Supplementary Information

Microwave assisted reaction, photophysical studies and antibacterial activities of simple sugar chalcone derivatives

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Experimental Section

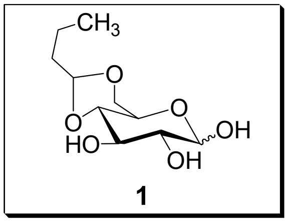
General Methods

D-Glucose and various aldehydes were purchased from Sigma-Aldrich Chemicals Pvt. Ltd., USA and were of high purity. Butyraldehyde and the organic catalyst (pyrrolidine) were obtained from SRL, India. Other reagents, such as, hydrochloric acid, sodium hydrogencarbonate, ammonium chloride and solvents (AR Grade) were obtained from Sd-fine, India, in high purity and were used without any further purification. Acetylacetone were purchased from Loba-Chemie, India. The solvents were purified according to the standard methods. Microwave oven is used for the synthesis. Column chromatography was performed on silica gel (100-200 mesh). NMR spectra were recorded on a Bruker DRX 300 MHz instrument in either $CDCl_3$ or DMSO-d_6. Chemical shifts are referenced to internal TMS. Absorption studies were carried out on 1800 Shimadzu UV spectrophotometer in the range 190-800 nm. Elemental analysis was performed using Perkin-Elmer 2400 series CHNS/O analyzer.

Synthesis of 4,6-*O*-protected D-glucose

Protection of D-glucose was carried out following the literature procedure.[10]

Synthesis, physicochemical and spectral data of 4,6-O-butylidene-D-glucopyranose (1)



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Compound, **1** was obtained as a white solid by the reaction of **D**-glucose with butyraldehyde in the presence of conc. HCl.

Mp : 162-164 °C.

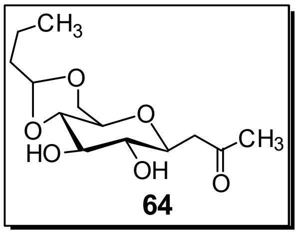
^{1}H NMR(300 MHz, $CDCl_3$ + DMSO-d_6): δ 5.14 (d, J = 3.6 Hz, 1H, Sac-H), 4.58-4.54 (m, 1H, Sac-H), 4.11-4.03 (m, 2H, Sac-H), 3.88-3.76 (m, 2H, Sac-H), 3.60-3.50 (m, 2H, Sac-H), 3.47-3.43 (m, 1H, Sac-H), 3.30-3.17 (m, 2H, Sac-H), 1.62-1.58 (m, 2H, -CH_2), 1.47-1.40 (m, 2H, CH_2), 0.93 (t, J = 7.5 Hz, 3H, -CH_3).

^{13}C NMR (75 MHz, $CDCl_3$ + DMSO-d_6): δ 100.8, 96.7, 84.1, 79.2,76.3, 72.9, 69.3, 36.6, 14.4, 13.2.

Synthesis of *β-C*-glycosidic ketone derivatives, (2)

β-C-Glycosidic ketone, **2** was synthesized following the literature procedure.[11]

Synthesis, physicochemical and spectral data of 4,6-O-butylidene-β-D-glucopyranosylpropane-2-one (2)



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Knoevenagel condensation of compound, **1** with acetyl acetone and $NaHCO_3$ gave **2** as a colourless fluffy solid.

Mp : 102-104 °C.

^{1}H NMR(300 MHz, $CDCl_3$ + DMSO-d_6): δ 4.53 (t, J = 5.1 Hz, 1H, Sac-H), 4.13 (dd, J = 4.5 Hz, 5.0 Hz, 1H, Sac-H), 3.84-3.82 (m, 1H, Sac-H), 3.68 (t, J = 9.0 Hz, 1H, Sac-H), 3.42 (t, J = 9.9 Hz, 1H, Sac-H), 3.35-3.31 (m, 2H, Sac-H), 3.21 (t, J = 9.2 Hz, 1H, Sac-H), 2.90 (dd, J = 3.6 Hz, J = 16.4 Hz, 1H, -CH_2), 2.66 (dd, J = 8.1 Hz, J = 16.2 Hz, 1H, -CH_2), 2.20 (s, 3H, -CH_3), 1.67-1.61 (m, 2H, -CH_2), 1.42 (q, J = 8.1 Hz, 2H, -CH_2), 0.92 (t, J = 7.4 Hz, 3H, -CH_3).

^{13}C NMR(75 MHz, $CDCl_3$ + DMSO-d_6): δ 207.0, 102.2, 80.2, 75.8, 74.8, 73.9, 70.3, 68.0, 45.8, 35.9, 30.6, 17.1, 13.6.

Table S1 — Different solvents in microwave oven method for the synthesis of compound 3

S. No.	**Solvents used**	**Yield (%)**
1	DMF	25
2	EtOH	38
3	MeOH	40
4	CH_3CN	20
5	DCE	85

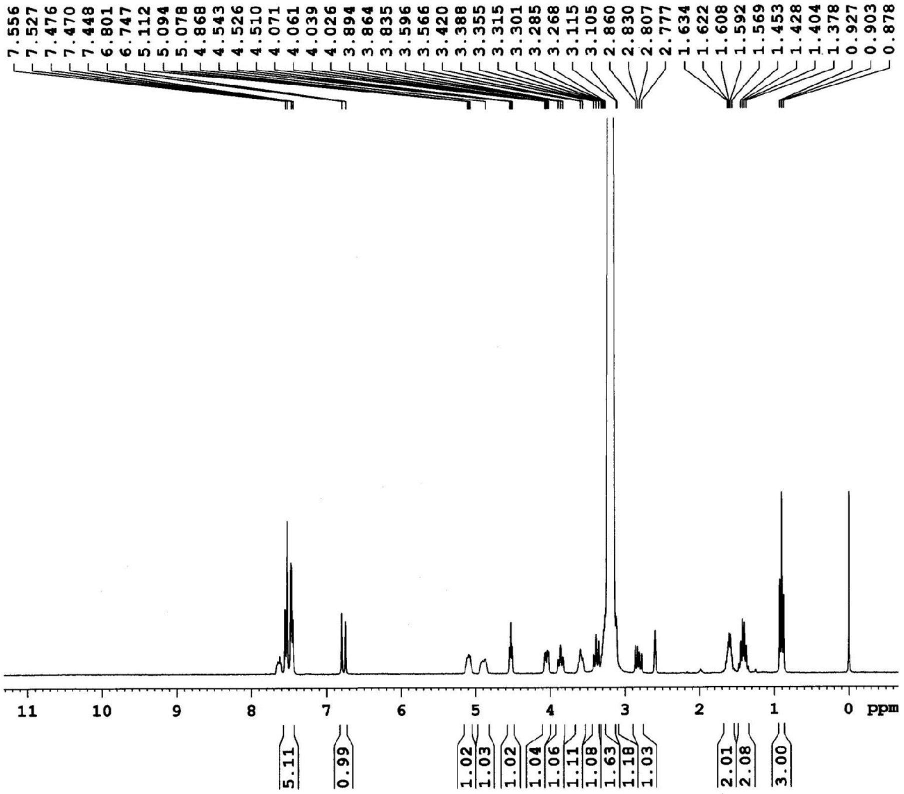


Fig. S1 — ^{1}H NMR spectra (300 MHz, $CDCl_3$) of sugar chalcone derivative, 3

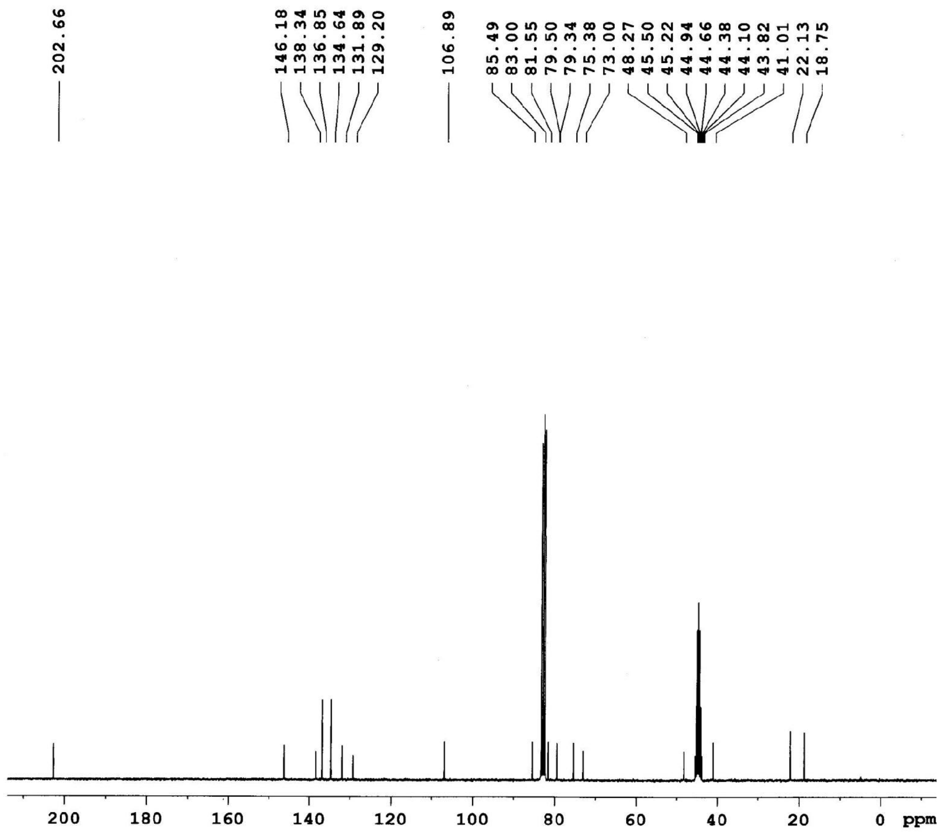
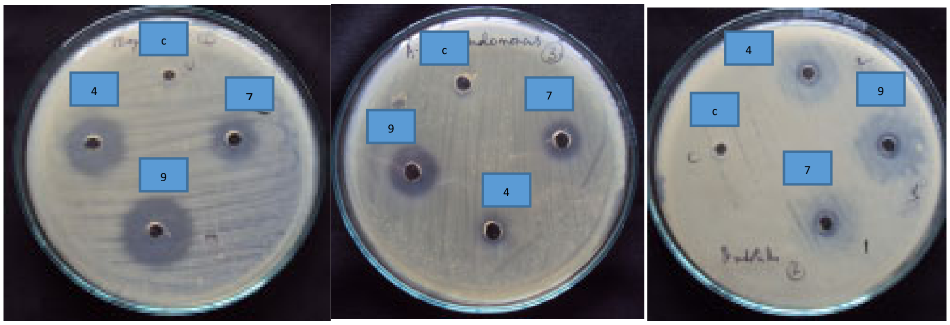


Fig. S2 — ^{13}C NMR (75 MHz, $CDCl_3$) spectra of sugar chalcone derivative, 3



(a) (b) (c)

Fig. S3 — Image of inhibition effect of compound **4, 7, 9** on growth of (a) Bacillus subtilis at 75 µL, (b) Pseudomonas aureginosa at 75 µL and (c) Klebsiella Pneumonia at 25 µL; C - control, (only Chloroform)

Table S2 — Inhibition effect of compounds 4, 7 and 9 on growth of bacteria at 75 μL concentration

S. No.	Bacteria	Zone of inhibition of compounds (diameter in mm)		
		Compound 4	Compound 7	Compound 9
1	Bacillus subtilis	10	7	13
2	Pseudomonas aureginosa	6	2	11
3	Klebsiella Pneumonia	12	5	13
4	Control	No Inhibition	No Inhibition	No Inhibition