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New Designed Monosaccharide's Epimeric Diagram (Chart) Using Monosaccharide's Barcode

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Abstract

In this research a new epimeric diagram (chart) introduced for easy determination of the kind of epimers in each monosaccharide using the corresponding barcode. This new epimeric chart is facilitating the determination and the prediction of any kind of epimers in each monosaccharide. It is convenient to attach this new chart on the laboratory and/or library board as the reference of graduate, undergraduate and carbohydrate researchers.

Keywords: Epimeric chart, Monosaccharide barcode, Monosaccharide lines, Centrosymmetry

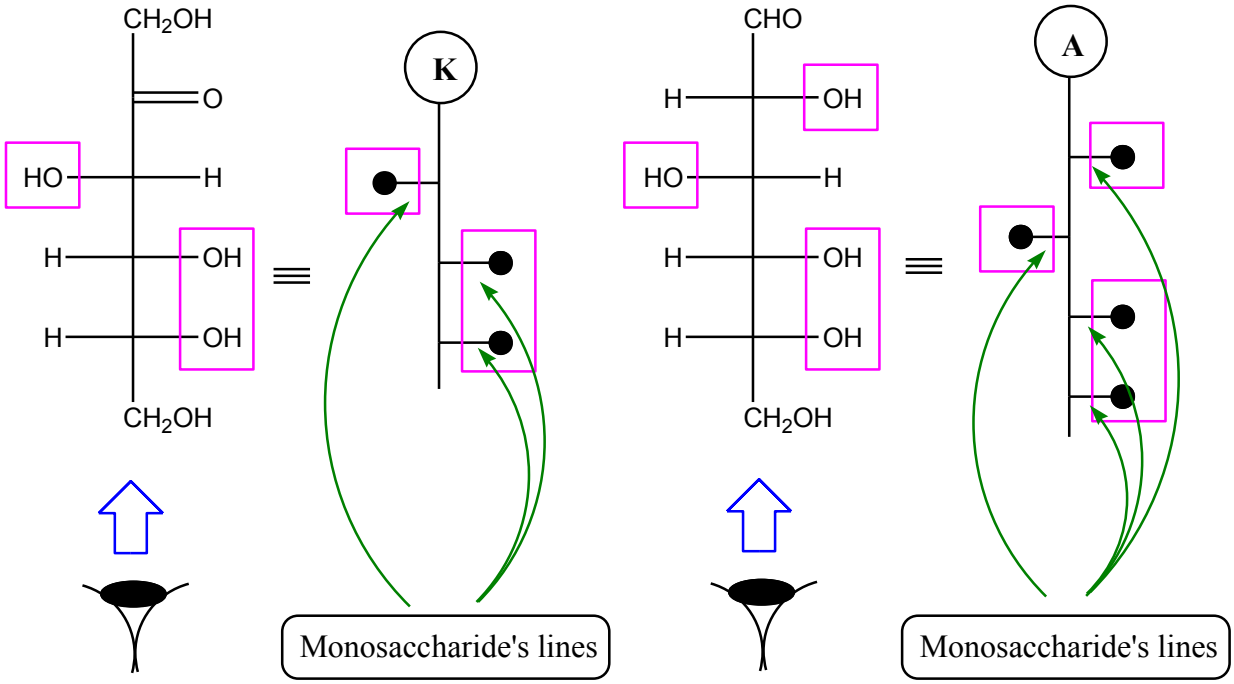
Contents

Introduction

Carbohydrates are the most abundant class of organic compounds found in living organisms. Another type of isomer that carbohydrates that can take on are epimers. Epimers are two diastereomers that differ only at one stereocenter [1]. For example; D-glucose and D-mannose are an example of an epimer. The -OH group on the first carbon of glucose is in the axial position and opposite the -OH group on carbon C-4. Instead, the -OH group of galactose is oriented in the same direction, the equatorial position [2]. In stereochemistry, epimer is one of a pair of stereoisomers and the two isomers differ in their configuration at only one stereogenic center. All other stereo centers in the molecules are the same.

Many chemists have described new methods to solve the problems in monosaccharides. For example: the work of Fischer and Van't Hoff in carbohydrate chemistry [3], the use of schematic formulas for representing configurations for monosaccharides [4], to indicate the carbohydrates structure [5] and the nomenclature of carbohydrate's history [6] have been presented.

Monosaccharides have multiple stereocenters and the presence of these multiple stereocenters contributes to the rich structural diversity of carbohydrates, resulting in serving as "molecular (cellular) barcodes" [7]. Monosaccharide cycles (*MoCycle*) is an interesting method for determination of the general stereochemical relationships of both D and L monosaccharides, as has been reported by Hunsen [7]. Arita and Tokimatsu [8] reported the stereo parities of four chiral positions (from C5 to C2) for D-hexose monosaccharides. Recently, we have reported the new monosaccharide's barcoding that made drawing of Fischer projection of the linear monosaccharaides easier [9]. This new barcodes forced the invention of the new monosaccharide's osazone chart [10]. In the present research and educational work, we introduce a simple and convenient diagram (chart) for determination and elucidation of epimers using our recently reported monosaccharide barcodes. In the present educational work, a novel epimeric chart was introduced for detection of the all monosaccharide epimers without spending the time for drawing of the monosaccharide's structures. It is sufficient only to attach this new chart on the laboratory and/or library board for detecting any epimers of monosaccharides.



D-Fructose (**21K**) D-Glucose (**211A**)

Figure 1 The introduction of monosaccharide's lines in D-Fructose and D-glucose.

Results and Discussion

This paper describes a new interesting monosaccharide's epimeric diagram (chart). This chart is useful for learning of undergraduate and graduate students at the university and some useful aspects are as below;

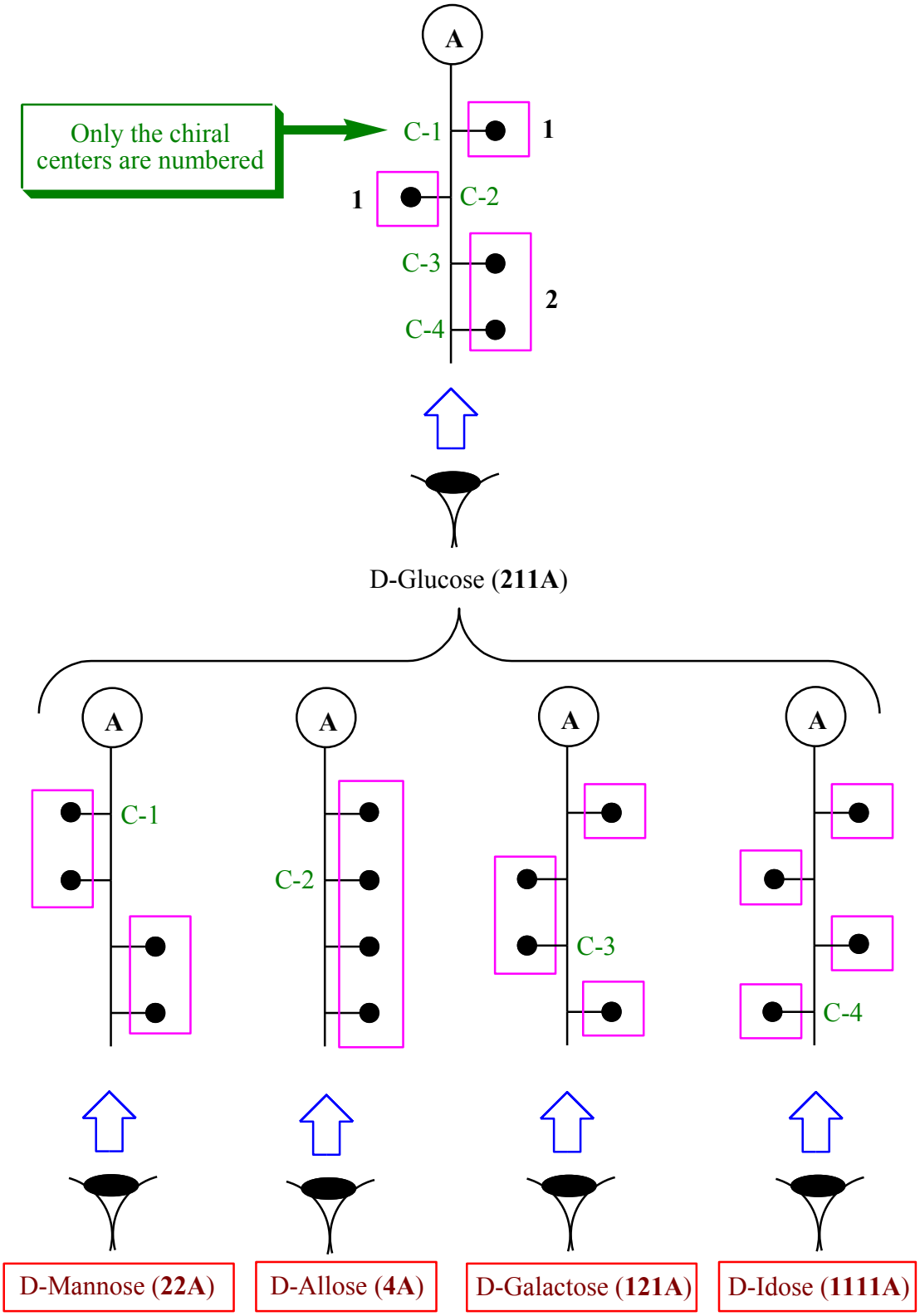


Figure 2 All the epimers derived from D-glucose and only the chiral centers are numbered.

(a) Determination of epimers using monosaccharide's lines.
(b) Determination of epimers using Arita and Tokimatsu barcoding method.
(c) Conversion of Arita and Tokimatsu's barcodes to our barcodes (Noroozi-Rahbari-Elahirad's barcode [9]) and *vice versa*.
(d) Symmetry and determination of epimers using new presented epimeric symmetry diagram.

(a) Determination of epimers using monosaccharide's lines

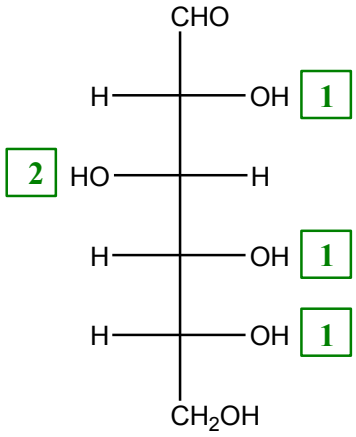
Definition of monosaccharide lines;

When we draw the monosaccharide (aldose or ketose) Fischer projection, the carbon chain and the OH substituents linked to the chiral centers can be shown as a dense dot (●) in horizontal lines, and the lines are called *monosaccharide's lines* (**Figure 1**). The capital letters **A** and **K** represents the aldose and ketose functional groups, respectively.

First, we draw the monosaccharide's lines for each monosaccharide (an aldose or a ketose). Then we change position of the OH substituent at the first chiral center in the monosaccharide's lines. (If the OH group to be located at the right hand side of chiral center, it will be changed to the left hand side and *vice versa*) as other chiral centers to be fixed. Therefore, the obtained monosaccharide's lines become boxation and barcoding according to our new barcoding method that has recently been reported [9]. In this case, the first epimer can be obtained as the result of changing of the first chiral center (Figure 2, bottom left). Then, we change the second chiral center in a similar manner to the first chiral center and the second epimer is obtained. We continued this until we obtain all epimers of each monosaccharide and so on (**Figure 2**).

(b) Determination of epimers using Arita and Tokimatsu barcoding method

The glucose barcoding by the Arita and Tokimatsu's method is shown in **Figure 3**. All four epimers barcodes (by the Arita and Tokimatsu's method) derived from glucose are also shown in **Figure 4**. In these barcodes, the first to final chiral centers are shown from right to left, respectively.



D-Glucose (1121)

Figure 3 The glucose barcoding by the Arita and Tokimatsu's method [8].

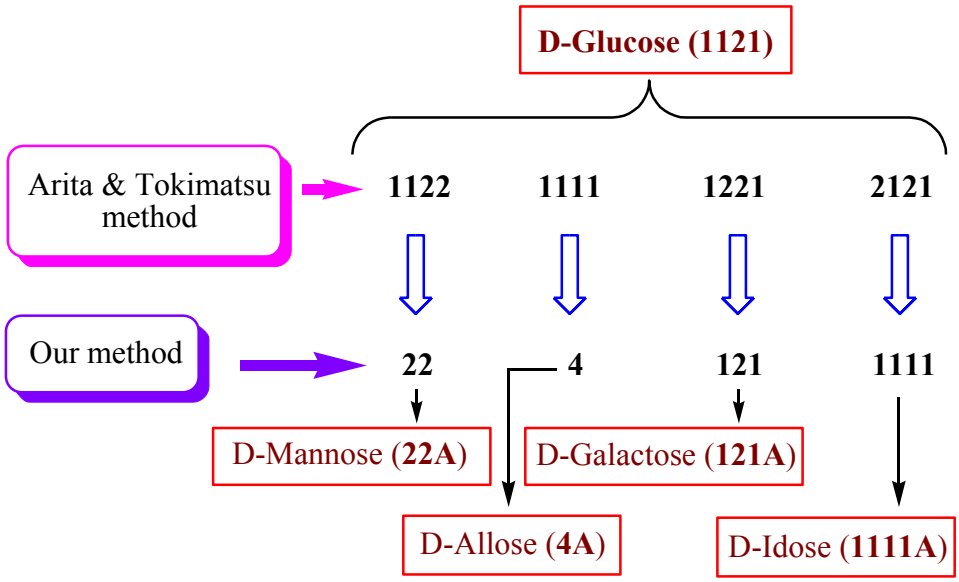


Figure 4 All four epimers barcodes derived from glucose by the Arita and Tokimatsu's method [8] and our method [9].

Table 1 Conversion of Arita and Tokimatsu's barcodes to our monosaccharide's barcodes and *vice versa*.

Talose	Idose	Galactose	Altrose	Monosaccharide
1222	**1212**	**1221**	**1112**	Arita & Tokimatsu's barcode
⇩⇧	⇩⇧	⇩⇧	⇩⇧	
RLLL	**RLRL**	**RLLR**	**RRRL**	Convertor
⇩⇧	⇩⇧	⇩⇧	⇩⇧	
13	**1111**	**121**	**31**	Our barcode

(c) Conversion of Arita and Tokimatsu's barcodes to our barcodes (Noroozi-Rahbari-Elahirad's barcode) and *vice versa*

(c-1) Conversion of Arita and Tokimatsu's barcodes to our barcodes

Table 1 exemplifies the procedure for the conversion of Arita and Tokimatsu's barcodes to our barcodes with four monosaccharides. First, we replace the letters "**R**" and "**L**" to in the place of "**1**" and "**2**", respectively, from left to right (from row 2 to row 3; the letters of "**R**" and "**L**" represents the "Right" and "Left" hand, respectively). Then the numbers of consecutive same letters are summed, and one obtains a series of mathematical digits, which corresponding to our barcode. For example, **R = 1**, **L = 1**, **RR = 2**, **LL = 2**, **RRR = 3**, **LLL = 3**, **RRRR = 4**, **LLLL = 4**, **RLLL = 13**, **RLRL = 1111**, **RLLR = 121**, **RRRL = 31** and so on (from **Table 1** row 3 to row 4, marked by ⇩).

Table 2. The square table barcodes of aldotetroses and ketopentoses.

Threose	Erythrose
11	2
11	2

Xylulose	Ribulose
11	2
11	2

Table 3 The square table barcodes of aldopentoses and ketohexoses.

Xylose	Lyxose	Arabinose	Ribose
111	12	21	3
111	12	21	3
111	12	21	3
111	12	21	3

Sorbose	Tagatose	Fructose	Psicose
111	12	21	3
111	12	21	3
111	12	21	3
111	12	21	3

Table 4 The square table barcodes of aldohexoses.

Idose	Gulose	Galactose	Talose	Glucose	Mannose	Altrose	Allose
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4
1111	112	121	13	211	22	31	4

(c-2) Conversion of our barcodes to Arita and Tokimatsu's barcodes

In this conversion, we assign the letters "**R**" and "**L**" to the number of boxes from left to tight, respectively (**Table 1**, rows 2 and 3, marked by ⇧).

(d) Symmetry and determination of epimers using new presented epimeric symmetry diagram

We introduced an epimeric symmetry diagram that facilitates the prediction of all the epimers of each monosaccharide based on our new monosaccharide barcodes that recently we reported [9]. We use the square table barcodes in **Tables 2-4** for designing new epimeric diagrams in **Figures 5-8**.

(d-1) How we can use the epimeric diagrams in Figs. 5 and 7?

The both **Figures 5** and **7** are divided to four sections (Ⅰ to Ⅳ). For instance, in **Figure 5,** we assumed period 2 in parallel of X-vector (assigned by pink horizontal line (——) in the sections I and II). For example; the monosaccharides ribose (as an aldose) or psicose (as a ketose) that corresponds to barcode **3** is assigned with dense violet dot ( ) on the symmetrical diameter (assigned as violet line (——)). The location of each monosaccharide on the diameter is shown by a blue mark ( ). Now, arabinose (**21**) is the C-1 epimer of ribose that is assigned with red dense dot ( ) on the above-mentioned pink horizontal line (——). Lyxose (**12**) is the C-3 epimer of ribose and Xylose (**111**) is the C-2 epimer of ribose on the same pink horizontal line. The symmetric nature of this chart is shown in **Figure 5**. Another example; Fructose as a ketohexose, its C-1, C-2 and C-3 epimers are psicose, tagatose and sorbose, respectively (In period 1 from right to left, respectively). For lyxose; the C-1, C-2 and C-3 epimers are xylose, arabinose and ribose, respectively. For xylose; the C-1, C-2 and C-3 epimers are lyxose, ribose and arabinose, respectively. **Figures 5** and **7** have a centrosymmetric case that are shown in **Figures 6** and **8**, respectively. All full epimeric correlations for aldopentoses and ketohexoses are shown in **Tables 5** and **6**, respectively.

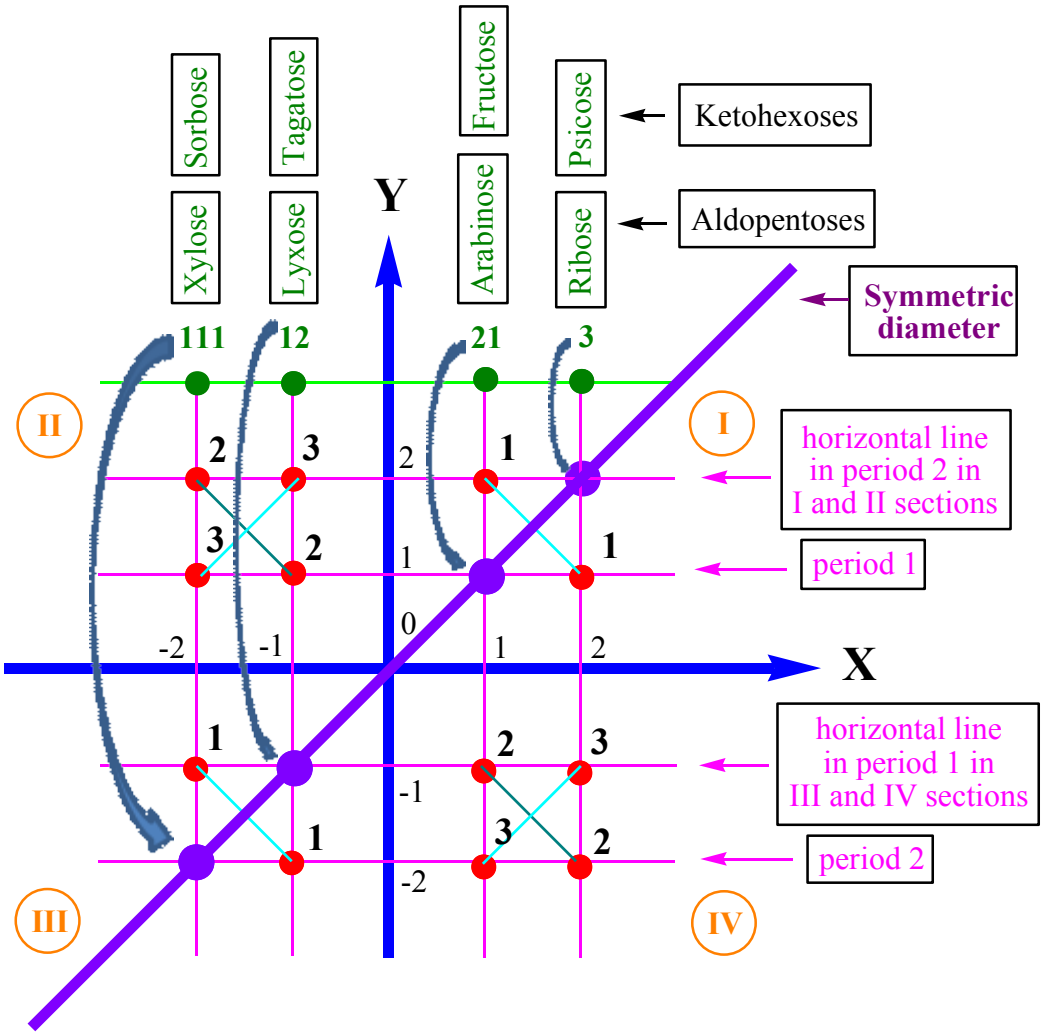


Figure 5 An epimeric diagram for aldopentoses and ketohexoses.

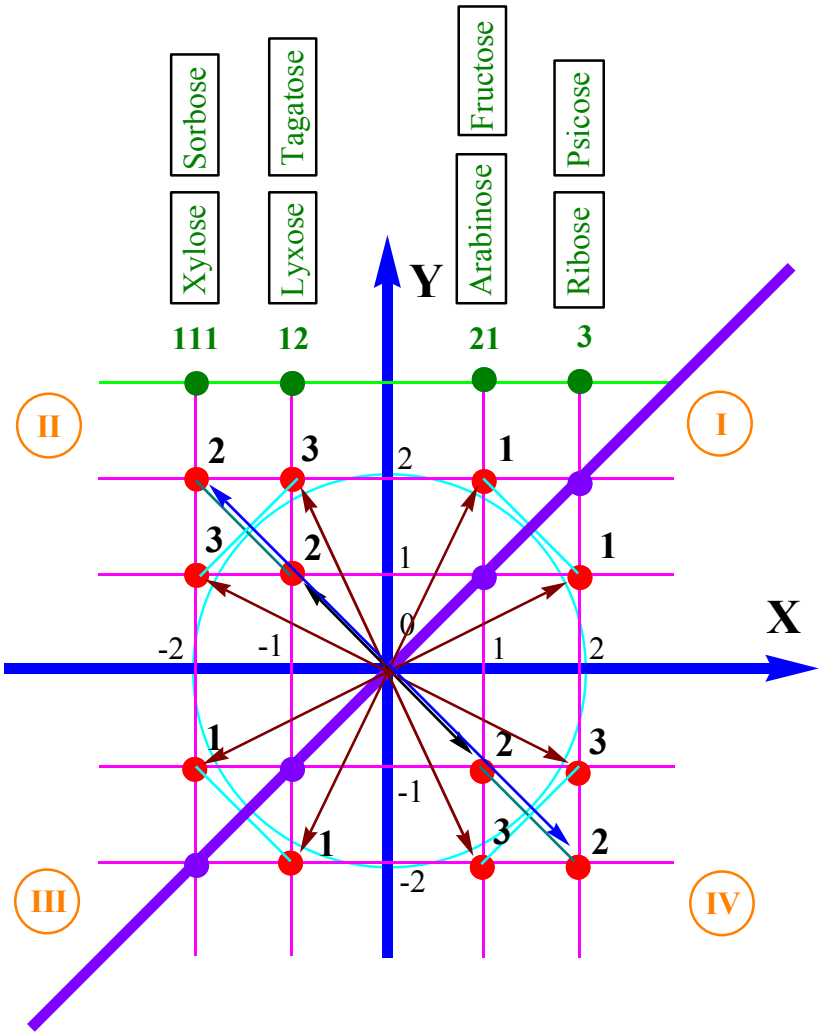


Figure 6 A centrosymmetric case in epimeric diagram for aldopentoses and ketohexoses.

Table 5 Full epimeric correlations between aldopentoses.

Aldopentose	C-1 epimer	C-2 epimer	C-3 epimer
Ribose (3)	arabinose (21)	xylose (111)	lyxose (12)
Arabinose (21)	ribose (3)	lyxose (12)	xylose (111)
Lyxose (12)	xylose (111)	arabinose (21)	ribose (3)
Xylose (111)	lyxose (12)	ribose (3)	arabinose (21)

Table 6. Full epimeric correlations between ketohexoses.

ketohexose	C-1 epimer	C-2 epimer	C-3 epimer
Psicose (3)	fructose (21)	sorbose (111)	tagatose (12)
Fructose (21)	psicose (3)	tagatose (12)	sorbose (111)
Tagatose (12)	sorbose (111)	fructose (21)	psicose (3)
Sorbose (111)	tagatose (12)	psicose (3)	fructose (21)

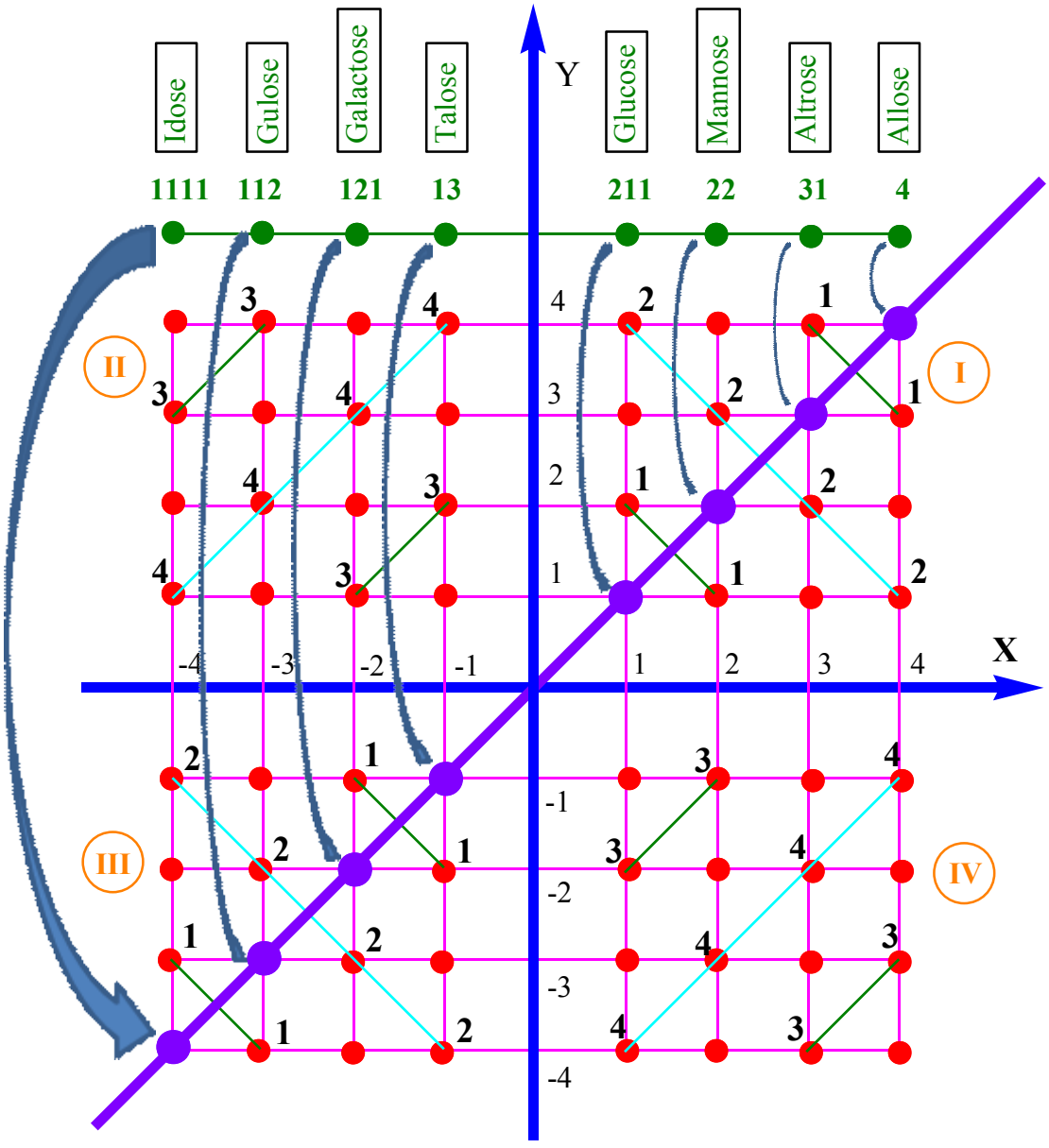


Figure 7. An epimeric diagram for aldohexoses.

Among aldohexoses (**Figure 7**), for example; we assume allose (4) as an aldehexose (Section I, period 4). The C-1 epimer of allose is altrose (**31**), its C-2 epimer is glucose (**211**), its C-3 epimer is gulose (**112**) and finally, its C-4 epimer is talose (**13**). All these epimers are assigned as the red dense dot (●) with the corresponding epimeric carbon number. Other epimeric correlations are also described below and the full epimeric correlations of all aldohexoses are summarized in **Table 7**. It is sufficient that this chart to stick in the board of laboratory and/or library for detecting any epimer of each monosaccharide.

Example 1: For allose: the C-1, C-2, C-3 and C-4 epimers are altrose, glucose, gulose and talose, respectively.

Example 2: For altrose: the C-1, C-2, C-3 and C-4 epimers are allose, mannose, idose and galactose, respectively.

Example 3: For mannose: the C-1, C-2, C-3 and C-4 epimers are Glucose, altrose, talose and gulose, respectively and so on.

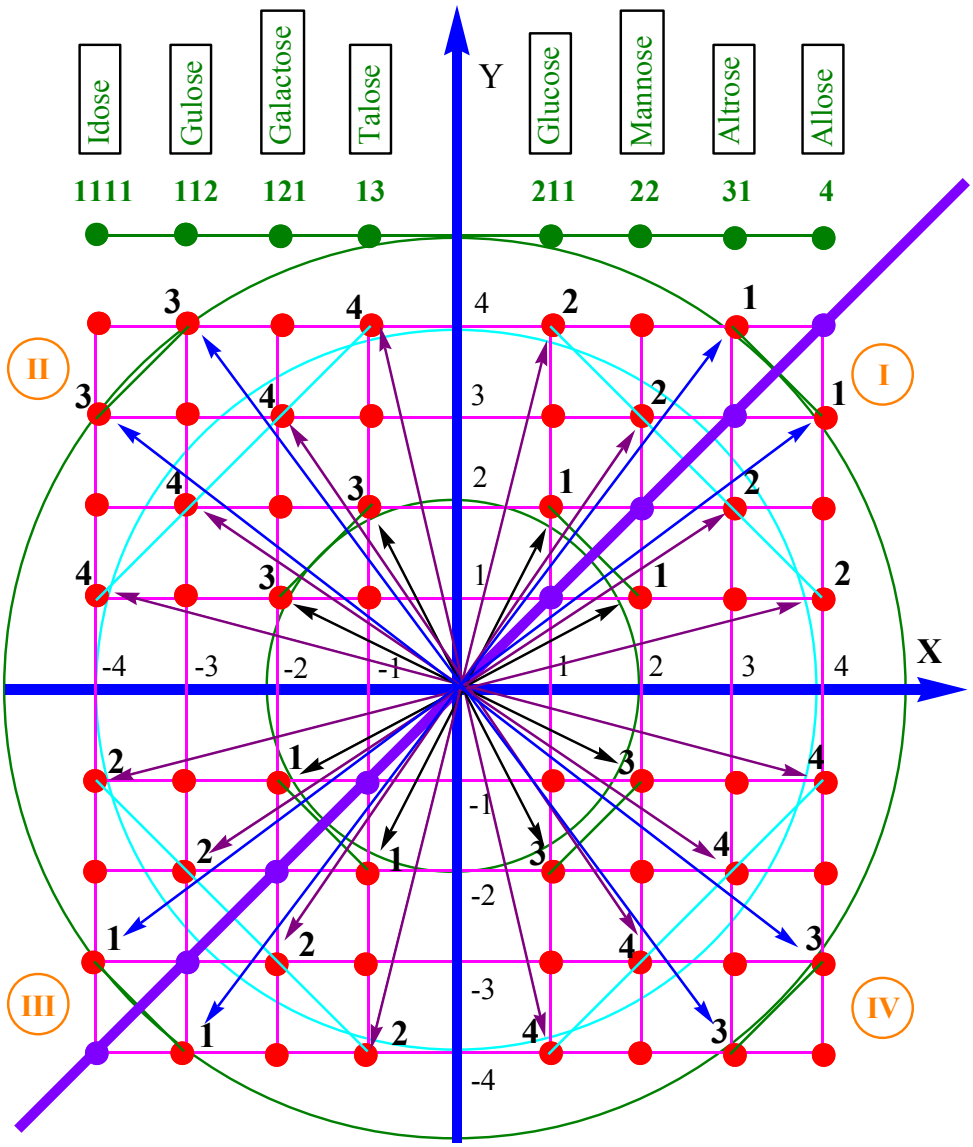


Figure 8. A centrosymmetric case in epimeric diagram for aldohexoses.

Table 7. Full epimeric correlations between aldohexoses.

Aldohexose	C-1 epimer	C-2 epimer	C-3 epimer	C-4 epimer
Allose (4)	altrose (31)	glucose (211)	gulose (112)	talose (13)
Altrose (31)	allose (4)	mannose (22)	idose(1111)	galactose (121)
Mannose (22)	glucose (211)	altrose (31)	talose (13)	gulose (112)
Glucose (211)	mannose (22)	allose (4)	galactose (121)	idose (1111)
Talose (13)	galactose (121)	idose (1111)	mannose (22)	allose (4)
Galactose (121)	talose (13)	gulose (112)	glucose (211)	altrose (31)
Gulose (112)	idose (1111)	galactose (121)	allose (4)	mannose (22)
Idose (1111)	gulose (112)	talose (13)	altrose (31)	glucose (211)

Finally, in this work, we have extracted new monosaccharide's epimeric chart by the results of our reported monosaccharide's barcoding. The Arita and Tokimatsu's barcoding offered each monosaccharide barcode, so there is no any relation between monosaccharides barcodes (Arita and Tokimatsu's barcoding). In their method, the parity **1** and **2** corresponds to right and left orientation of the Fischer projection from the bottom up, respectively. The keto group is represented by '_' to distinguish hexoses and pentoses [8,9]. Therefore, there are no osazone and epimeric charts were extracted from their barcoding. In our barcoding, there are distinguished relations between monosaccharides barcodes, so we also extracted and designed new interesting osazone chart (ref. [10] in the manuscript text). Therefore, the osazone and epimeric charts of monosacharides are the results of our new monosaccharide barcoding and are of our barcoding advantages.

Conclusion

In summary, in this work, a novel epimeric chart was introduced for detection of the all monosaccharide's epimers without any spending the time for drawing of the monosaccharide's structures. It is convenient to attach the charts like **Tables 6** and **7** on the board for detecting any epimers of each necessary monosaccharide.

Acknowledgement

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