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Synthesis of Some Novel 2-*S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-*O*-benzoyl-β-D-lactosyl-2-isothiobiurets

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ABSTRACT

The study of S-and N-glycosides is important in carbohydrate chemistry. Sugar isocyanate is good precursors and versatile intermediate for synthesis of S- and N-glycosides. Carbohydrates play an important role in the number of biological events and play an important role in their synthetic strategy as well. Similarly the amino sugars are an important class of glycosidase inhibitors and are arousing great interest as potential therapeutic agents. Several 2-S-tetra-O-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-O-benzoyl-β-D-lactosyl-2-isothiobiurets have been synthesized for the first time by the interaction of hepta-O-benzoyl-β-D-lactosyl isocyanate and S-tetra-O-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides. All the synthesized compounds were characterized on the basis of elemental analysis and IR, [1]HNMR and Mass spectral analysis. The polarimetric study of the compounds was carried out.

Key words: Lactosyl isocyanate, glucopyranosyl isothiocarbamides, lactosyl isothiobiurets.

INTRODUCTION

Glycosyl amines, glycosyl guanidine derivatives, glycosyl thiocarbamides have several medicinal applications such as antitumor agent[1], antilukemic agent[2], antibacterial properties[3], antimetastatic compounds[4] and in many other ways[5]. *S*-and *N*-glycosylated derivatives and their utilities in medicinal chemistry have been extensively studied[6-19]. The synthesis and pharmacological evaluation of the varieties of glycosyl isothiobiurets and isodithiobiurets have been reported.

In present communication we report the synthesis of 2-*S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-*O*-benzoyl-β-D-lactosyl-2-isothiobiurets **(III)** by the interaction of hepta-O-benzoyl-β-D-lactosyl isocyanate **(I)** and various *S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides **(II)**.

MATERIALS AND METHODS

Optical rotations $[\alpha]_D^{31}$ were measured on the Equip-Tronics EQ-800 Digital Polarimeter at 31^0C in $CHCl_3$. IR Spectra were recorded on Perkin-Elmer spectrum RXI FTIR Spectrometer. ^{1}H NMR was obtained on Bruker DRX-300 NMR Spectrometer. Samples were prepared in $CDCl_3$ with TMS as an internal reference. The mass spectra were obtained on Thermo Fennigan LCQ Advantage max ion trap mass spectrometer.

General Procedure:-

2-*S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-*O*-benzoyl-β-D-lactosyl-2-isothiobiurets (IIIa-g) (Scheme 1)

A 0.005M of *S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides **(IIa-g)** in a 5ml of benzene was added to a 0.005M solution of hepta-*O*-benzoyl-β-D-lactosyl isocyanate **(I)** in 15ml benzene the reaction mixture was reflux over boiling water bath for 5hr. After refluxing, the solvent was distilled off and the sticky residue obtained was triturated with petroleum ether (60-80 ^{0}C) to afford a solid **(IIIa-g)**. The product was purified by chloroform petroleum ether. The product was checked by TLC. The percent yield, M.P., Optical rotation, elemental analysis shown in **Table 1**.

IIIa: IR (KBr):- ν 3068 (Ar-H), 1729 (C=O), 3465 (N-H), 1653 (C=N), 1269 (C-N), 771(C-S), 1101 & 1027 cm^{-1} (Characteristic of Lactose); ^{1}H NMR ($CDCl_3$):- δ 8.02-7.11 (42H, Ar-H), δ 6.28-3.89 (14H, lactosyl and glucosyl protons); Mass: - m/z 1825 (M^+), 1053, 948,932, 579, 531, 135. Anal. Calcd. for $C_{103}H_{83}O_{27}N_3SCl$, Requires: C, 67.72; H, 4.54; N, 2.30; S, 1.75; Found: C, 67.68; H, 4.50; N, 3.24; S, 1.71%.

Table 1:- Characterization data of 2-*S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-*O*-benzoyl-β-D-lactosyl-2-isothiobiurets (IIIa-g).

Reactants: -

1) Hepta-*O*-benzoyl-β-D-lactosyl isocyanate **(I)** [0.005M].
2) *S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides **(IIa-g)** [0.005M].

Sr. No.	Compd.	%Yield	m. p. (^{o}C)	$[\alpha]_D^{31}$ ($CHCl_3$)	Analysis Found (Required)	
					N	S
1.	IIIa	60.10	130-132	+50.01 ^{o} (c, 0.930)	2.30 (3.24)	1.71 (1.75)
2.	IIIb	49.45	118	+66.4^o (c, 0.930)	2.21 (2.28)	1.70 (1.74)
3.	IIIc	53.26	110	+82.9^o (c, 0.930)	2.22 (2.28)	1.71 (1.74)
4.	IIId	54.34	122	+42.32^o (c, 0.930)	2.23 (2.28)	1.72 (1.74)
5.	IIIe	69.89	112	+52.14^o (c, 0.930)	2.21 (2.25)	1.67 (1.72)
6.	IIIf	53.76	127	+69.28^o (c, 0.930)	2.19 (2.25)	1.68 (1.72)
7.	IIIg	44.08	108	+ 35.59^o (c, 0.930)	2.22 (2.25)	1.69 (1.72)

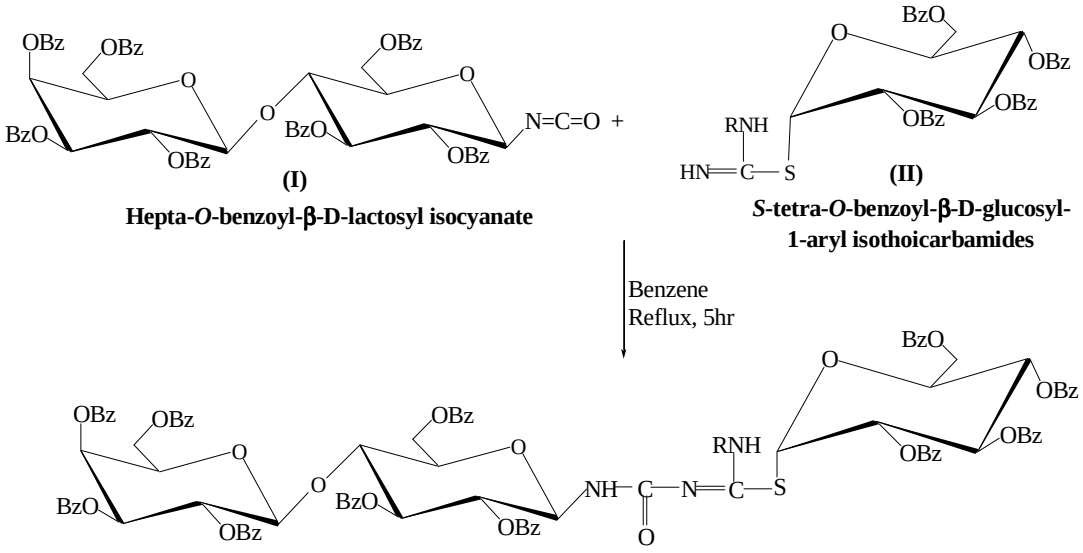
IIIc: IR (KBr):- ν 3066 (Ar-H), 1730 (C=O), 3451 (N-H), 1653 (C=N), 1270 (C-N), 709 (C-S), 1069 & 1025 cm^{-1} (Characteristic of Lactose); ^{1}H NMR ($CDCl_3$):- δ 8.20-7.12 (44H, Ar-H),δ 6.22-3.73 (14H, lactosyl and glucosyl protons); Mass: - m/z 1839 (M^+), 1053, 948,932, 579, 531, 135. Anal. Calcd. for $C_{104}H_{85}O_{27}N_3SCl$, Requires: C, 67.86; H, 4.62; N, 2.28; S, 1.74; Found: C, 67.79; H, 4.59; N, 2.22; S, 1.71%.

IIIf: IR (KBr):- ν 3067 (Ar-H), 1729 (C=O), 3448 (N-H), 1601 (C=N), 1270 (C-N), 772 (C-S), 1099 & 1025 cm^{-1} (Characteristic of Lactose); ^1H NMR ($CDCl_3$):- δ 8.28-7.19 (44H, Ar-H),δ 5.88-4.19 (14H, lactosyl and glucosyl protons); Mass: - m/z 1859 (M^+), 1053, 948,932, 579, 531, 135. Anal. Calcd. for $C_{103}H_{82}O_{27}N_3SCl$, Requires: C, 66.46; H, 4.40; N, 2.25; S, 1.72; Found: C, 66.40; H, 4.32; N, 2.19; S, 1.68%.

RESULTS AND DISCUSSION

2-*S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl-5-hepta-*O*-benzoyl-β-D-lactosyl-2-isothiobiurets **(IIIa-g) (Scheme 1)** were prepared by the interaction of hepta-*O*-benzoyl-β-D-lactosyl isocyanate **(I)** and various *S*-tetra-*O*-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides **(IIa-g)** in benzene medium for 5 hr. After condensation, solvent was distilled off and sticky residue obtained which was triturated with petroleum ether (60-80 ^{0}C) to afford product. It was purified by chloroform-Petroleum ether.

Scheme 1



2-*S*-tetra-*O*-benzoyl-β-D-glucosyl-1-aryl-5-hepta-*O*-benzyl-β-D-lactosyl-2-isothiobiurets

Where, ***Bz-*** COC_6H_5

R = a) phenyl, b) o-tolyl, c) m-tolyl, d) p-tolyl, e) o-Cl-phenyl, f) m-Cl-phenyl, g) p-Cl-phenyl.

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