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Research Paper

Synthesis and Glucosylation of Chalcone-3'-Carboxylic Acids using Glucosyl Donor

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ABSTRACT: *Condensation of Tetra-O-acetyl-α-D-glucopyranosyl bromide (glucosyl donor) with 5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acids furnishes 3-(2,3,4,6-tetra-O-acetyl-3-acyl-β-D-glucopyranosyl)-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazoles. Deacetylation of 3-(2,3,4,6-tetra-O-acetyl-3-acyl-β-D-glucopyranosyl)-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazoles with sodium methoxide in dry methanol affords β-D-glucopyranosyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates. The structure of these compounds have been characterized on the basis of their sophisticated instrumental analysis like FT-IR, ^{1}H-NMR, FAB-MS, specific rotation, elemental analysis and chemical properties.*

KEYWORDS*: 1,2-Benzisoxazole, Chalcones, Carboxylic acid, β-D-Glucosides.*

I. INTRODUCTION

A monosaccharide (or sugar fragment of any size) is condensed with either an aliphatic or aromatic alcohol, or another sugar moiety through oxygen, a glycoside bond is formed. *O*-Glucosylation reaction is the key reaction for the synthesis of many carbohydrate based biomolecules, oligosaccharides, complex carbohydrate conjugates and many complex glycosides. *O*-Glycosides have been the subject of considerable interest in carbohydrate chemistry because many carbohydrate derivatives exhibit very interesting biological activities such as antitumor activity and inhibitors of metabolic processes[1]. Thus, a modification of carbohydrates *via* carbon-oxygen bond formation receives increasing interest among synthetic organic chemists and also provides valuable synthons suitable for the synthesis of complex molecules since carbohydrate derivatives contain a large number of chiral centers and functional groups. Multidrug resistance (MDR) of cancer cells is one of the main reasons of failure of antineoplastic therapy. The phenomenon involves acquisition of resistance neoplastic cells to cytostatic drugs of various groups manifesting distinct chemical structure and mechanism of action by (Gillet and Gottesman, 2010). Pharmacological agents can cause drug resistance usually when incorrectly dosage. Another reason involves cellular factors which can change: (1) the rate of absorption of the drug or rate of its elimination from the cell (resistance *via* transport), (2) the level of activation/inactivation of pharmaceuticals (metabolic resistance), (3) the amount or affinity of enzymes representing target for cytostatic agents (target resistance), (4) the processes of DNA repair, (5) the ability of malignant cells to undergo apoptosis. So far, the best understood mechanism by which drugs are eliminated from the cell is associated with the activity of membrane proteins[2].

A large number of chalcones have displayed interesting antineoplastic, diuretic, choleretic and antidiabetic properties. Various derivatives of benzylidene acetophenone show anti-inflammatory, antibacterial, antiviral and gastric protectant activities. It possesses insecticidal, antimicrobial and antipicorhenovirus activities. Chalcones find applications in industries and some of the chalcones are used as artificial sweeteners. Various chalcones find their applications in photosensitive polymers, produce nematic liquid crystals and as an antioxidant for oils[3-16].

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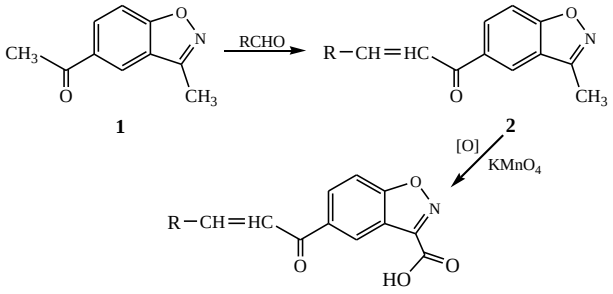
O-Glucosylation reaction of carboxylchalcones has been carried out because they possess higher degree of antibiotic, antifungal and anti-HIV activity. Glucosylation often improves solubility of various drugs without affecting their activity. Moreover, β-glucosylation can improve the drug targeting to the cells due to their solubility in the membrane components. The glucosylation reactions of 4′-hydroxychalcones have been described herein since no synthetic chalcone glucosides have been reported till now. *O*-Glucosylation has been carried out without using any Lewis acid catalyst or heavy metal salts but by modified *Koenigs-Knorr* method[17].

II. RESULT AND DISCUSSION

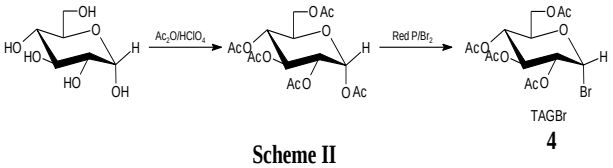
In view of the pronounced biological and pharmacological applications of the compounds containing these moieties, *O*-glucosylation reactions have been performed by condensing α-acetobromoglucose (ACBG) **4** and 5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acids **3a-o** in the presence of tetrabutylammonium bromide (PTC). This reaction affords β-D-glucopyranosyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates **6a-o** in good yield (**Scheme III**).



1 **2** **3**

Scheme I

The acids **3a-o** were synthesized by the oxidation of 3-methyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazoles **2a-o** using alkaline $KMnO_4$ and the products **2a-o** were prepared from 3-methyl-5-acetyl-1,2-benzisoxazole **1** as reported in literature[18].



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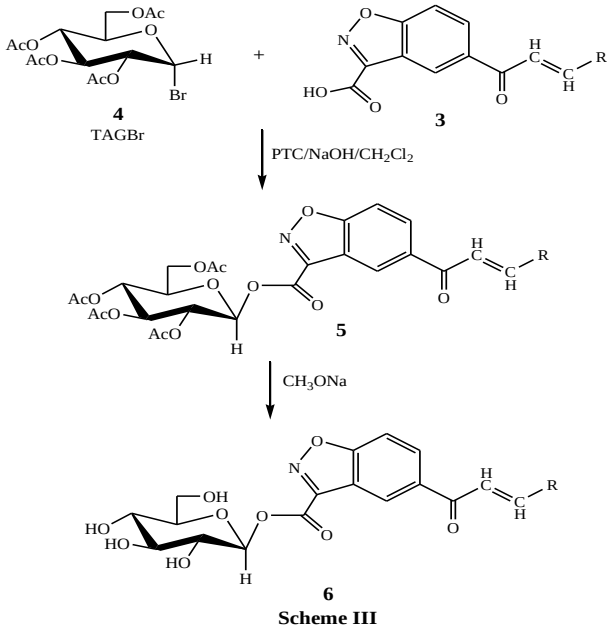
Scheme II



Scheme III

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R= a; C_6H_5 i; *m*-$NO_2C_6H_4$
b; *o*-OHC_6H_4 j; 2-C_5H_4N
c; *p*-OHC_6H_4 k; 3-C_5H_4N
d; 2,4-$(OH)_2C_6H_3$ l; 4-C_5H_4N
e; *p*-OH-*m*-$OCH_3C_6H_3$ m; 3-C_4H_3O
f; *o*-ClC_6H_4 n; 3-C_8H_5N
g; *p*-ClC_6H_4 o; *p*-*N*$(CH_3)_2C_6H_4$
h; *o*-$NO_2C_6H_4$

III. CONCLUSION

The Glucoside derivatives β-D-glucopyranosyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates **6a-o** were synthesized successfully and these compounds were evaluated for in vitro antibacterial activity against *Escherichia coli* and *Bacillus subtilis* strains as well as for antifungal activity against *Candida albicans* and *Aspergillus niger* strains using cup-plate method. Most of Glucosides gave excellent results against bacterial and fungal strains. All newly synthesized products are confirmed by elemental analysis, optical activity, FT-IR, ^{1}H-NMR and FAB-MS.

IV. EXPERIMENTAL

4.1 Materials and methods

All the starting materials and reagents were obtained from Merk, Aldrich and Rankem Pvt Ltd and were used without further purification. The course of reaction and purity were ascertained by performing Thin Layer Chromatography. Melting points were determined in open capillaries and are uncorrected. IR spectra were recorded as KBr pallets on Shimadzu-810 IA and Perkin Elmer FT-IR spectrometer and only significant absorption levels (cm^{-1}) are listed. ^{1}H-NMR spectra were recorded on Bruker AC-300F ($300M_{HZ}$) instrument with TMS as internal standard and the chemical shift are expressed in ppm values. FAB-MS were recorded on a JEOL SX 102/DA-6000 mass spectrometer using *m*-nitrobenzyl alcohol (NBA) matrix. The FLASH EA 1112 C, H and N analyzer, made by Thermo Finigen, Itali for elemental analysis.

4.2 Synthesis

3-Methyl-5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole (2a)

3-Methyl-5-acetyl-1,2-benzisoxazole (0.1mol, 17.5g), benzaldehyde (15ml), ethyl alcohol (25ml) and a few drops of piperidine was warmed for 1h. It was cooled to 0^0C, the yellow solid formed was filtered, washed with distilled water and dried. It was crystallized from distilled water (9.0g, 50.9%), m.p. 120^0C. It gave dark red color with conc. H_2SO_4. FT-IR (KBr): 1715 (C=O str. Aryl ketone), 1562 (C=C), 1362 (C-O), 3005 (Ar-H); ^{1}H-NMR signal at δ2.2 (s, CH_3), 7.4-9.3 (8H, m, aromatic protons), 6.0-6.7 (2H, d, CH=CH); FAB-MS: M^+ 264, m/z 248, 185, 174 and 160.

In the same way, other 3-methyl-5-(3`-aryl prop-`2-enoyl)-1,2-benzisoxazoles **2a-o** were prepared (**Scheme I**).

5-(3`-Phenyl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acid (3a)

In round bottomed flask a mixture of 3-Methyl-5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole (0.01mol, 2.6g), potassium permanganate (1.5g), sodium carbonate (1.2g) and distilled water (100ml) was refluxed under water bath for 1-4hrs, until the purple color of the permanganate has disappeared, cool and acidify with dilute H_2SO_4, heat the mixture for 30 minutes under refluxed and cool, remove excess manganese dioxide by the addition of little sodium metabisulphite, filtered and washed acid compound with distilled water. It was crystallized with distilled water (yield 2.1g, 80.7%), m.p. 104^0C. It gave effervescences of carbon dioxide with sodium bicarbonate. FT-IR (KBr): 3560 (br, OH), 1715 and 1745 (C=O *str*, two), 902 (=N-O), 1615 (C=C *str*), 773 (isoxazole ring *str*), 1362 (C=N, ter. amine) and 3005 (Ar-H); ^{1}H-NMR signal at δ9.5-10.5 (s, Ar-COOH), aromatic protons at 7.68-8.15 (m, 10H), 6.2-6.8 (2H, in ethylenic –CO-CH=CH-, dd); FAB-MS: M^+ 2964, m/z 284, 215, 204, 192 and 160.

In the same way, various 5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acids **3a-o** were synthesized (**Scheme I**).

β-D-Glucopyranosyl-5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates (6a)

We performed the glucosylation reaction by condensing acetobromoglucose (ACBG) with 5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acids in the presence of tetrabutylammonium bromide (PTC). The glucosylation reaction was accomplished by means of the following steps.

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(i) Glucose pentacetate

To an ice cold solution of acetic anhydride (40ml) was added perchloric acid (0.25ml) as catalyst. To this pale yellow solution was added gradually anhydrous D-glucose (10g) with constant stirring. After the addition of D-glucose the reaction mixture was kept for 10-15min at room temperature. The contents of the conical flask were then poured in to ice-cold water, when glucose pentacetate was precipitate out. It was filter, washed with sodium bicarbonate solution to remove excess of perchloric acid and water. The solid was filtered, dried and it was crystallized from ethanol, (yield 8.7g, 87%), m. p. 110^0C, $[\alpha]_D^{25}$ = $+101^0$ (c, 0.28 in $CHCl_3$).

(ii) Brominating agent

Glacial acetic acid (30ml) and red phosphorus (3g) was taken in a conical flask. To this mixture, molecular bromine (7ml) was added gradually with constant shaking and cooling. The resulting mixture was allowed to stand at room temperature for about 15mins. It was then filtered through glass wool to remove suspended impurities and used immediately.

(iii) Tetra-*O*-acetyl-α-D-glucopyranosyl bromide (TAGBr) or Glucosyl donor or α-Acetobromoglucose (ACBG)

The finely powdered glucose pentacetate (21.6g) was added gradually in several installments to the brominating agent (30ml). After the addition, the contents of the flask were kept at room temperature for 2 hrs. The reaction mixture was then mixed with chloroform and the mixture was shaken vigorously for about 15mins. It was poured on to ice cold water. The chloroform layer was separated. It was washed several times with sodium bicarbonate solution to remove excess of bromine and finally 2-3 times with water. The chloroform was dried over anhydrous calcium chloride. Afterword, the solvent was removed through vacuum distillation when a solid tetra-*O*-acetyl-α-D-glucopyranosyl bromide was obtained, (yield 14.5g, 67%), $[\alpha]_D^{25}$ = $+196^0$ (c, 2 in $CHCl_3$), (**Scheme II**).

(iv) β-D-Glucopyranosyl-5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylate (6a)

To a solution of 5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acid (0.01mol, 2.94g) and 2,3,4,6-tetra-*O*-acetyl-α-D-glucopyranosyl bromide (3g) in dichloromethane was added tetrabutylammonium bromide (0.32g) with stirring at 5^0C. Sodium hydroxide (10%, 10ml) was added to it drop wise over a period of 30mins and the reaction mixture further stirred for 24hrs. The organic layer was separated, washed with water, 5% aq. $NaHCO_3$, distilled water and dried.

Deacetylation. The tetraacetyl derivative was deacetylated with 0.5% sodium methoxide solution by following the reported procedure[18]. To a solution of 3-(2,3,4,6-tetra-*O*-acetyl-4`-*O*-$\beta$-D-glucosidoxyphenyl)-5-(3`-phenyl prop-2`-enoyl)-1,2-benzisoxazole in absolute methanol (25ml) was added (1.5ml) of 0.5% of sodium methoxide solution and kept at room temperature for 45mins. The reaction mixture was neutralized with ion exchange resin (Amberlite IR 120), filters and dried. A semi-solid mass so obtained was purified on a column of silica gel and crystallized from ethanol as brown syrupy compound **6a** was obtained (1.8g, 62%). The compound was found to be optically active and the specific rotation $[\alpha]_D^{25}$ in water was found to be $+44.8^0$. FT-IR (KBr): 3296 (br, -OH peak of carbohydrate residue), 1655 and 1779 (2C=O), 1362 (C-O), 3009 (Ar-H str), 1163 (C-O-C, ester linkage), 1510 (C=C), 1581 (C=N, isoxazole ring) and 1222 (ring stretching vibration in isoxazole ring). ^{1}H-NMR signal at δ6.5-7.0 (dd, 2H, in ethylenic –CH=CH-), 7.0-8.9 (m, 8H, in aromatic), 5.10 (1H, d, *J*=7.5Hz, H-1 of sugar), The PMR spectrum displayed no signals of a acetyl protons, signals due to protons of the carbohydrate hydroxyl groups were not observed in the spectrum because of the fast exchange of all non-hydrogen bonded -COOH groups and the acidic carboxylic function. FAB-MS: M^+ 455, m/z 293, 248, 216, 206, 163 and 131.

Following the above procedure, other β-D-glucopyranosyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates **6a-o** were prepared (**Scheme III**).

V. MICROBIAL ACTIVITIES

5.1 Antimicrobial Activity

The obtained products were tested for their antibacterial activities by using cup-plate method against *Bacillus Subtilis* (gram positive) and *Escherichia Coli* (gram negative) at concentration of 100µg/ml in DMF. Pure Norfloxacin was used as standard antibiotic for the comparison of the results. The sterilized Muller-Hinton

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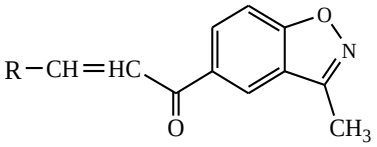
agar medium 50ml was inoculated with test organism and poured into petridishes. Then four holes of 6mm were completely filled with different test solution. The plates were then incubated for 24hrs at 37^0C and zones of inhibitions were measured. Similar procedure was adopted for pure Norfloxacin and the corresponding zone diameters were compared. Screening results indicate that compounds **6a-o** showed to excellent bacteriocidal activities against both the organisms (**Table 3**).

5.2 Antifungal Activity

The antifungal activity of newly synthesized products was evaluated by the using above same procedure (cup-plate) against *Aspergillus Niger* and *Candida Albicans* at concentration 100µm/ml in DMF. The plates were incubated for 8 days at 37^0C. The zones of inhibitions were measured. A commercial fungicide Gresiofulvin was also tested under similar condition with a view of comparing the results. The compounds showed significant fungi toxicity against both the fungi (**Table 3**).

Table 1. Characterization data of 3-methyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazoles



2a-o

Comp	R	Molecular Formula	Mol. wt.	M.P. ^{0}C	Yield %	R_f value	Found (calcd) % C	H	N
1.	C_6H_5-	$C_{17}H_{13}NO_2$	263	120	50.9	0.12	77.50 (77.55	4.95 4.98	5.30 5.32)
2.	*o*-OHC_6H_4-	$C_{17}H_{13}NO_3$	279	97	41.23	0.20	73.10 (73.11	4.70 4.69	5.05 5.02)
3.	*p*-OHC_6H_4-	$C_{17}H_{13}NO_3$	279	155	51.54	0.18	73.09 (73.11	4.65 4.69	5.06 5.02)
4.	2,4-$(OH)_2$-C_6H_3-	$C_{17}H_{13}NO_4$	295	105	42.34	0.24	69.00 (69.15	4.40 4.44	4.70 4.74)
5.	*p*-OH-*m*-$OCH_3C_6H_3$-	$C_{18}H_{15}NO_4$	309	109	49.84	0.23	69.86 (69.89	4.90 4.89	4.51 4.53)
6.	*o*-ClC_6H_4-	$C_{17}H_{12}ClNO_2$	297	92	45.30	0.20	68.57 (68.58	4.00 4.06	4.70 4.70)
7.	*p*-ClC_6H_4-	$C_{17}H_{12}ClNO_2$	297	194	48.54	0.28	68.57 (68.58	4.05 4.06	4.64 4.70)
8.	*o*-$NO_2C_6H_4$-	$C_{17}H_{12}N_2O_4$	308	187	43.75	0.34	66.24 (66.23	3.91 3.92	9.08 9.09)
9.	*m*-$NO_2C_6H_4$-	$C_{17}H_{12}N_2O_4$	308	127	50.0	0.27	66.21 (66.23	3.90 3.92	9.10 9.09)
10.	2-C_5H_4N-	$C_{16}H_{12}N_2O_2$	264	126	43.47	0.30	72.70 (72.72	4.57 4.58	10.61 10.6)
11.	3-C_5H_4N-	$C_{16}H_{12}N_2O_2$	264	118	57.97	0.34	72.72 (72.72	4.56 4.58	10.58 10.6)
12.	4-C_5H_4N-	$C_{16}H_{10}N_4O_3$	306	161	54.34	0.27	72.69 (72.72	4.60 4.58	10.56 10.6)
13.	3-C_4H_3O-	$C_{15}H_{11}NO_3$	253	120	52.83	0.28	71.12 (71.14	4.33 4.38	5.55 5.53)
14.	3-C_8H_5N-	$C_{19}H_{14}N_2O_2$	302	154	44.58	0.25	75.45 (75.48	4.65 4.67	9.29 9.27)
15.	*p*-*N*$(CH_3)_2$-C_6H_4-	$C_{19}H_{18}N_2O_2$	306	165	47.16	0.30	65.52 (74.49	4.60 5.92	15.96 9.14)

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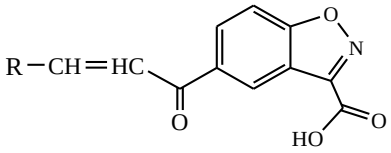
Table 2. Characterization data of 5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylic acids



3a-o

Comp	R	Molecular Formula	Mol. wt.	M.P. ^{0}C	Yield %	R_f value	Found (calcd) % C	H	N
1.	C_6H_5-	$C_{17}H_{11}NO_4$	294	104	80.7	0.29	69.60 (69.62	3.68 3.78	4.75 4.78)
2.	*o*-OHC_6H_4-	$C_{17}H_{11}NO_5$	309	111	48.0	0.30	66.85 (66.02	3.40 3.58	4.57 4.53)
3.	*p*-OHC_6H_4-	$C_{17}H_{11}NO_5$	309	99	61.0	0.29	65.85 (66.02	3.55 3.58	4.51 4.53)
4.	2,4-$(OH)_2$-C_6H_3-	$C_{17}H_{11}NO_6$	325	104	66.8	0.41	62.70 (62.77	3.31 3.41	4.12 4.31)
5.	*p*-OH-*m*-$OCH_3C_6H_3$-	$C_{18}H_{13}NO_6$	339	145	68.2	0.27	63.15 (63.72	3.91 3.86	4.18 4.13)
6.	*o*-ClC_6H_4-	$C_{17}H_{10}ClNO_4$	327	120	54.1	0.31	63.01 (62.30	3.10 3.08	4.26 4.27)
7.	*p*-ClC_6H_4-	$C_{17}H_{10}ClNO_4$	327	179	52.3	0.34	62.29 (62.30	2.98 3.08	4.24 4.27)
8.	*o*-$NO_2C_6H_4$-	$C_{17}H_{10}N_2O_6$	338	154	56.2	0.31	60.32 (60.36	3.02 2.98	8.23 8.28)
9.	*m*-$NO_2C_6H_4$-	$C_{17}H_{10}N_2O_6$	338	112	61.2	0.23	60.28 (60.36	2.89 2.98	8.19 8.28)
10.	2-C_5H_4N-	$C_{16}H_{10}N_2O_4$	294	118	67.7	0.24	65.30 (65.31	3.39 3.43	9.51 9.52)
11.	3-C_5H_4N-	$C_{16}H_{10}N_2O_4$	294	114	59.0	0.28	65.28 (65.31	3.42 3.43	9.52 9.52)
12.	4-C_5H_4N-	$C_{16}H_{10}N_2O_4$	294	148	55.7	0.29	65.32 (65.32	3.35 3.43	9.48 9.52)
13.	3-C_4H_3O-	$C_{15}H_9NO_5$	283	139	61.5	0.23	63.57 (63.61	3.09 3.20	4.94 4.95)
14.	3-C_8H_5N-	$C_{19}H_{12}N_2O_4$	332	185	53.5	0.35	68.60 (68.67	3.62 3.64	8.41 8.43)
15.	*p*-*N*$(CH_3)_2$-C_6H_4-	$C_{19}H_{16}N_2O_4$	336	171	72.0	0.26	67.82 (67.85	4.71 4.79	8.30 8.33)

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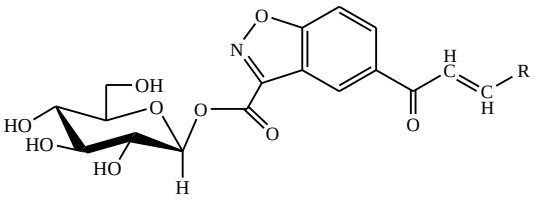
Table3. Characterization data of β -D-glucopyranosyl-5-(3`-aryl prop-2`-enoyl)-1,2-benzisoxazole-3-carboxylates



6a-o

Comp	R	Molecular Formula	Mol. wt.	$[\alpha]_D^{25}$ (^{0})	Yield %	R_f value	Found (calcd) % C	H	N
1.	C_6H_5-	$C_{23}H_{21}NO_9$	455	+44.8	62.06	0.30	60.64 (60.66	4.63 4.65	2.98 3.08)
2.	*o*-OHC_6H_4-	$C_{23}H_{21}NO_{10}$	471	+43.4	50.18	0.25	57.90 (58.60	4.49 4.49	2.98 2.97)
3.	*p*-OHC_6H_4-	$C_{23}H_{21}NO_{10}$	485	+39.8	59.42	0.32	58.53 (58.60	4.39 4.49	2.88 2.97)
4.	2,4-$(OH)_2$-C_6H_3-	$C_{23}H_{21}NO_{11}$	487	+46.0	61.16	0.19	56.61 (56.68	4.33 4.34	2.85 2.87)
5.	*p*-OH-*m*-$OCH_3C_6H_3$-	$C_{24}H_{23}NO_{11}$	501	+47.5	59.31	0.27	57.47 (57.49	4.63 4.62	2.80 2.79)
6.	*o*-ClC_6H_4-	$C_{23}H_{20}ClNO_9$	489	+46.7	60.98	0.22	56.34 (56.39	4.10 4.12	2.86 2.86)
7.	*p*-ClC_6H_4-	$C_{23}H_{20}ClNO_9$	489	+39.8	57.43	0.20	55.76 (56.39	4.08 4.12	2.79 2.86)
8.	*o*-$NO_2C_6H_4$-	$C_{23}H_{20}N_2O_{11}$	500	+33.9	69.09	0.28	55.20 (55.20	4.05 4.03	5.58 5.60)
9.	*m*-$NO_2C_6H_4$-	$C_{23}H_{20}N_2O_{11}$	500	+47.1	47.29	0.21	55.15 (55.20	4.02 4.03	5.59 5.60)
10.	2-C_5H_4N-	$C_{22}H_{20}N_2O_9$	456	+42.5	54.30	0.18	57.89 (57.90	4.40 4.42	6.13 6.14)
11.	3-C_5H_4N-	$C_{22}H_{20}N_2O_9$	456	+39.6	63.41	0.26	56.89 (57.90	4.41 4.42	6.11 6.14)
12.	4-C_5H_4N-	$C_{22}H_{20}N_2O_9$	456	+44.6	58.77	0.37	57.85 (57.90	4.43 4.42	6.13 6.14)
13.	3-C_4H_3O-	$C_{21}H_{19}NO_{10}$	445	+41.7	58.38	0.29	56.59 (56.63	4.27 4.30	3.12 3.14)
14.	3-C_8H_5N-	$C_{25}H_{22}N_2O_9$	494	+46.5	63.20	0.36	59.90 (60.73	4.45 4.48	5.65 5.67)
15.	*p*-*N*$(CH_3)_2$-C_6H_4-	$C_{25}H_{26}N_2O_9$	489	+50.0	58.57	0.23	60.21 (60.24	5.24 5.26	5.59 5.62)

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