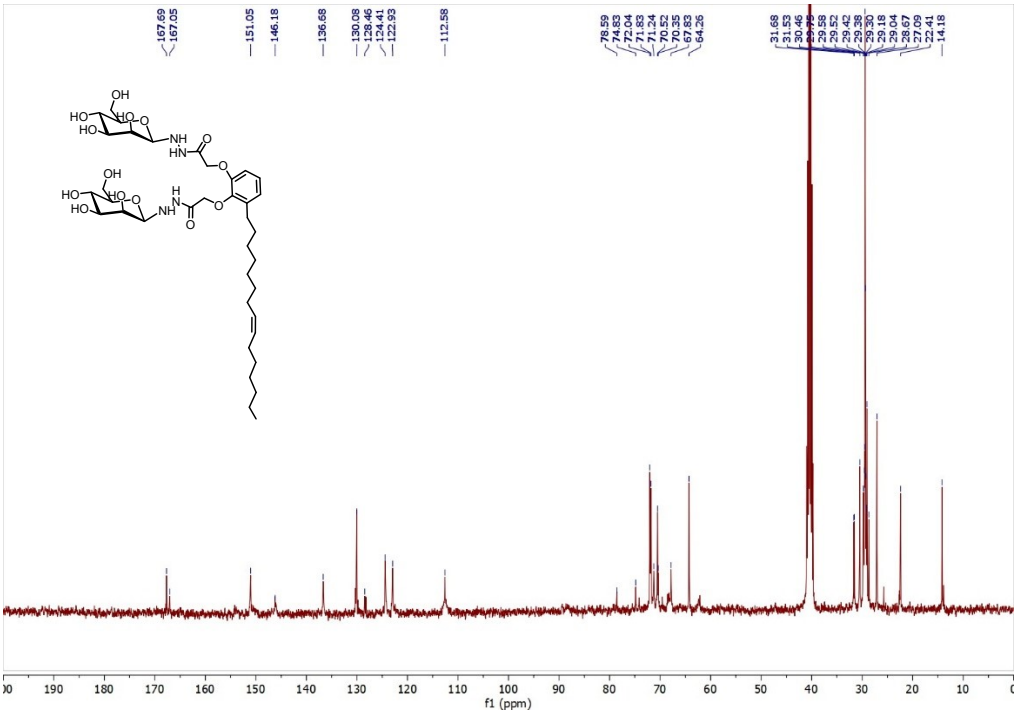

Figure S15. ^{13}C NMR spectrum of compound 5c (DMSO-d_6 100MHz) at 80 °C

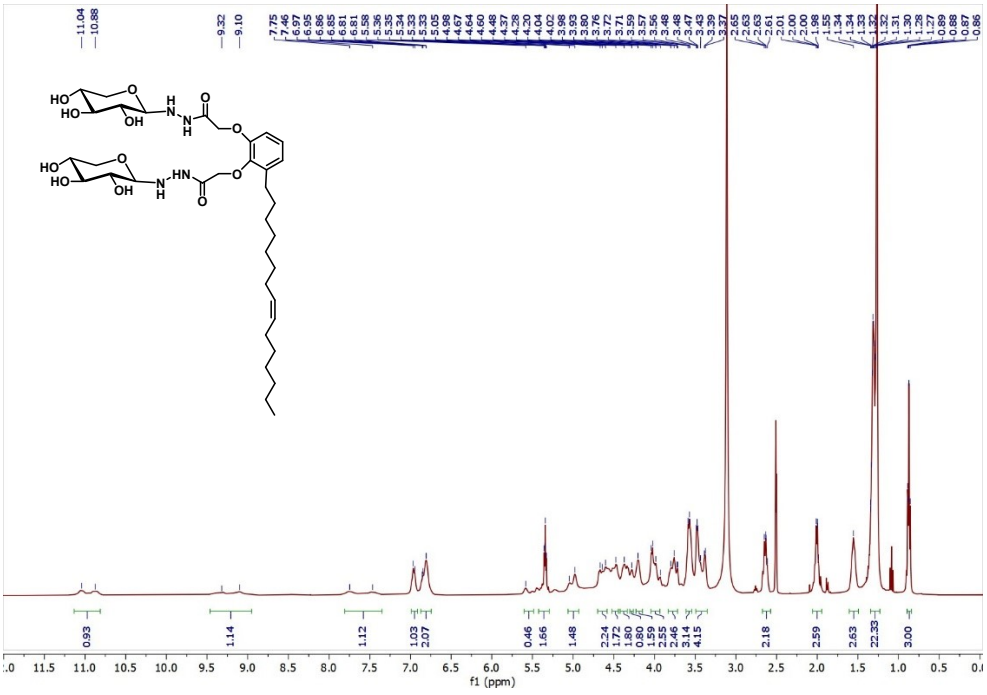

Figure S16. ^{1}H NMR spectrum of compound 5d (DMSO-d_6 400MHz) at 80 °C

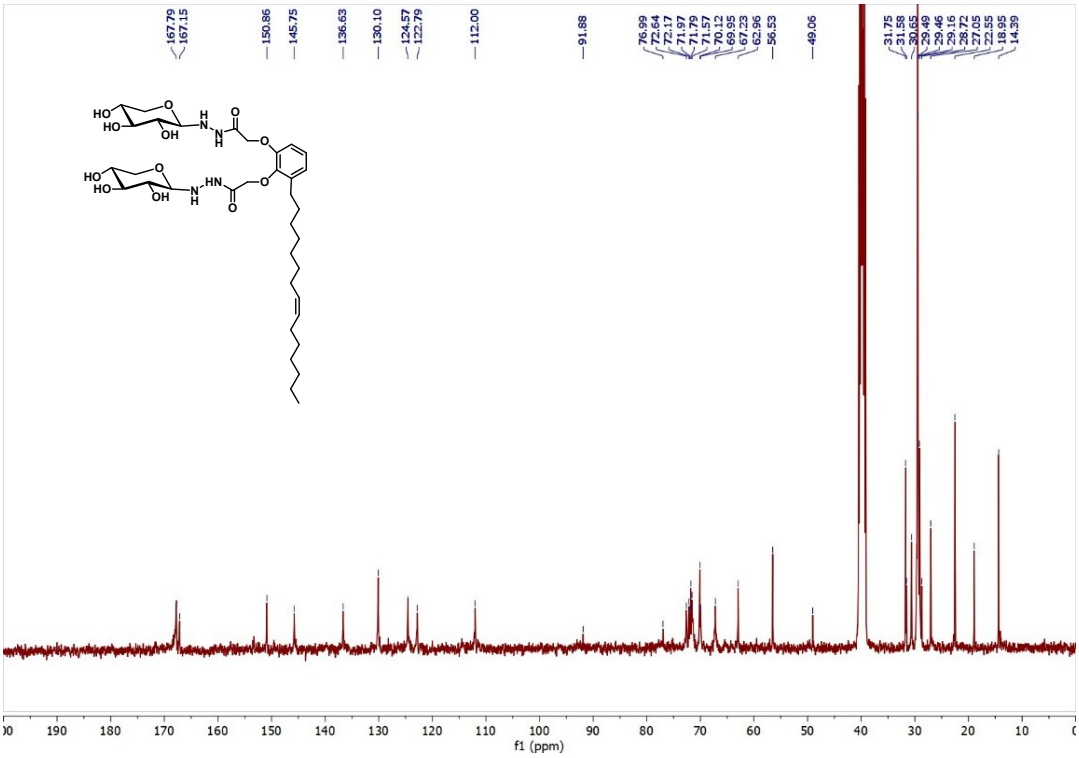

Figure S17. ^{13}C NMR spectrum of compound 5d (DMSO-d_6 100MHz) at 80 °C

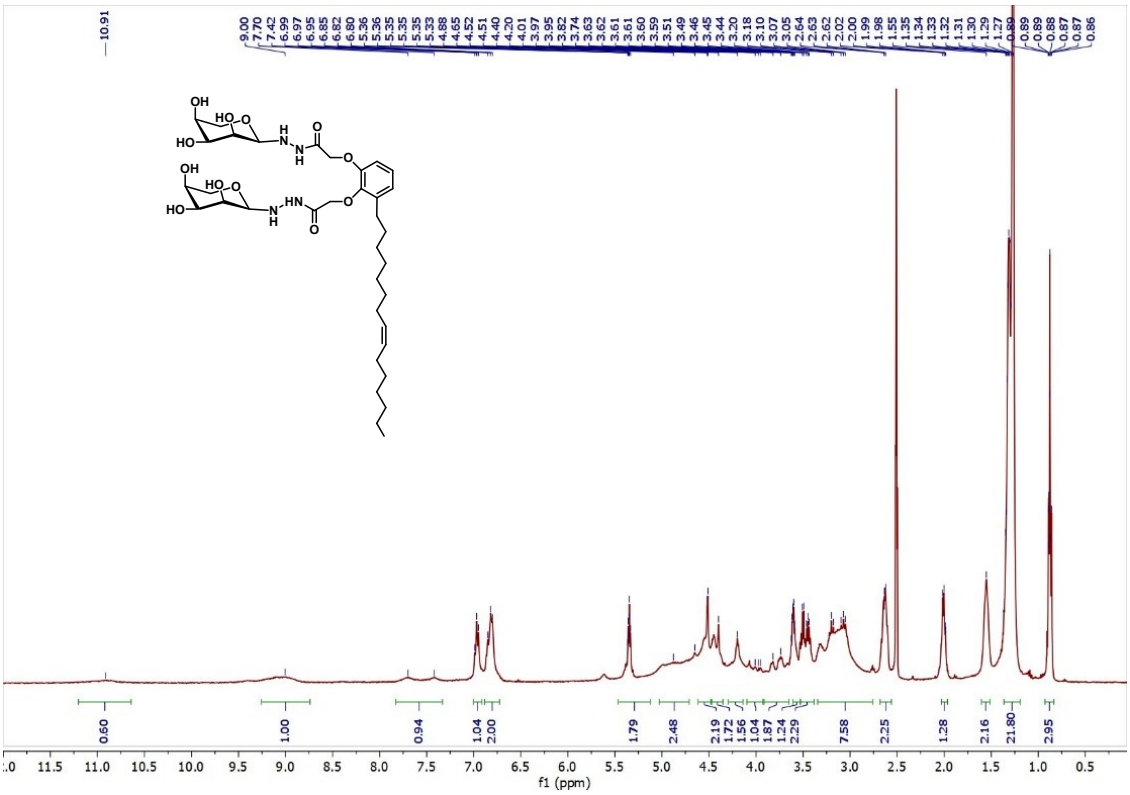

Figure S18. ^{1}H NMR spectrum of compound 5e (DMSO-d_6 400MHz) at 80 °C

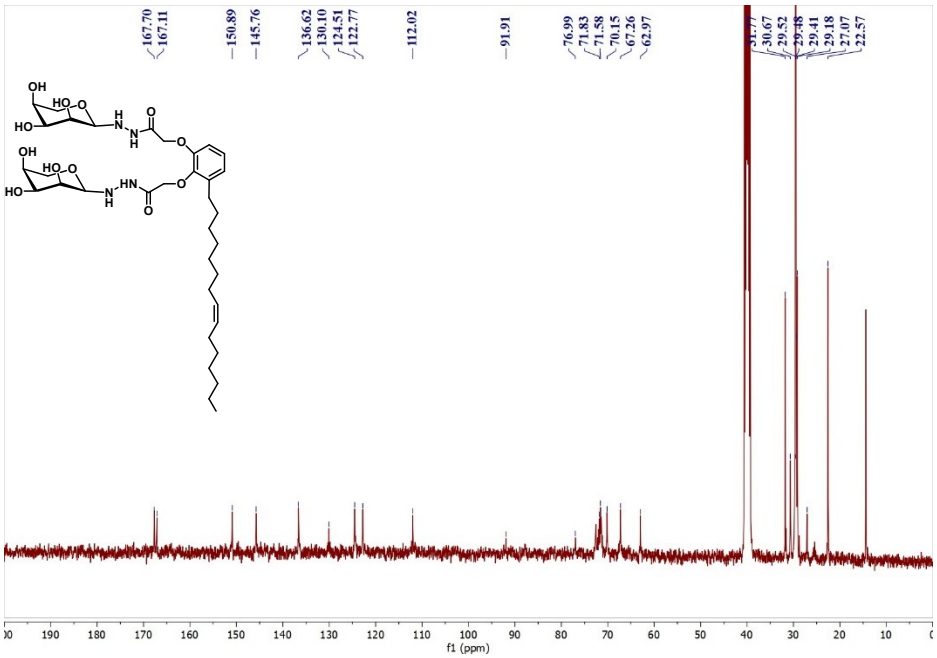

Figure S19. ^{13}C NMR spectrum of compound 5e (DMSO-d_6 100MHz) at 80 °C

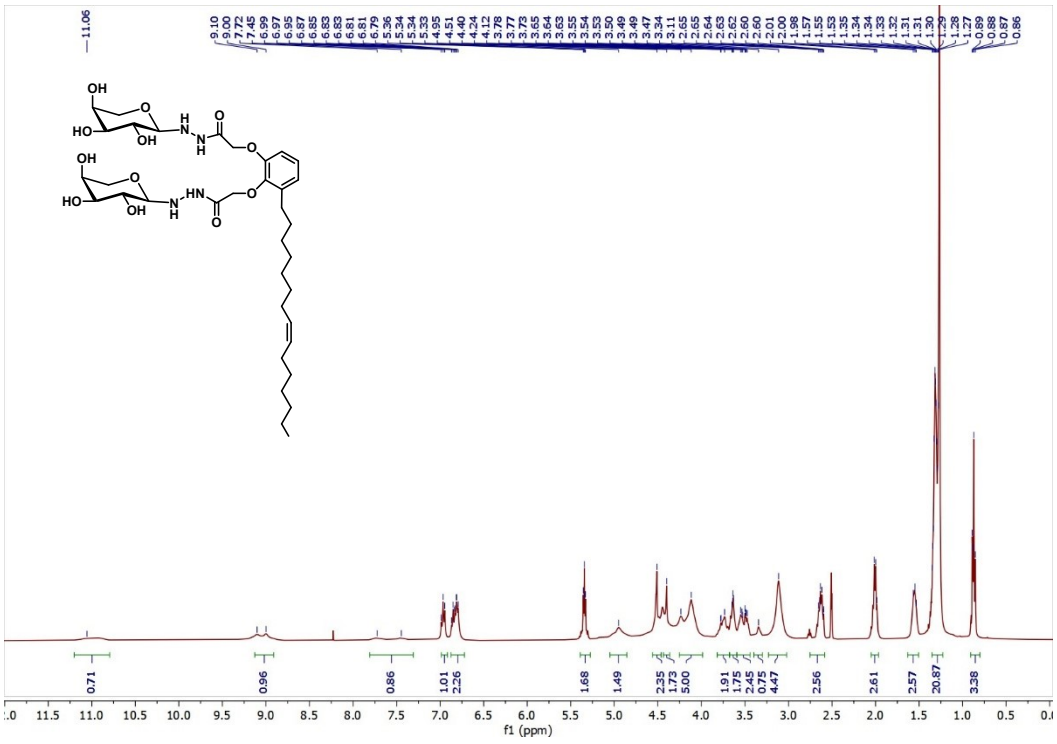

Figure S20. ^{1}H NMR spectrum of compound 5f (DMSO-d_6 400MHz) at 80 °C

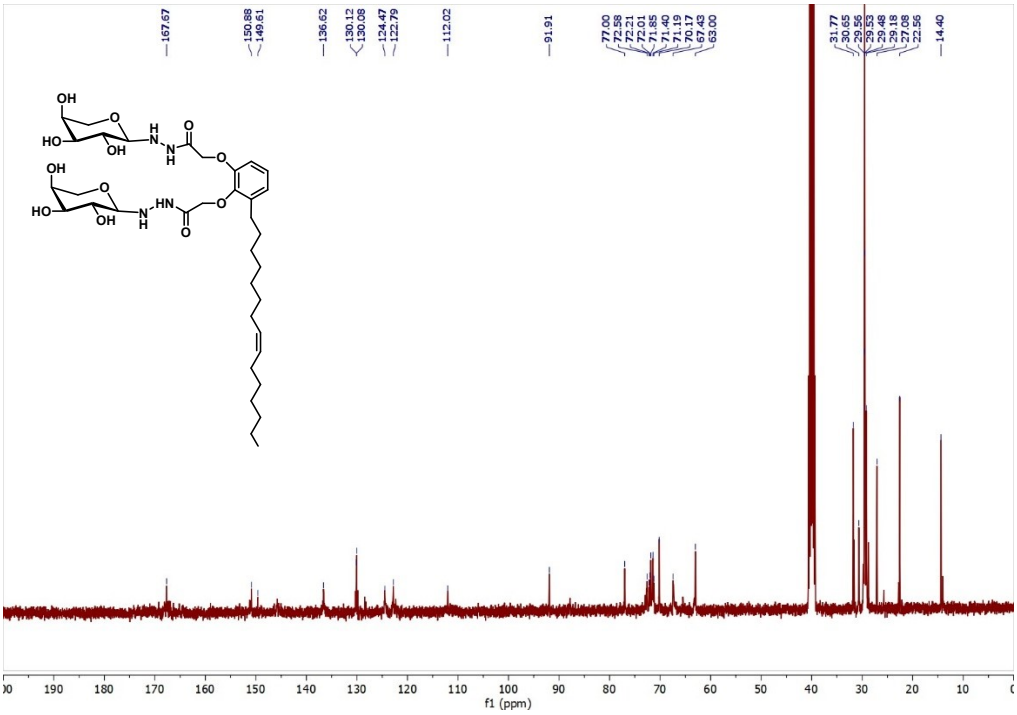

Figure 21. ^{13}C NMR spectrum of compound 5f (DMSO-d_6 100MHz) at 80 °C

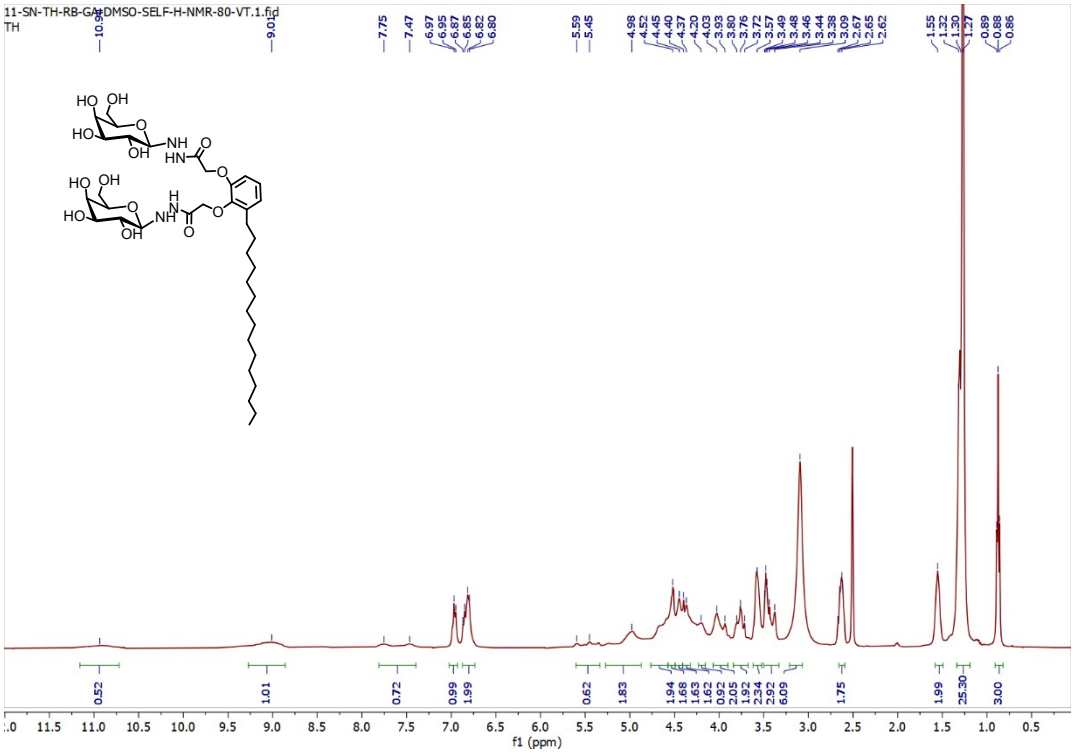

Figure S22. ^{1}H NMR spectrum of compound 6a (DMSO-d_6 400MHz) at 80 °C

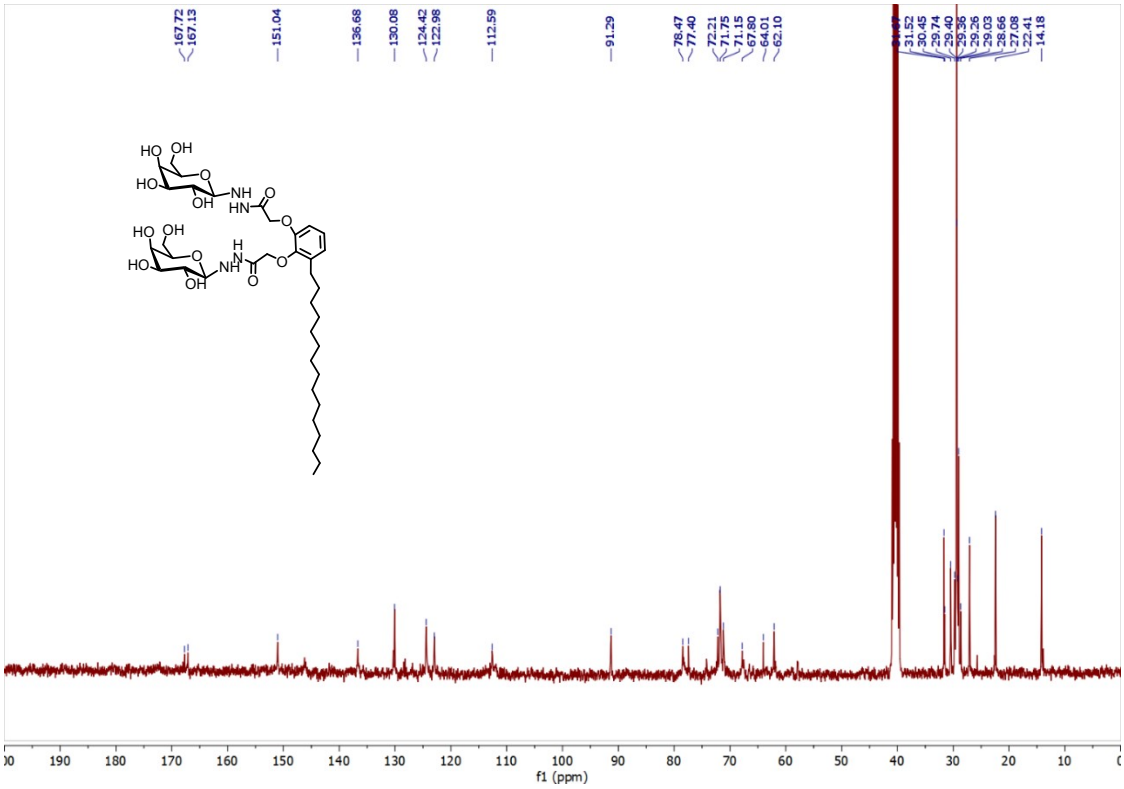

Figure S23. ^{13}C NMR spectrum of compound 6a (DMSO-d_6 100MHz) at 80 °C

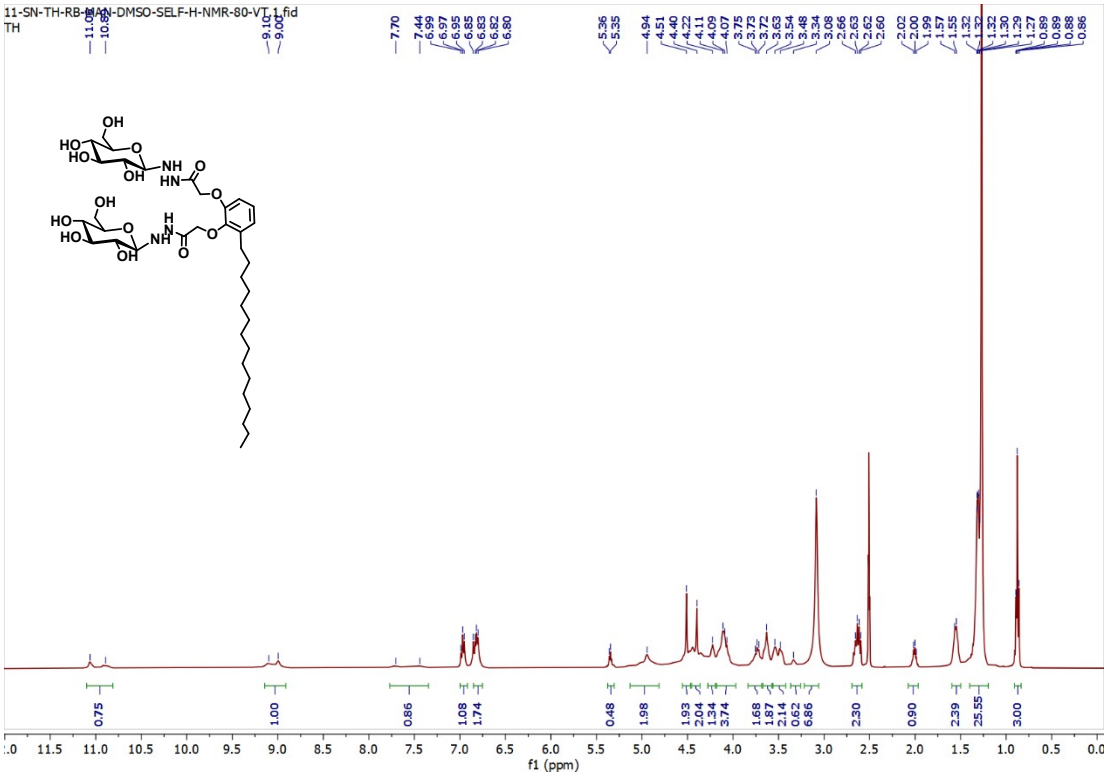

Figure S24. ^{1}H NMR spectrum of compound 6b (DMSO-d_6 400MHz) at 80 °C

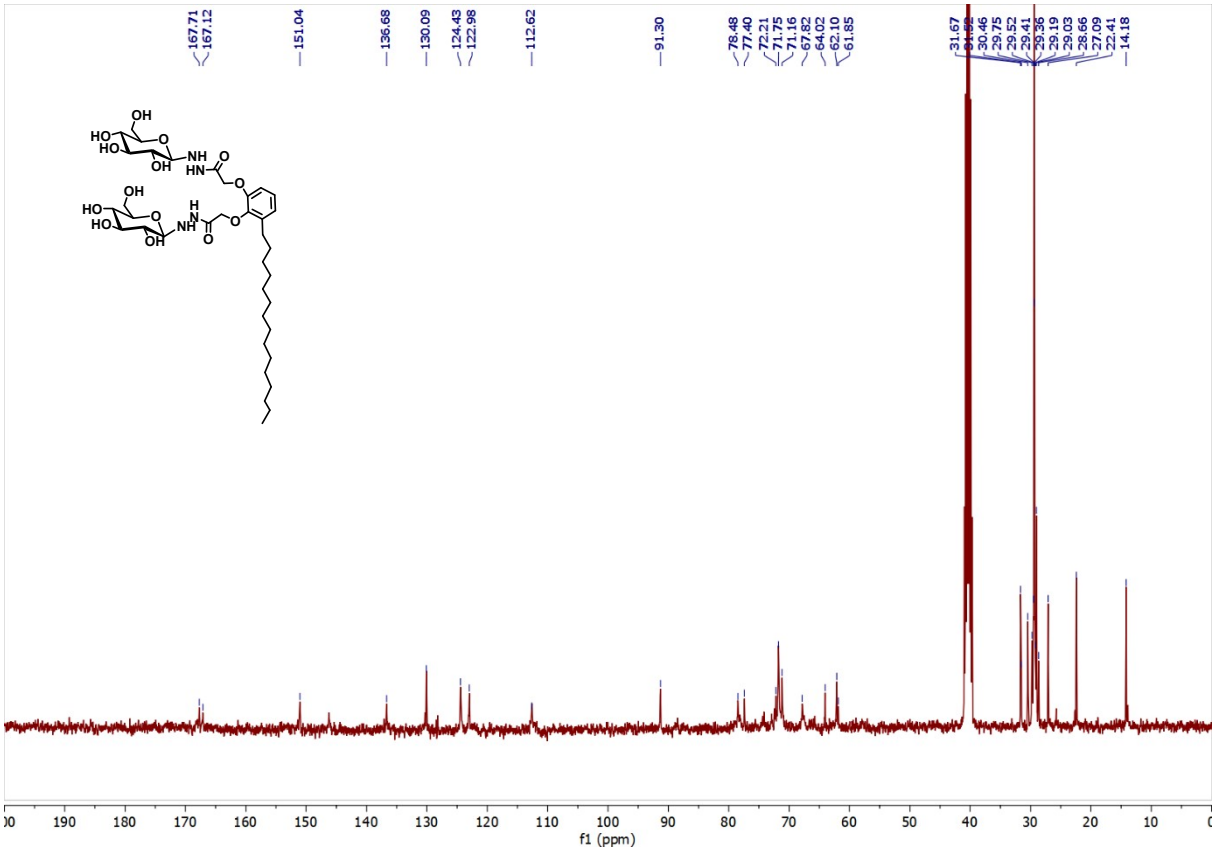

Figure S25. ^{13}C NMR spectrum of compound 6b (DMSO-d_6 100MHz) at 80 °C

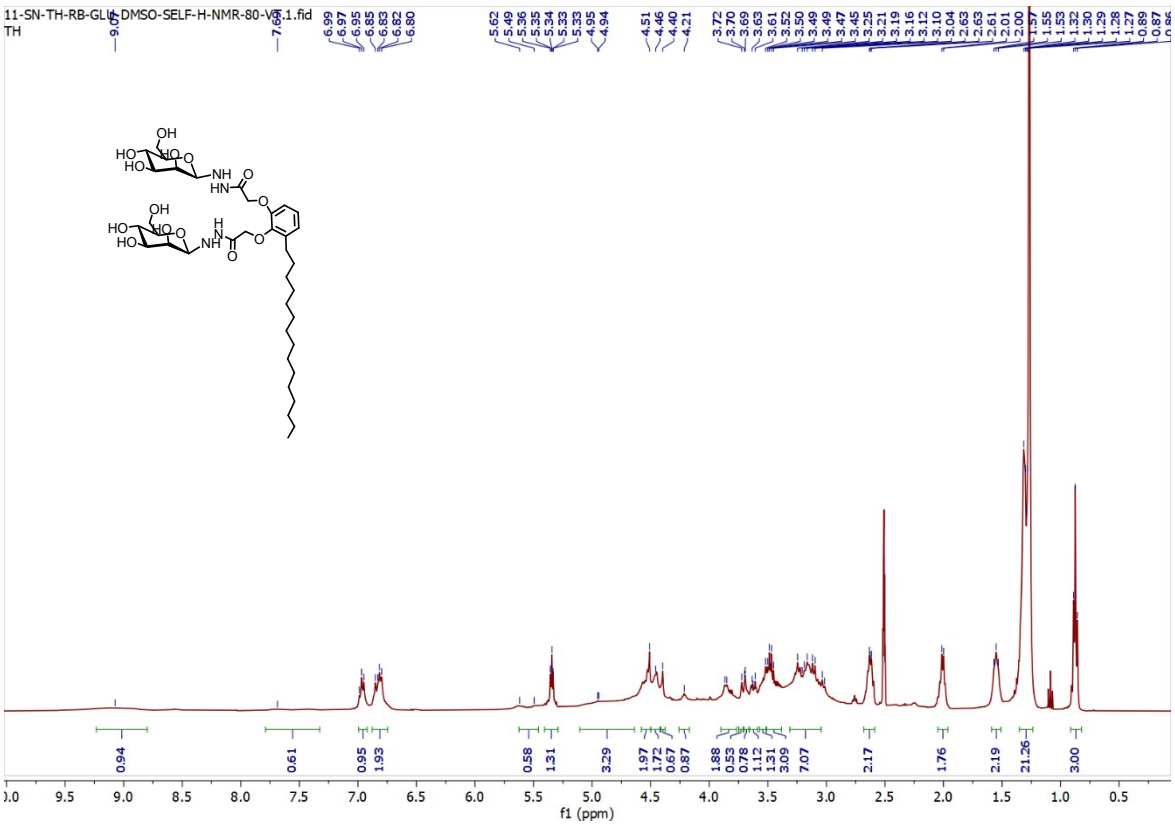

Figure S26. ^{1}H NMR spectrum of compound 6c (DMSO-d_6 400MHz) at 80 °C

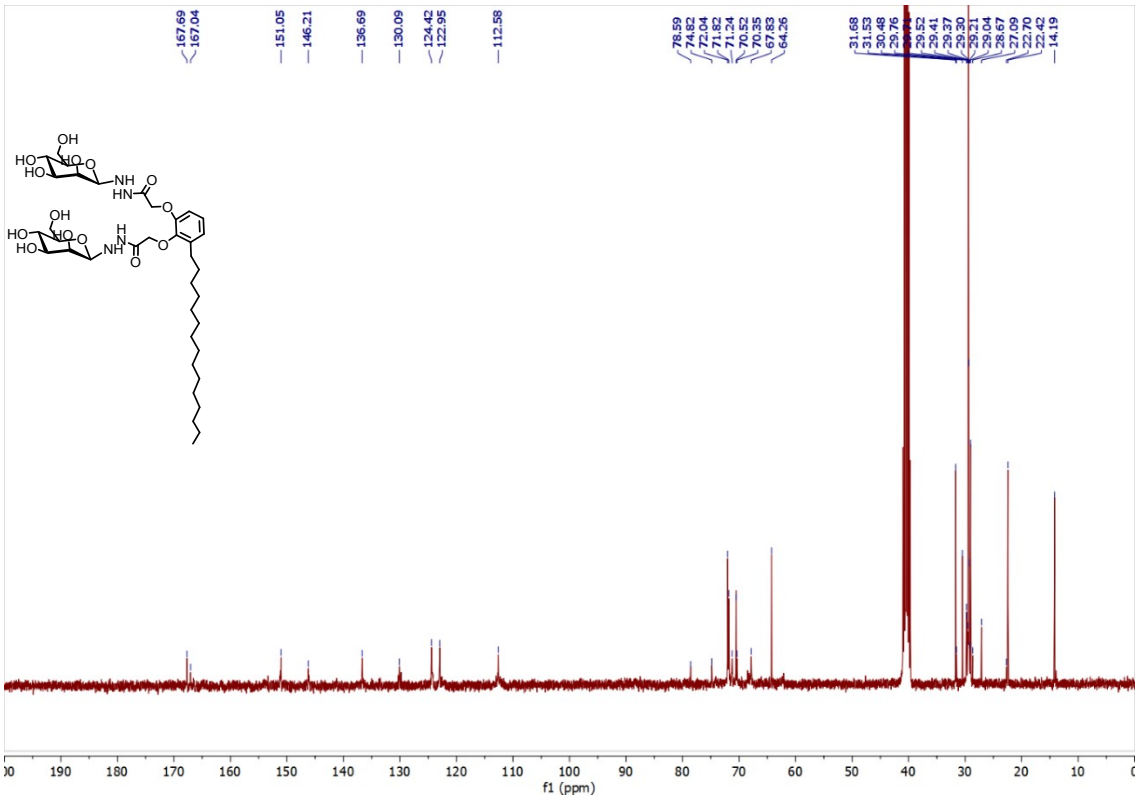

Figure S27. ^{13}C NMR spectrum of compound 6c (DMSO-d_6 100MHz) at 80 °C

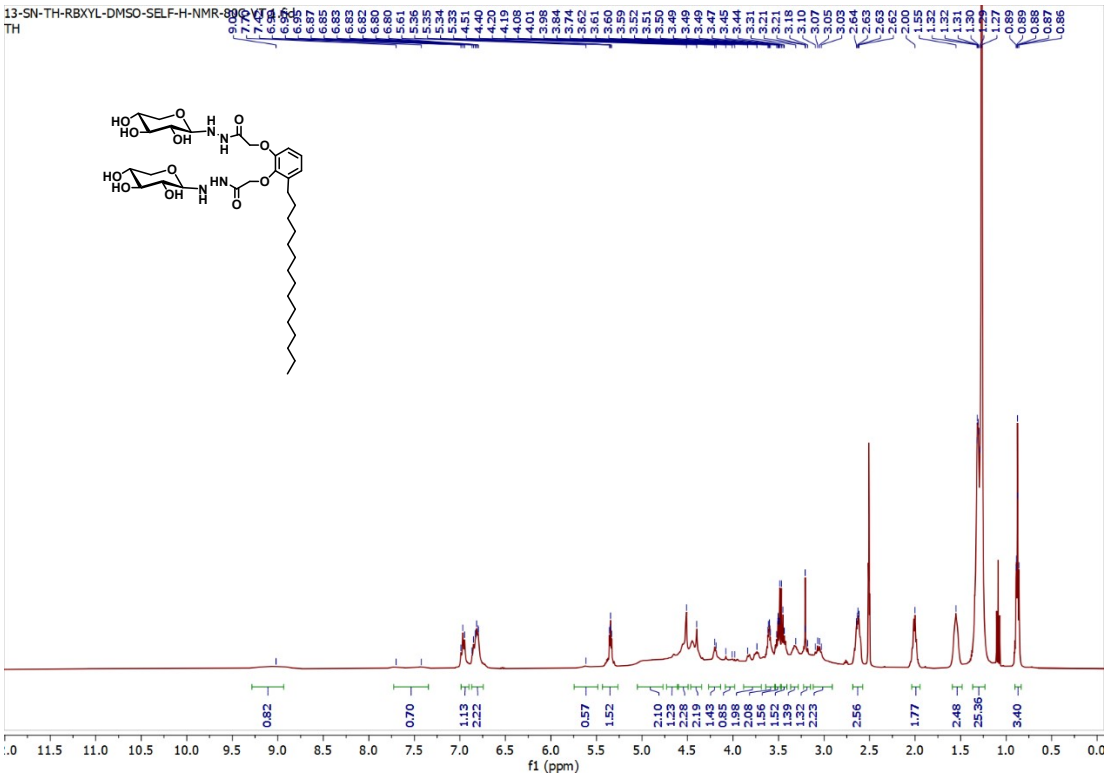

Figure S28. ^{1}H NMR spectrum of compound 6d (DMSO-d_6 400MHz) at 80 °C

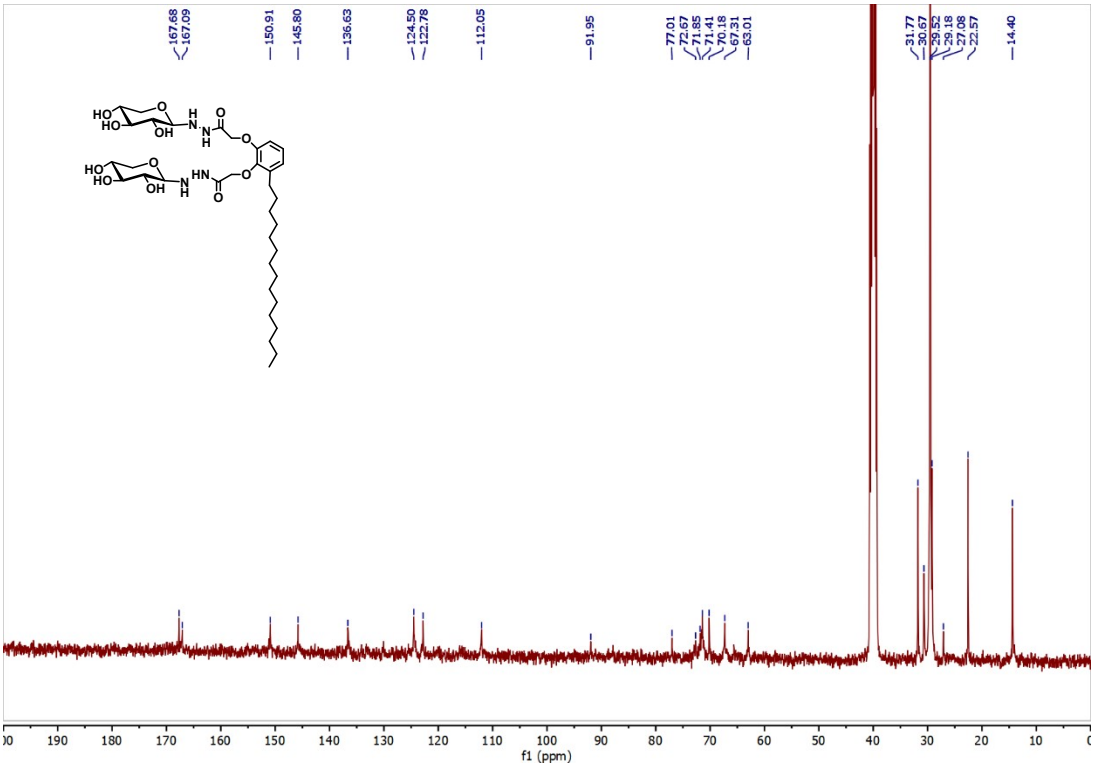

Figure S29. ^{13}C NMR spectrum of compound 6d (DMSO-d_6 100MHz) at 80 ^{o}C

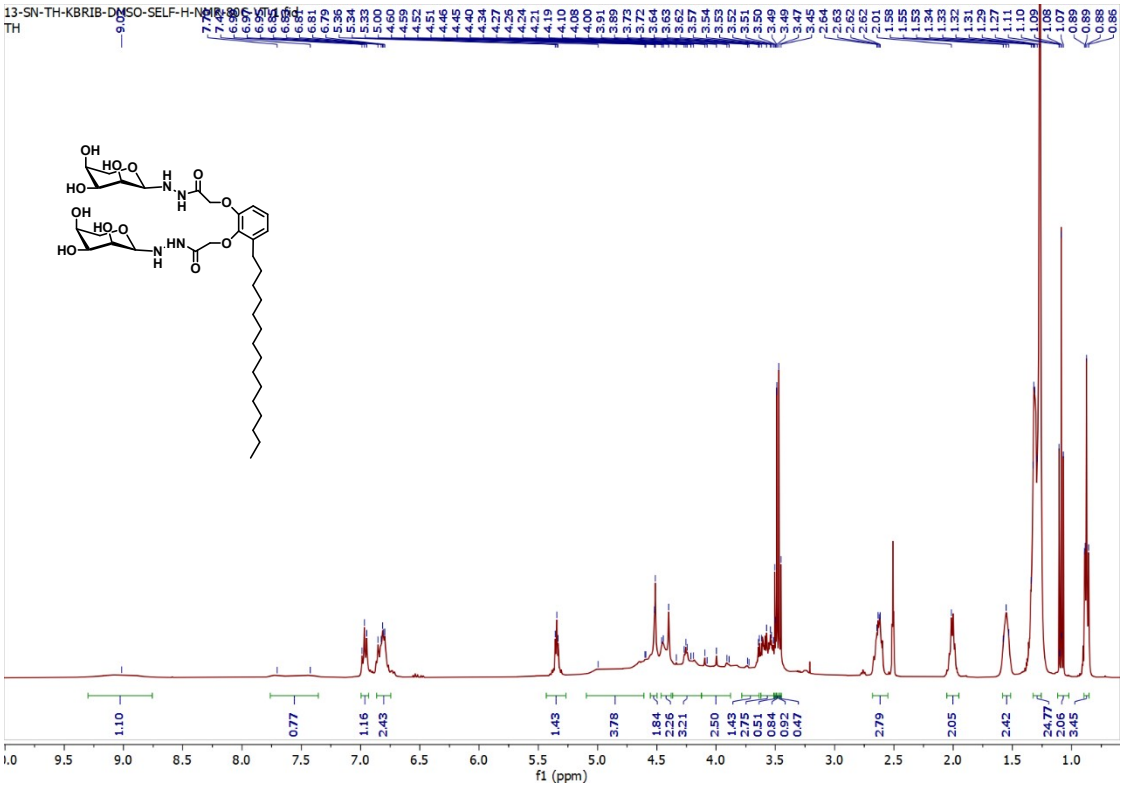

Figure S30. ^{1}H NMR spectrum of compound 6e (DMSO-d_6 400MHz) at 80 ^{o}C

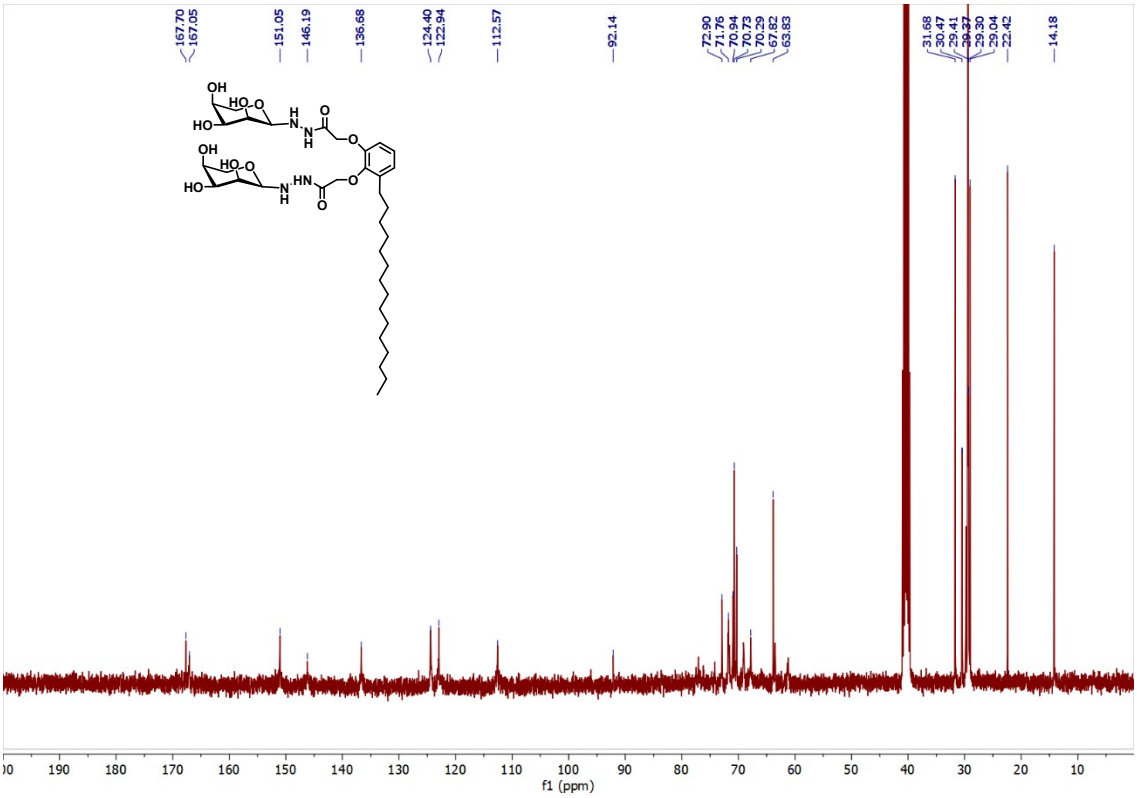

Figure S31. ^{13}C NMR spectrum of compound 6e (DMSO-d_6 100MHz) at 80 °C

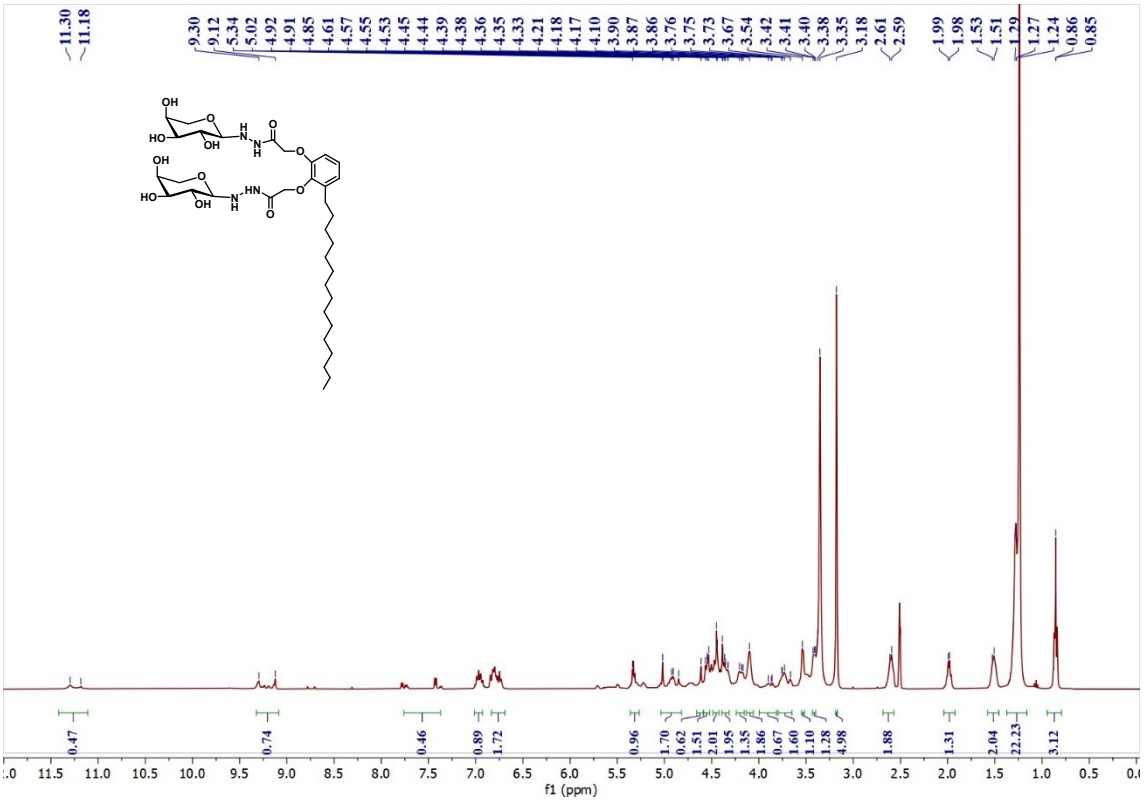

Figure S32. ^{1}H NMR spectrum of compound 6f (DMSO-d_6 400MHz) at 80 °C

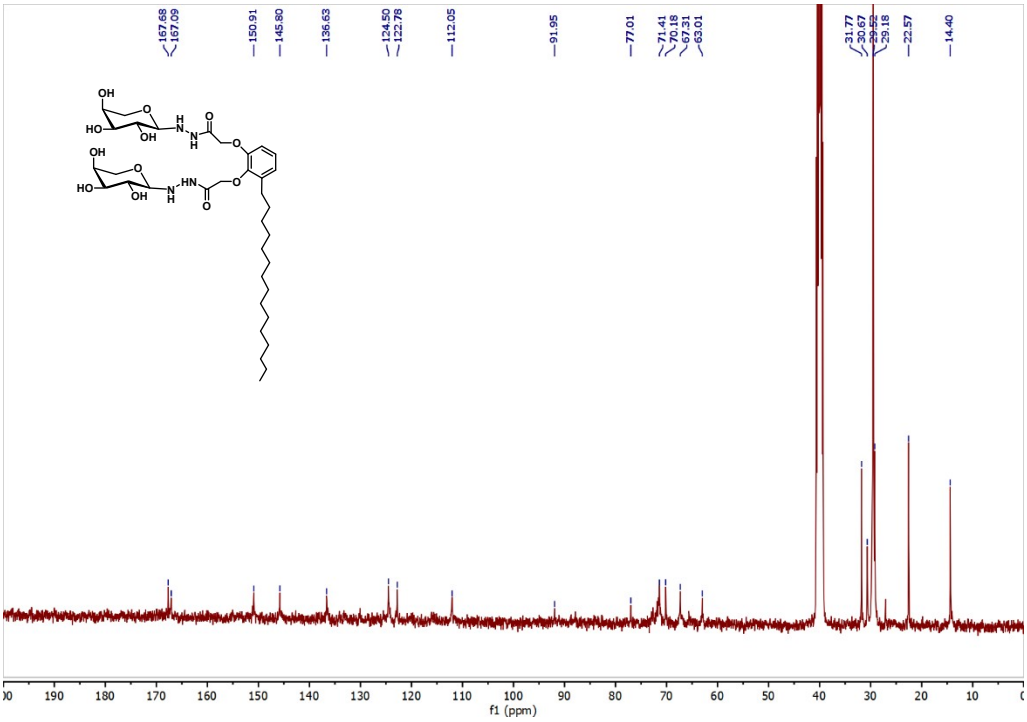

Figure S33. ^{13}C NMR spectrum of compound 6f (DMSO-d_6 100MHz) at 80 ^{o}C

HRMS SPECTRAL DATA

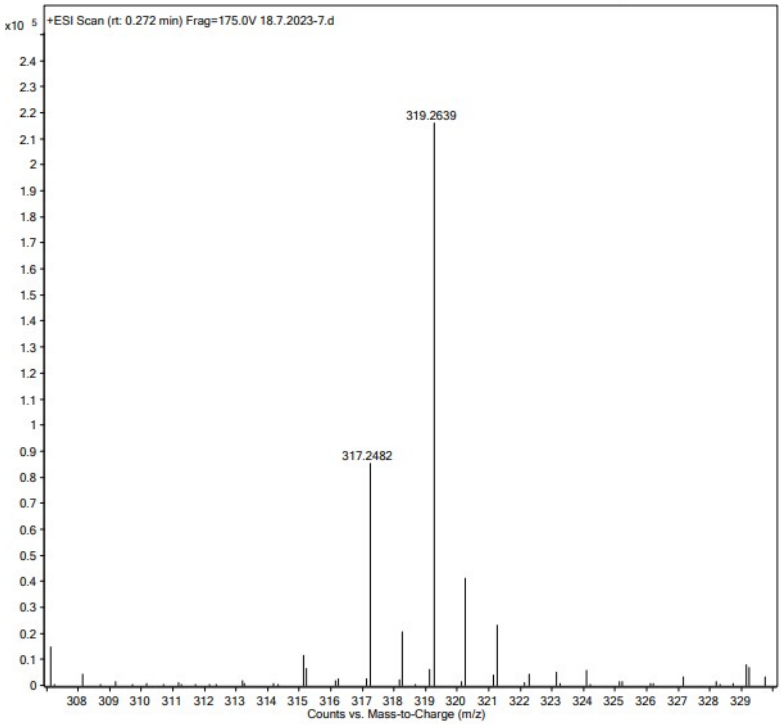

Figure S34. HRMS spectrum of compound 1a

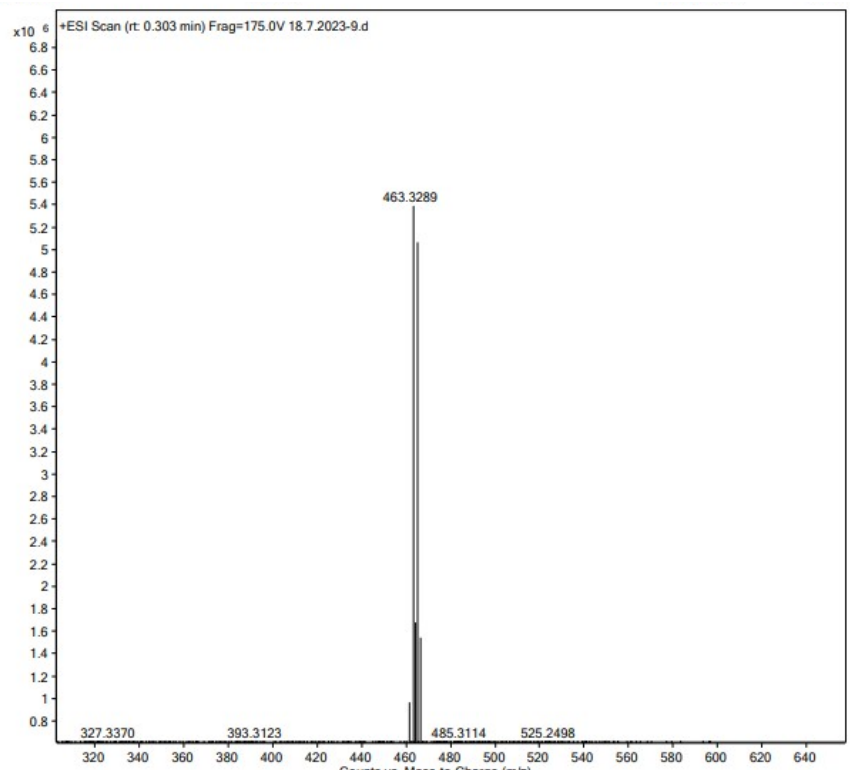

Figure S35. HRMS spectrum of compound 3a

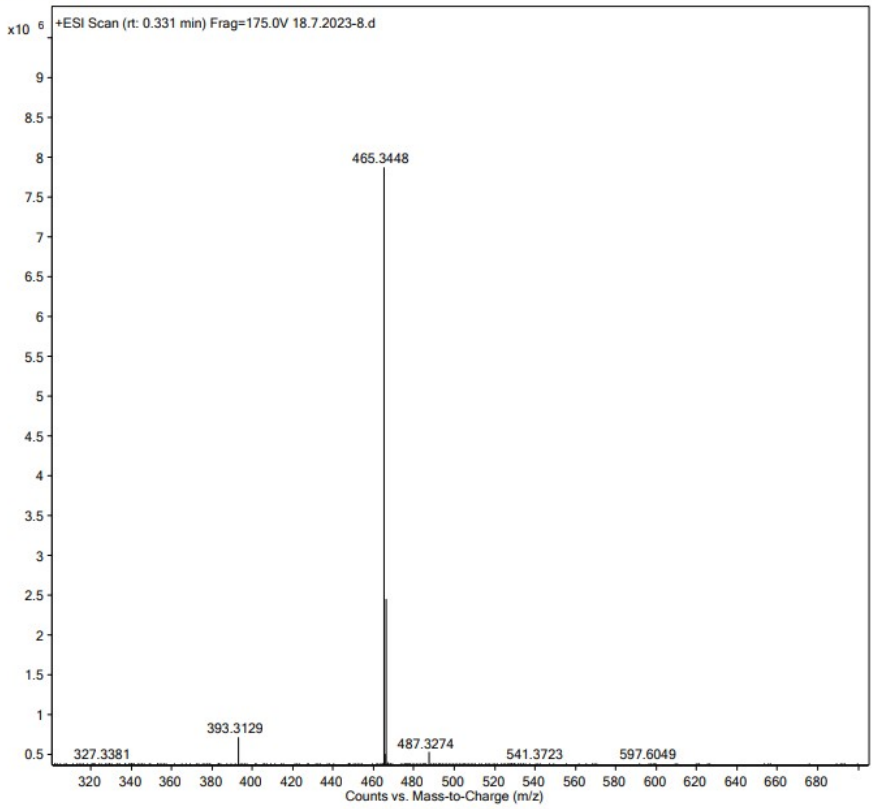

Figure S36. HRMS spectrum of compound 3b

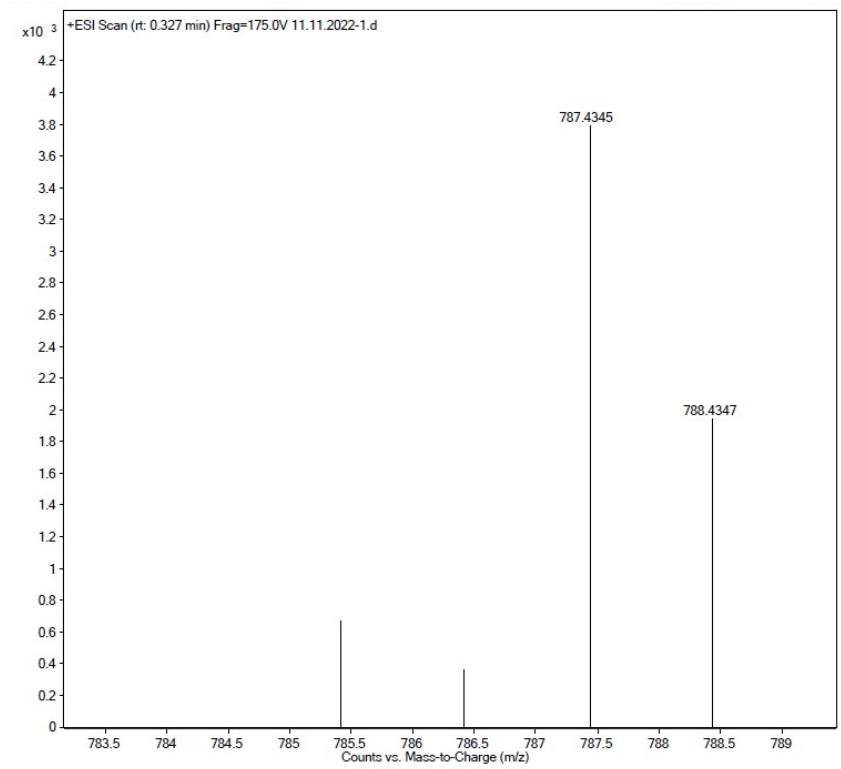

Figure S37. HRMS spectrum of compound 5a

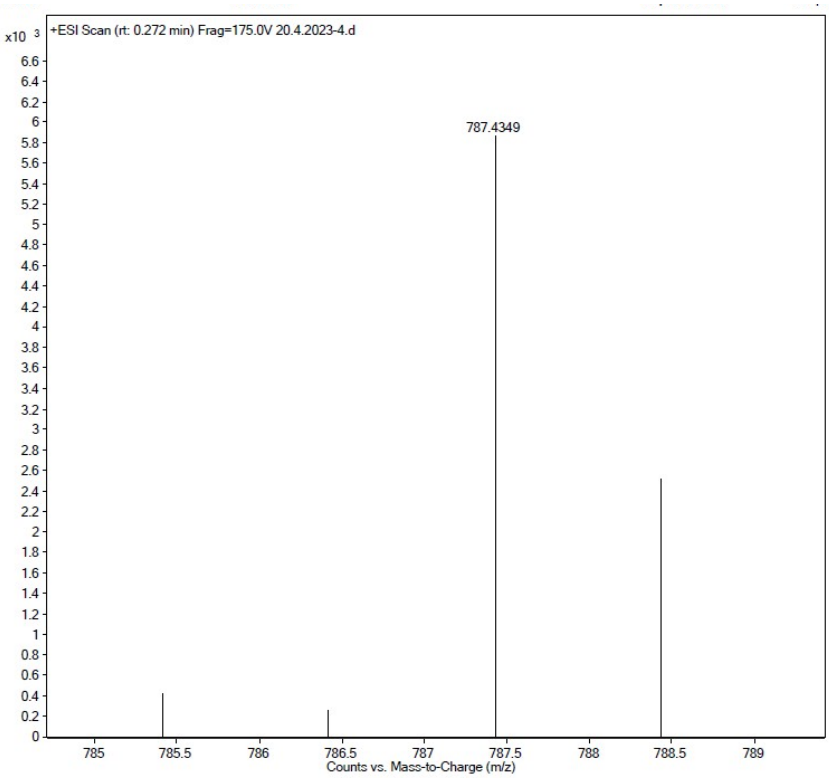

Figure S38. HRMS spectrum of compound 5b

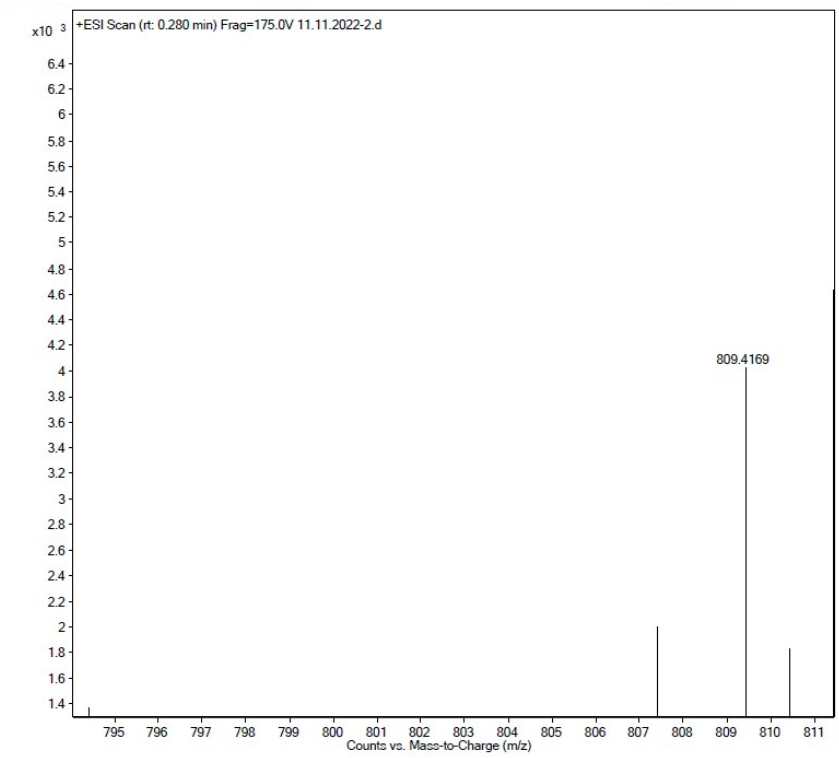

Figure S39. HRMS spectrum of compound 5c

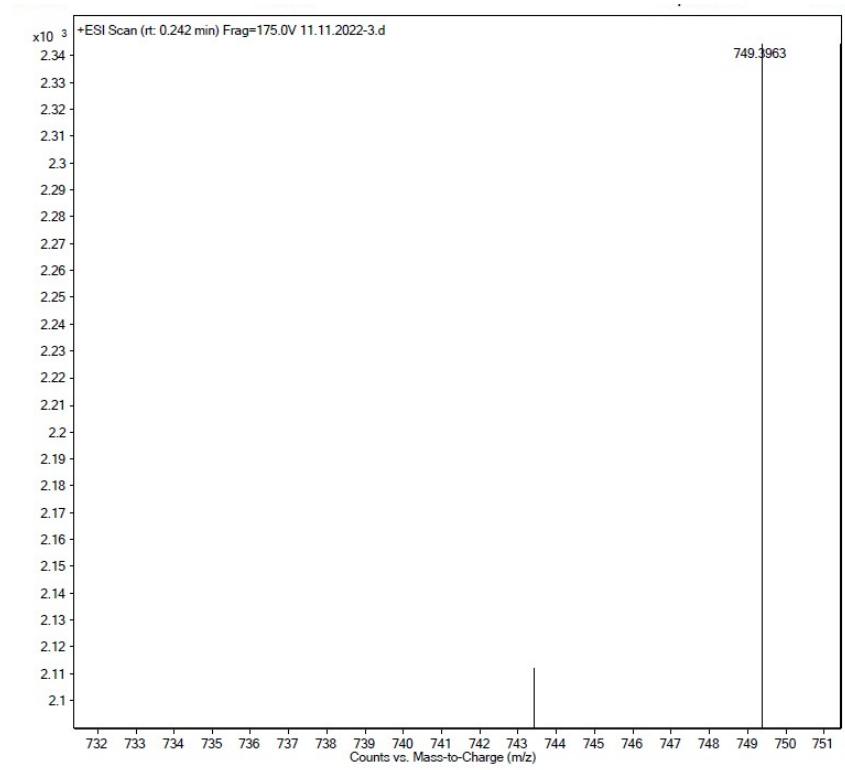

Figure S40. HRMS spectrum of compound 5d

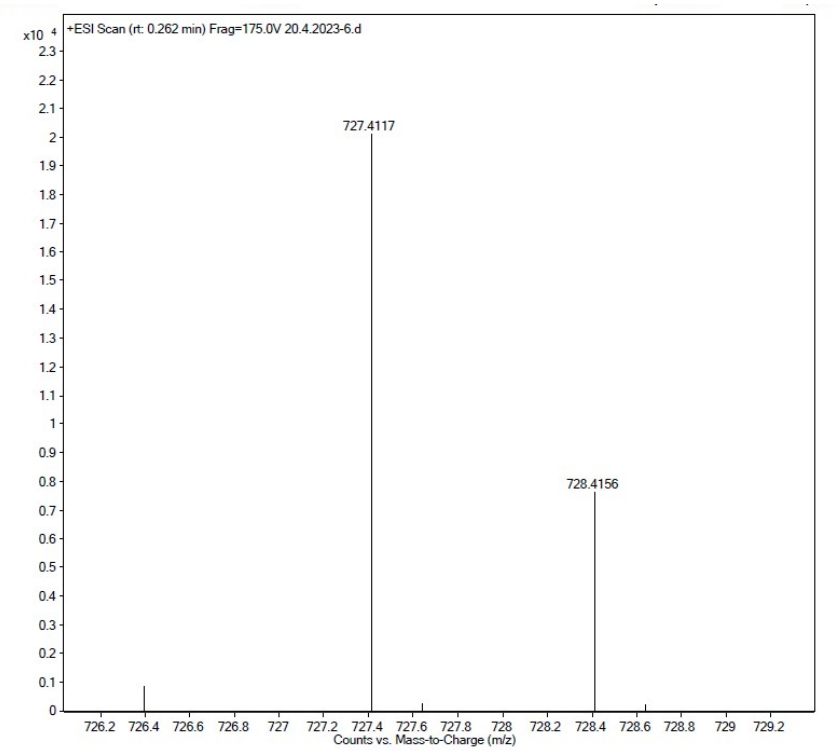

Figure S41. HRMS spectrum of compound 5e

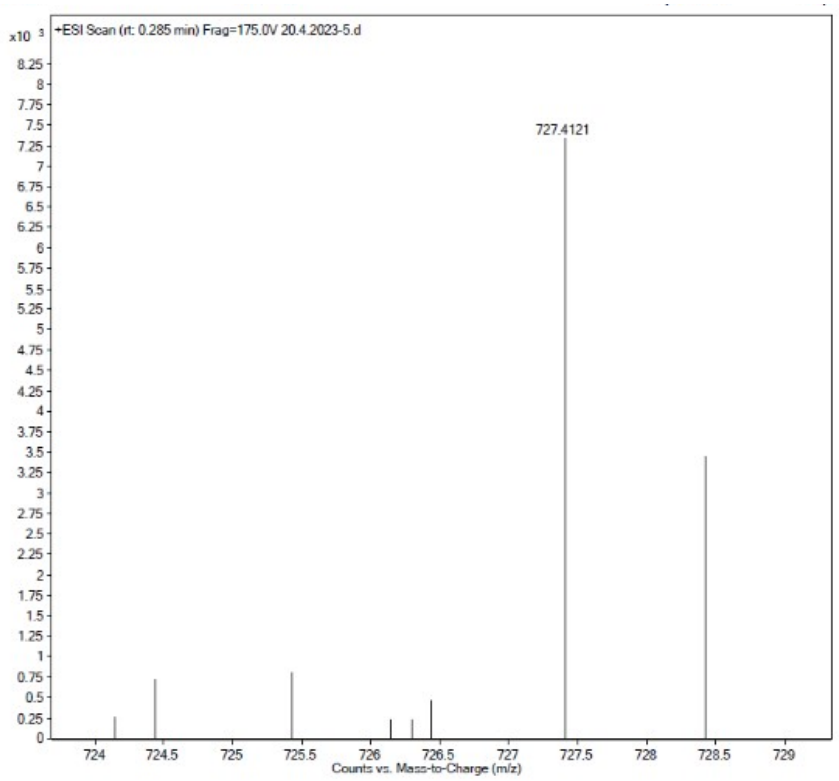

Figure S42. HRMS spectrum of compound 5f

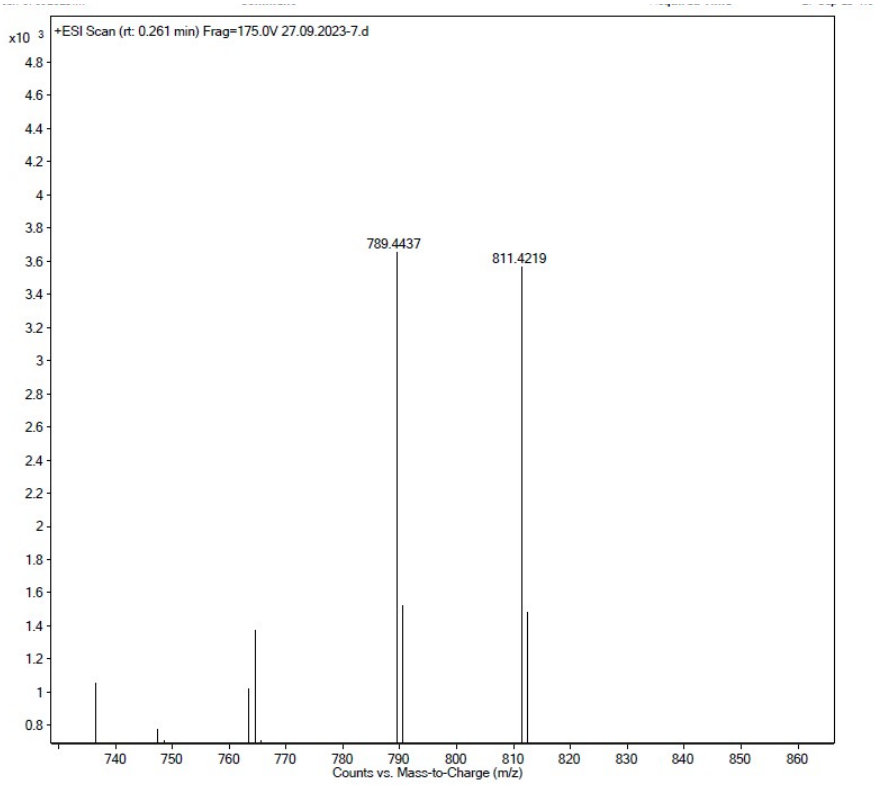

Figure S43. HRMS spectrum of compound 6a

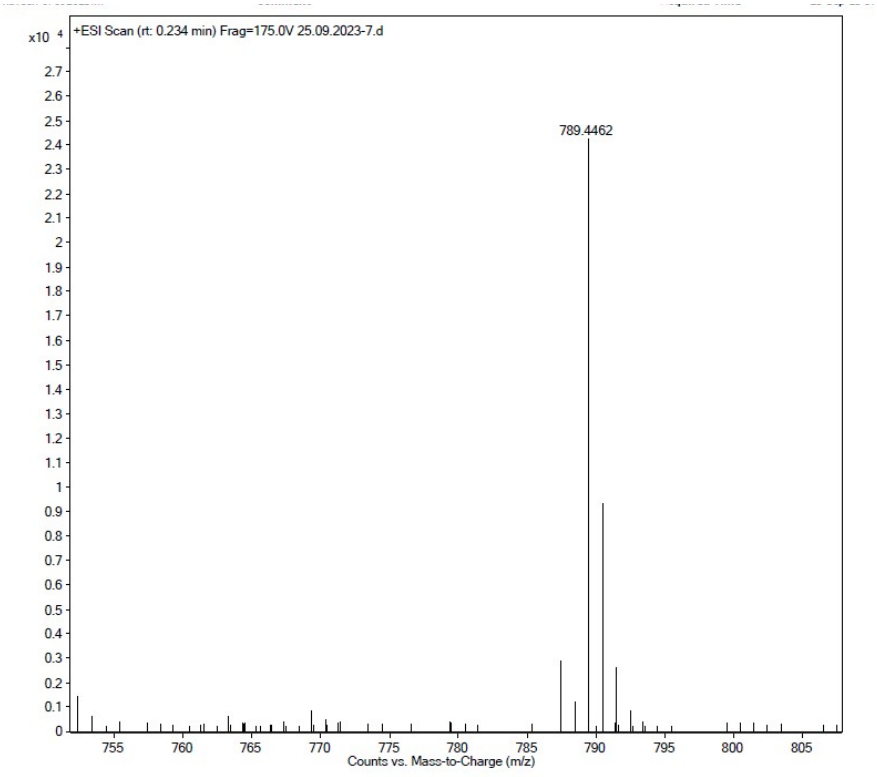

Figure S44. HRMS spectrum of compound 6b

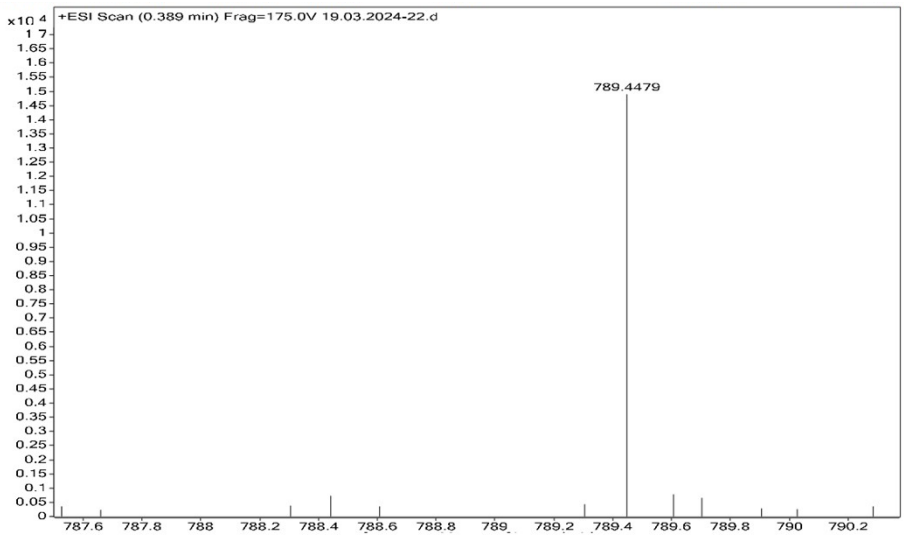

Figure S45. HRMS spectrum of compound 6c

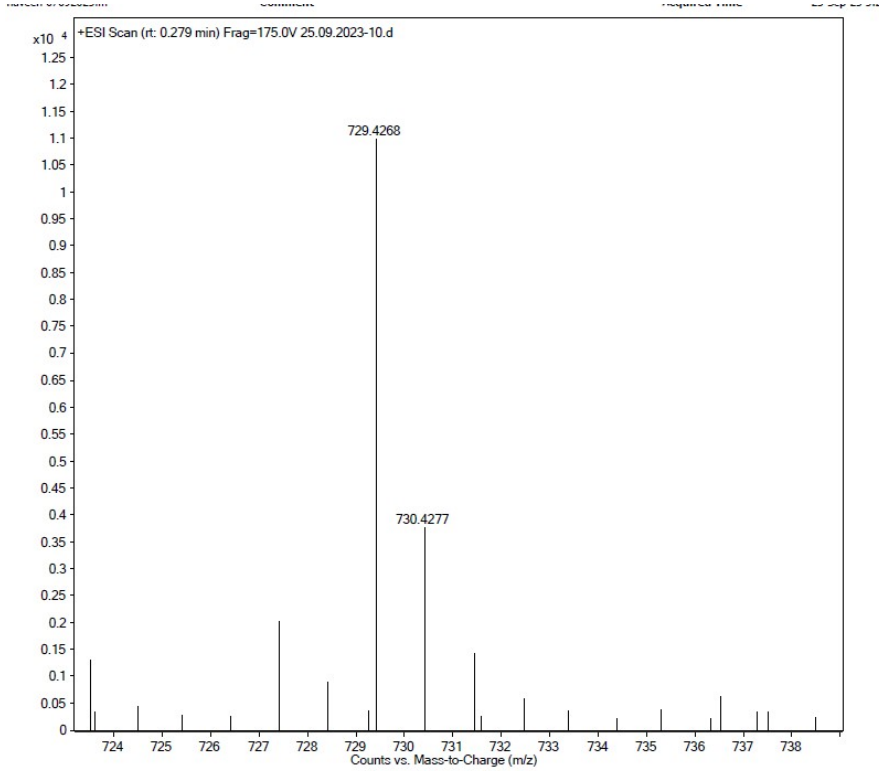

Figure S46. HRMS spectrum of compound 6d

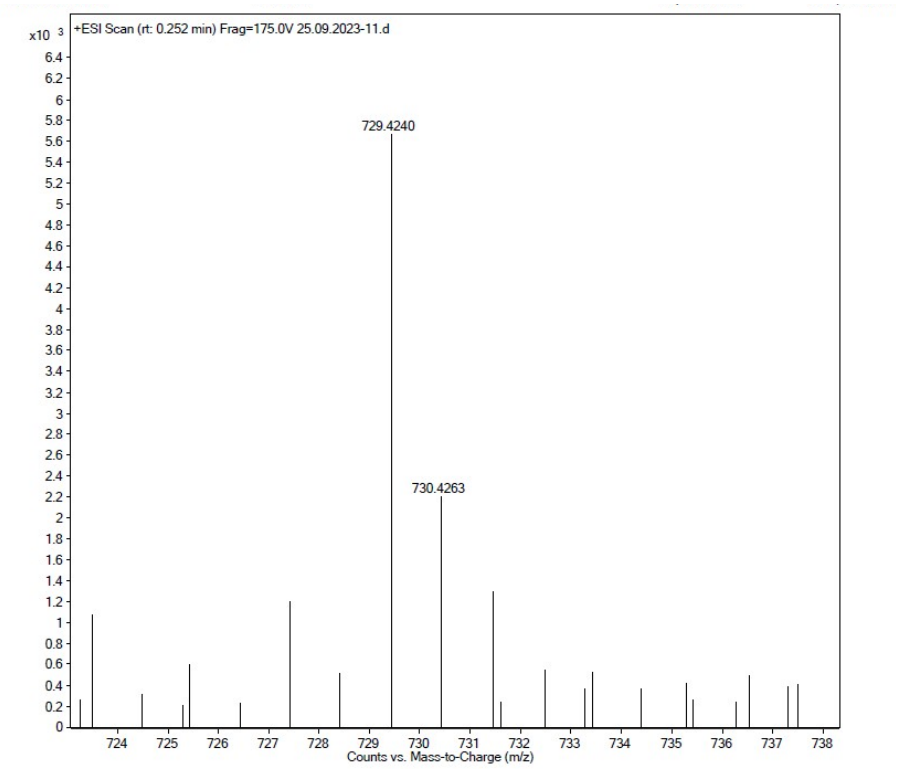

Figure S47. HRMS spectrum of compound 6e

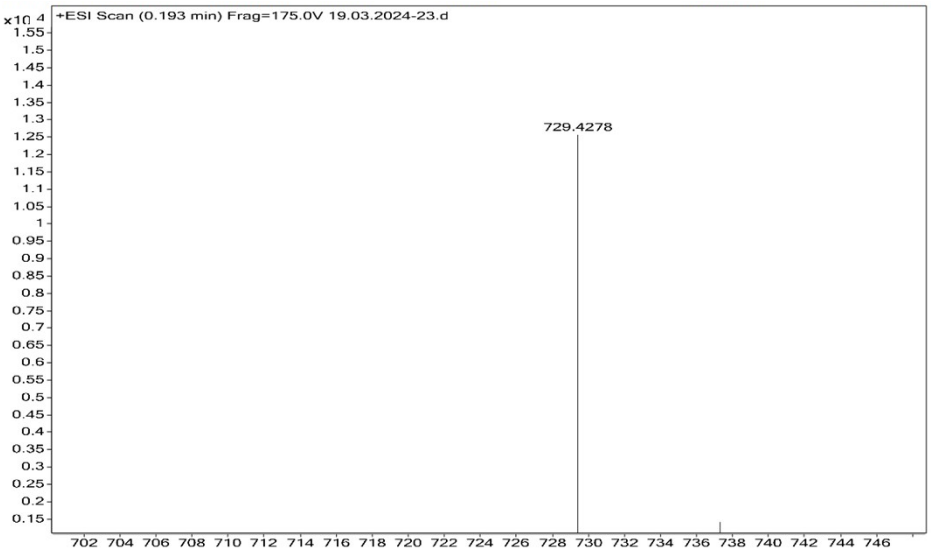

Figure S48. HRMS spectrum of compound 6f

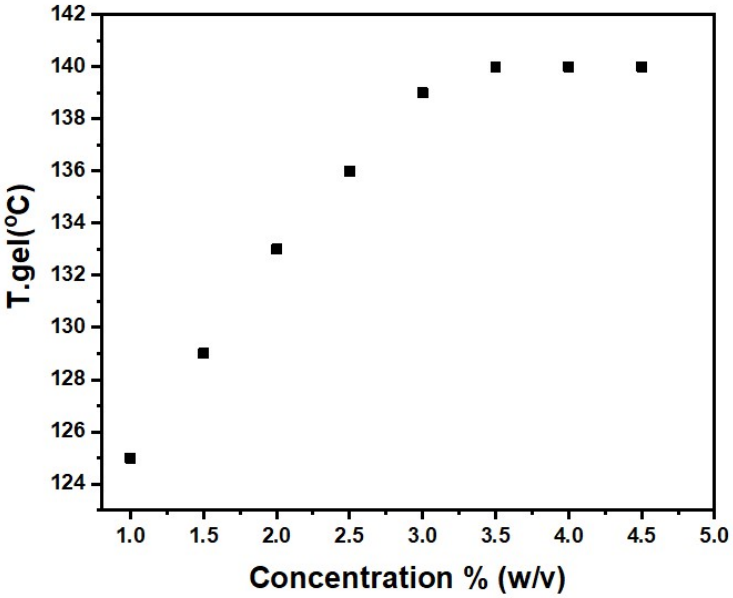

Figure S49. T(gel) of compound 6a with change in concentration.

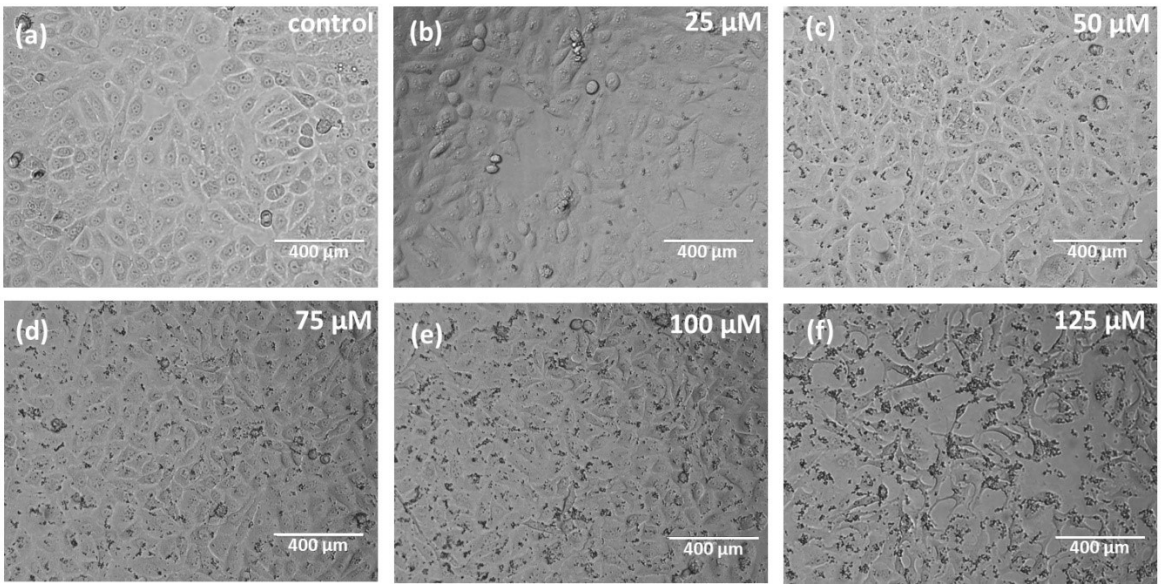

Figure S50. (a-e) microscopic images of compound (BCG 5a) with Hela cells at different concentrations.

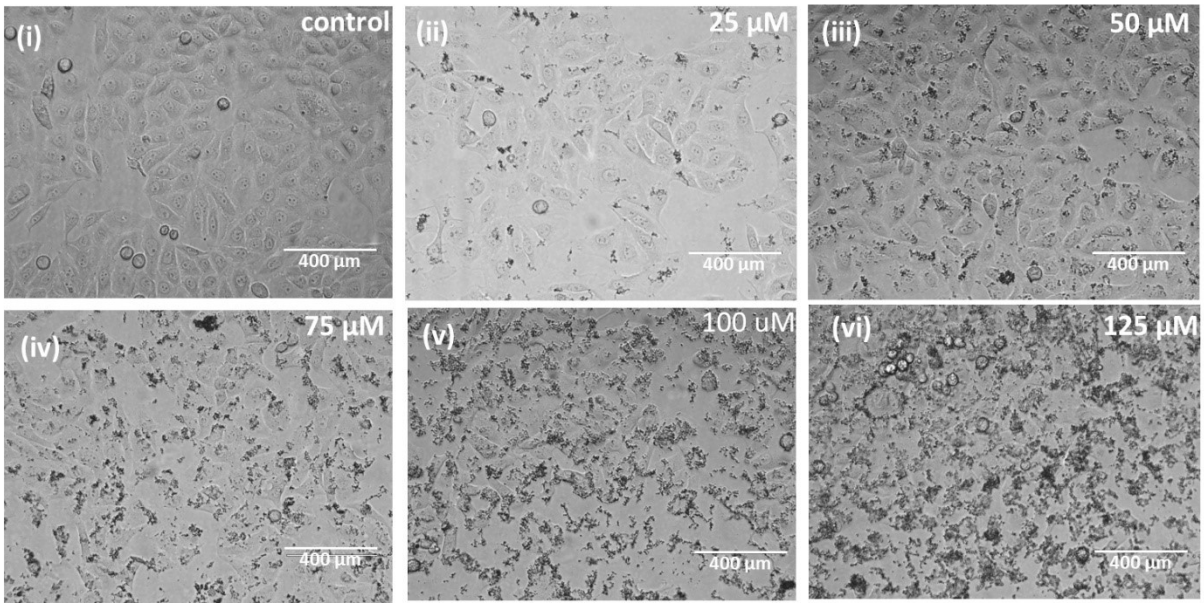

Figure. S51. (a-e) microscopic images of compound (BCG5b) with Hela cells at different concentrations.

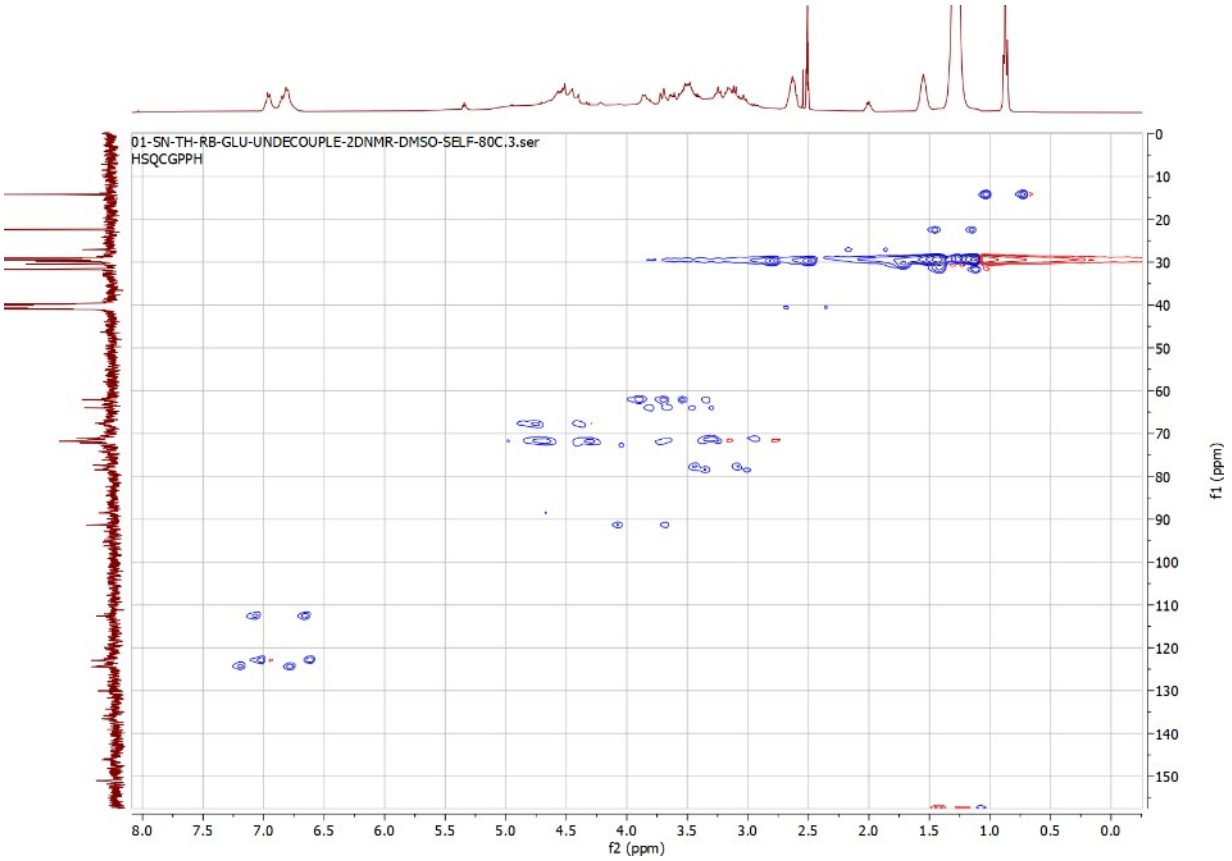

Figure. S52. $^{1}H,^{13}C$-HSQC NMR spectrum of compound BCG6b (DMSO-d_6 400MHz) at 80 ^{o}C

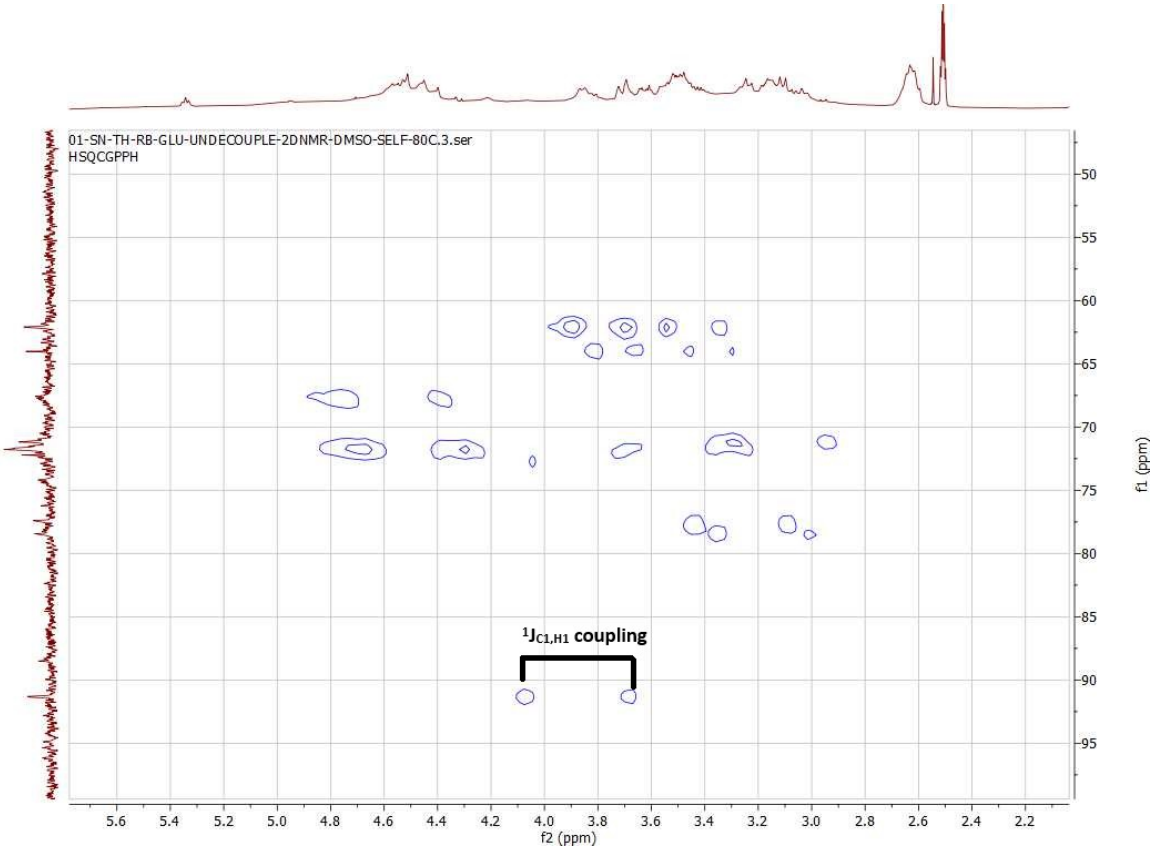

Figure. S53. $^{1}H,^{13}C$-HSQC NMR spectrum of compound BCG6b (DMSO-d_6 400MHz) at 80 ^{o}C (Expansion)