

# Creating an Adaptive Technology Using a Cheminformatics System To Read Aloud Chemical Compound Names for People with Visual Disabilities

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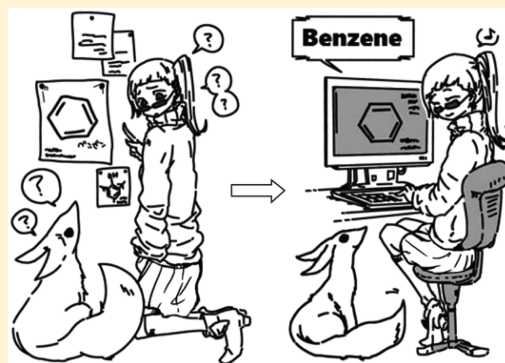
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**ABSTRACT:** Various tactile methods, such as Braille, have been employed to enhance the recognition ability of chemical structures by individuals with visual disabilities. However, it is unknown whether reading aloud the names of chemical compounds would be effective in this regard. There are no systems currently available using an audio component to assist in the recognition of chemical structures. This study aims to establish the essential requirements for the prototype Chemical Literature Extraction and Aloud-reading System (CLeArS) that enables visually impaired people to recognize a depicted chemical structure after hearing its name, which complies with the nomenclature adopted by the International Union of Pure and Applied Chemistry. Details of the methods employed in CLeArS and its execution are presented, in addition to the fundamental requirements for recognizing chemical structures using CLeArS. Experimental results on 450 images comprising both simple and complex chemical structures show a high recognition rate of 90% among subjects with visual disabilities. Thus, we conclude that reading aloud the names of chemical compounds is an effective method enabling students with impaired vision to recognize chemical structures.

**KEYWORDS:** High School/Introductory Chemistry, Cheminformatics, Computer-Based Learning, Computational Chemistry, Minorities in Chemistry, Student-Centered Learning



## INTRODUCTION

As supporting technology for those with visual disabilities to use a cheminformatics method, this research aimed to develop a method for reading-aloud text containing both characters and chemical structures.

From the viewpoint of education, understanding the structure and characteristics of chemical molecules is a fundamental and indispensable task in the broad natural science field dealing with molecules such as in chemistry and the life sciences. Moreover, this is one of the starting points of science education. At this stage, it is important for students to gain an understanding of and to develop intellectual curiosity about molecules. These can become major factors determining the direction of the courses undertaken by students. Therefore, it is desirable to have teaching materials that students can use to study and understand molecules with interest and in greater detail.<sup>1</sup>

In the chemistry field, when discussing an invisible object or concept such as molecules or reactions, a model (visual

expression, molecule model, molecular orbital, and so on) is indispensable and is used as a means of thinking about or communicating information. Various graphical systems visualized by computers have been developed and are currently used for research and education.<sup>2–5</sup> Since it is beneficial for visually disabled students to experience science phenomena and life processes using their tactile and/or hearing senses, various apparatus are used in studies and education for these students.<sup>6–13</sup> Specifically, several methods for changing visualized information into a tactile format have been developed. These are some of the leading methods for improving sight, showing that tactile systems are important for visually impaired students to understand the information contained in images.

**Special Issue:** Chemical Information

However, no study has investigated whether a reading-aloud system used prior to a tactile system can give those with visual disabilities greater understanding of chemical structures drawn in textbooks, chemical literature, and patents or even on a computer screen.

In recent years, research on character recognition methods using optical character recognition (OCR) has flourished with the advancement of computer technology.<sup>14,15</sup> Although OCR is effective for character recognition, because it cannot deal with anything other than characters, a method for recognizing information containing graphics other than characters needs to be built as support technology for those with visual disabilities.

In educational institutions specializing in a variety of fields, it is important to be proactive in attracting visually disabled students. However, traditional textbooks and experimental apparatus are not necessarily suitable for these students. In particular, because chemistry and life science textbooks typically contain many tables and images, it is important to ensure that visually disabled students can understand these tables and images. As another example, it is difficult for visually disabled students to convert teaching materials used in higher education, such as technical manuals, into an easily usable form. Generally, visually disabled students can use teaching materials incorporating text, tactile sense, and sound. A reading-aloud system for mathematical expressions has already been reported,<sup>16–18</sup> while the textbook “Japanese Braille Notation 2001” explains the Braille notation for printed characters only.<sup>19</sup> However, the notation does not cover graphical information like chemical structures. For this reason, tactile systems are used to present graphical information to visually disabled persons.<sup>20</sup> Although it is easy to depict graphical information using tactile systems, support methods that, for example, add Braille notation to such systems are required to understand graphical systems fully. Generally, those with some form of visual disability acquire information through hearing, such as face-to-face reading or reading-aloud by screen readers. However, it is more effective for such persons to listen to explanations of graphics with the support of drawing tools. Thus, a method that provides both hearing and tactile information is more effective.

In many cases, Braille users use Braille notation together with sound; according to ref 21, 10% of those with visual disabilities have been known to use audio guidance and Braille notation simultaneously. On the basis of the authors’ own experience of chemical education with a visual disability, no chemical structure recognition technique exists that is easy for persons with visual disabilities to use. Thus, we focused on the importance of acquiring information on chemical compounds, which is indispensable in chemical education. Previously, we reported a method for those with visual disabilities to write chemical structures by developing a text editor using XyMTeX/LaTeX, which is a well-known typesetting system.<sup>22,23</sup> However, no method exists that enables those with visually disabilities to acquire chemical structure information. In this article, we investigate a system for systematically searching and reading aloud compound names from chemical structures using the nomenclature of the International Union of Pure and Applied Chemistry (IUPAC).<sup>24</sup>

Various digital methods using OCR have been presented for converting graphical representations of chemical structures appearing in journal articles, patent documents, textbooks and trade magazines, among others.<sup>25–28</sup> These methods, which have advanced together with cheminformatics, convert chemical structures into plain text databases. Structure names

can be obtained directly from the plain text, which is effective as supporting technology for those with visual disabilities. Mol files, SMILES notation, and IUPAC names are ubiquitous file formats and systematic identifiers for chemical structures.<sup>29–31</sup>

Although commercial software that displays chemical structure names is available,<sup>32,33</sup> these software packages do not include the functionality of reading aloud the output depicted on a PC screen. Therefore, for ordinary use, additional supporting software must be used to read aloud the result.

Despite having an automatic nomenclature system and conversion systems from the analog representation of chemical graphics to a digital form, we suggest that as supporting technology, the conventional method is further extended by providing a reading-aloud system. Conventional techniques depend on a computer graphic user interface (GUI); however, even if the structure name is displayed on the screen, those with visual disabilities cannot benefit from this.<sup>34</sup> Text output systems without a computer GUI are also available. When using such systems to understand chemical structures, extraction of the chemical structure as well as the printed text from the document is required, and then it is necessary to integrate reading aloud the chemical structure names and printed text.

In this article, we propose an automatic reading-aloud system for structure names based on the IUPAC nomenclature system. We confirm that the proposed system is able to read aloud both the chemical structure and the printed text. Because our system can convert the extracted image of the chemical structure and the printed characters from a document into information required for reading aloud, it can be used by those with visual disabilities. Using the XyMTeX/LaTeX system mentioned above with the proposed system, we suggest that the prototype Chemical Literature Extraction and Aloud-reading System (CLEArS) developed in this research is a useful tool for communicating chemical structures to visually disabled users, and to support the searching and writing of academic papers by these users.

## ■ OUTLINE OF THE SYSTEM

### Basic Concept of CLEArS

CLEArS is aimed at visually disabled persons who wish to learn about chemistry, including students in higher education. The proposed reading-aloud system integrates the method for converting images of chemical structures into computer-searchable formats and the nomenclature method for chemical structures.

Given a document containing printed text and chemical structures as graphical images, CLEArS reads aloud the printed text and the names of the chemical structures using a screen reader. The proposed system aims to promote understanding of the whole document once the user has heard the name of the chemical structure.

### Functionality of CLEArS

CLEArS comprises components for reading a document with printed text and chemical structures and for capturing images. A flowchart of the process is depicted in Figure 1. In addition, with the aim of targeting users with visual disabilities, CLEArS was designed so that all operations can be carried out by the screen reader using shortcut keys only. Thus, chemical structures and indeed the whole document are read aloud after selecting the relevant image files using the up/down arrow keys and transferring the associated image file of the recognition result to the text-to-speech engine.<sup>35</sup> During the

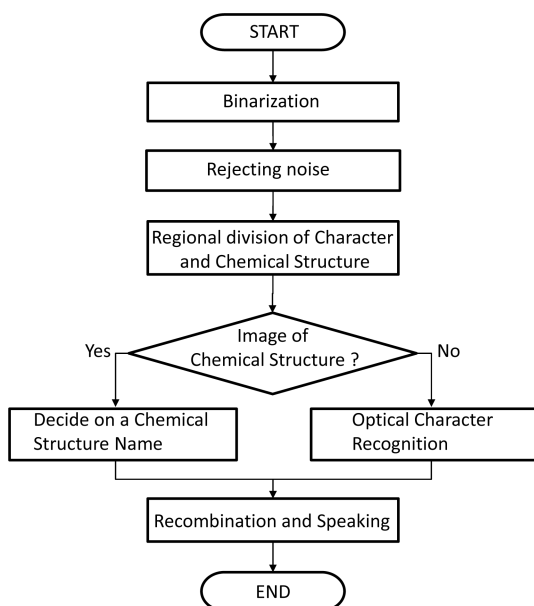


Figure 1. Flowchart of CLeArS.

reading of the document, CLeArS adds words, such as “text” or “structure”, at the beginning of each section, making it easy to understand whether what follows is indeed text or a chemical structure.

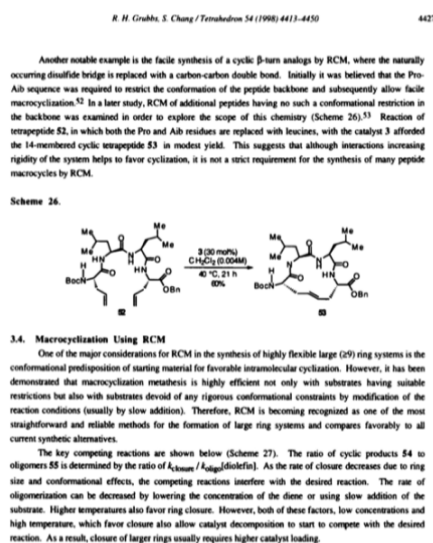
According to the extraction method described in the next section, the characters obtained from the area of printed text and those from the chemical structure area of the extracted image are transmitted to the Microsoft OCR engine and ChemAxon Marvin Beans (Molconvert),<sup>36</sup> respectively. Then, the characters to be read aloud are obtained by various recognition methods.

## Extraction of Chemical Structures from a Document

Initially, as preprocessing, the input image is binarized. A threshold is selected using Otsu's method.<sup>37</sup> Extractions are known to decrease the recognition rate of images like chemical structures substantially. As the possibility of false recognition is high for unregistered characters, we initially extract the character and chemical structure parts using Otsu's method, which is independent of specific fonts. After removing noise from the binarization using a median-type filter,<sup>38</sup> the areas with chemical structures and those with printed text are obtained from the captured image.

The image data used in CLeArS are bmp files, implying pixel groupings on a bitmap image. By considering object pixels horizontally, we have identified a trend whereby lines with text have low density and chemical structure lines have high density. Thus, using the density of object pixels, we can extract the various areas of printed text and chemical structures. We use two density measures in the standard method. The first is obtained by counting the number of pixels per line. This density is based on the assumption that the areas of printed text and chemical structures are identified by looking horizontally at the lateral text. Because vertical areas are not taken into consideration in this method, some of the printed characters and chemical structures may be misunderstood in certain images. The second density measure is defined as “area” given that the areas of printed text and chemical structures are identified by combining perpendicular continuous lines in the pixels of the object. Thus, this density measure is defined as the number of object pixels per size of the “area”, and the extraction is carried out using the two densities.

The result of the calculation of the number of pixels per line for the first density measure is either high or low. The histogram of the density of pixels per line (see Figure 2) shows the number of object pixels in each line of the image data. After removing lines that do not contain any objects in this histogram, the chemical structure and printed text areas are extracted using a binarization method for lines containing



Test Image

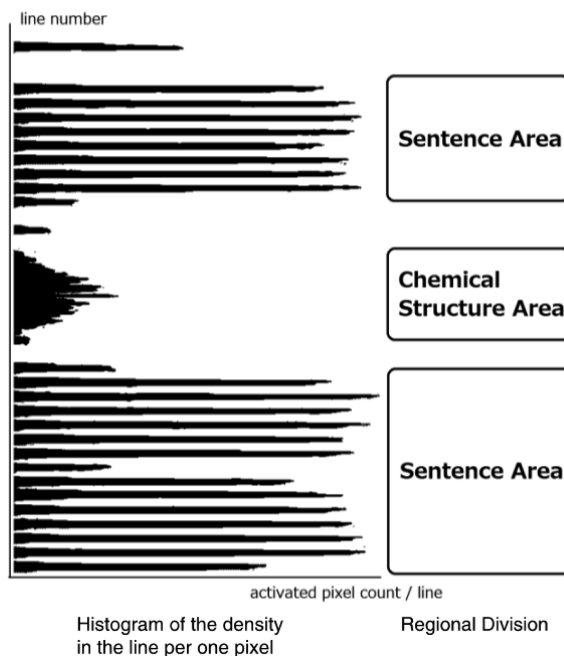
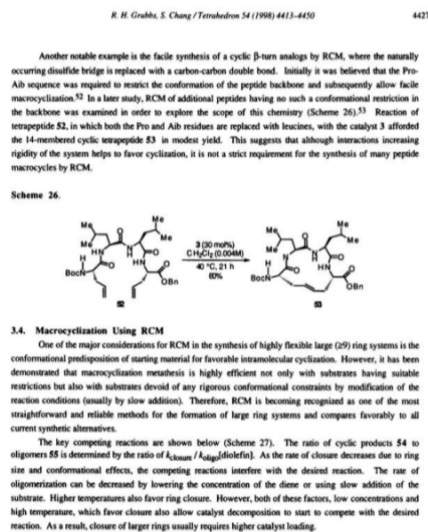
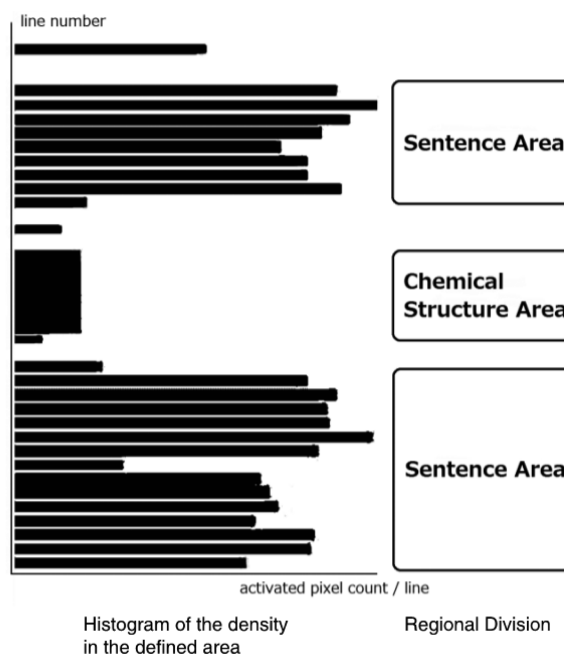


Figure 2. Histogram of the density of pixels per line. Left panels reproduced with permission from ref 39. Copyright 1998 Elsevier Science Ltd.



Test Image



**Figure 3.** Histogram of the density of pixels in defined areas. Left panel reproduced with permission from ref 39. Copyright 1998 Elsevier Science Ltd.

chemical structures and those with printed text only. A threshold is determined by Otsu's method. If many pixels exist in a line containing a chemical structure, or few pixels exist in a line of characters, the applicable pixel data are removed after smoothing.

The second density measure is calculated as the number of object pixels divided by the size of the area. The bar graph in Figure 3, with density depicted on the horizontal axis and area on the vertical axis, shows example values calculated for the second density measure. After removing lines with no object pixels from this histogram, the chemical structure and character areas are extracted using binarization based on lines containing chemical structure data and those containing characters only. A threshold is determined by Otsu's method, in the same way as for the first density measure.

## EXPERIMENTS

As mentioned above, digital books in pdf format are widely available on the Internet. Jpg files, converted from various file formats as explained below, were used in all the recognition experiments using CLArS. In the jpg images, only the chemical structures and text characters were printed; graphical information such as tables or photos was not printed.

Two separate experiments were carried out. The first was an extraction experiment to confirm whether extraction of the character and chemical structure areas had been performed correctly. The second experiment, involving nomenclature, investigated whether the well-extracted chemical structure image was correctly identified with the name of the corresponding compound. In the nomenclature recognition experiment, various text fonts were tested, since problems can occur when electronic data are exchanged through the Internet if the creators and users of data do not have the same font types installed. The experimental details are given below.

### Images Used in the Experiments

Two groups of chemical structure images were used in the experiments. The first group with 399 images was obtained

from the CLiDE validation set<sup>40</sup> (hereafter referred to as the CLiDE data set), while the second group with 51 images was selected from a Japanese high school textbook<sup>41</sup> (hereafter referred to as the textbook images). The main difference between these two groups was the complexity of the chemical structures. Because images in the first group were published in academic chemistry papers, they included complicated structures, whereas the latter images depict comparatively simple structures since they relate to structural formula taught in high-school chemistry. Poor quality data as well as illustrations without any chemical structures were included in the obtained images, fabricated by the chemical structure editor of CS ChemDraw prior to conducting the experiments. Because we set out to extract only characters and chemical structures in this experiment, no other information was considered. Graphical data for the experiments were obtained by combining chemical structure images with the characters annotated above and below the images.

These images represent the graphical data used in the following experiments; the same characters written above and below the chemical images were used in both groups of images. The horizontal resolution of the chemical structure was set to 1260 pixels, which is the default for sample images in Microsoft Word, while the perpendicular resolution was not fixed in the original images.

### Experiment on Extracting Images

The first experiment aimed to verify whether the character and chemical structure areas were extracted correctly. Division of the character and chemical structure areas in CLArS was investigated in 450 images, including 399 images taken from the CLiDE data set and 51 images from the textbook. Some images from the two sample data sets were excluded in our experiment: images drawn in white ink on a black background, which is the reverse of normal images; images containing several structures; images drawn with abbreviated functional groups, such as -R; images that were too large to fit on a page; and images containing experimental apparatus. In this experi-



ment, the accuracy of obtaining the correct nomenclature for the extracted chemical structure was not considered. After a series of iterations, the extraction was found to be successful in 405 of the 450 samples, yielding a 90.0% success rate. In the CLiDE data set, 356 samples were extracted correctly from the 399 samples (89.2%), while in the textbook, 49 samples were extracted correctly from the 51 samples (96.1%) (Table 1). Figures 4 and 5 show some failed extractions from some images; reasons for these are given in the Discussion section.

Table 1. Correct Extraction Rates

Image Sets	Number of Samples	Number of Correct Extractions	Yield (%)
CLiDE	399	356	89.2
Text book	51	49	96.1

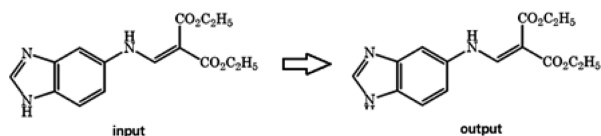


Figure 4. Partial image.

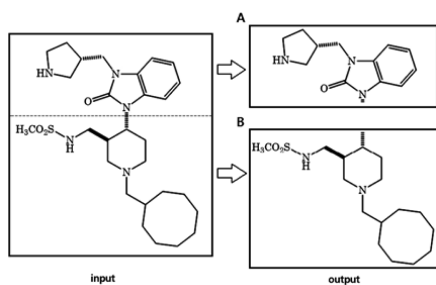


Figure 5. Image that is divided into several parts.

### Experiment on the Resulting Nomenclature for the Extracted Image

For recognition to be performed using different fonts, the structures in the CLiDE data set were drawn using the fonts available in CS ChemDraw, while those in the textbook were drawn using the fonts available in the Windows operating system. For each font, we examined whether the extracted chemical structure image was correctly identified as the corresponding compound name. In addition, the criterion for measuring the success of chemical name recognition was defined as correct answers for character strings obtained from the MolConvert conversions of both the original chemical image and the extracted chemical image. This experiment was performed on a computer running Windows 7.

### Experiment on Images Containing the Same Fonts

With the use of the CLiDE images, 172 of the 356 samples successfully extracted (48.3%) were correctly identified as the correct compound. Moreover, to investigate the misrecognition of chemical structure names, the kind and total number of elements for each chemical structure are given in Table 2.

In Table 2, the ground truth group (true) uses MDL Molfiles converted from the original chemical structures, while the output group (result) uses MDL Molfiles converted from the extracted chemical structures. The differences between the true and result values are explained in detail in the Discussion section.

Table 2. Comparison of the Number of Elements in the True and Result Images in the CLiDE Data Set

Element	True	Result	Difference
H	4	245	241
B	0	2	2
C	4886	4794	-92
N	619	530	-89
O	643	493	-150
F	81	27	-54
Na	2	0	-2
P	2	2	0
S	65	60	-5
Cl	70	74	4
Co	0	2	2
Se	1	0	-1
Br	22	4	-18
I	8	0	-8
Hf	0	10	10
Tl	0	2	2
U	0	7	7

### Experiment on Images Containing Different Fonts

The same operations were performed using the textbook images. For the textbook images, 29 of the 51 samples that were extracted successfully were identified as the correct chemical structure. The kind and total number of elements are given in Table 3. We believe that the reason for the decrease in

Table 3. Comparison of the Number of Elements in the True and Result Images in the Textbook<sup>a</sup>

Element	True	Result	Difference
H	124	82	-42
C	144	180	+36
N	4	4	0
O	49	48	-1
Cl	2	2	0

<sup>a</sup>The true and result groups were based on the same converted Molfiles as for Table 2.

correct answers for C and H in the textbook data set is that the number of elements was not recognized correctly because C and H are generally omitted in chemical structures. The differences between the true and result values are explained in detail in the Discussion section.

## DISCUSSION

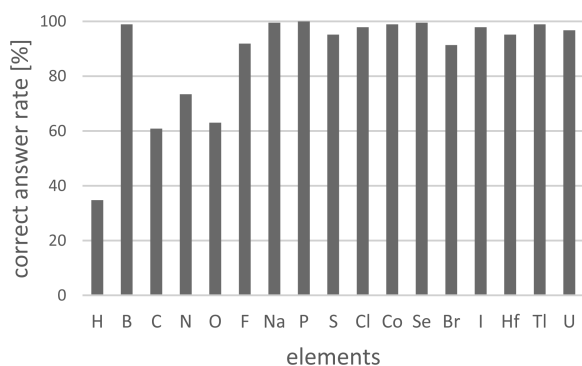
To improve the way visually disabled students learn chemistry, we constructed a new system to read aloud chemical structure names in image files. In this paper, we focused on media distributed on the Internet, such as chemical literature and patents.

In the case of documents containing both text and chemical structures, although various methods have been proposed for reading aloud text, tactile graphics have typically been used for images such as chemical structures.

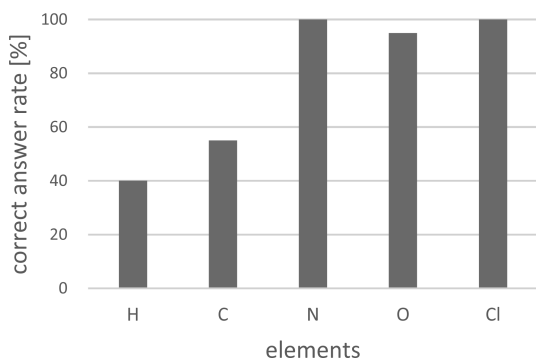
First, we investigated the extraction of text and chemical structures. In this article, we tried to improve the separation of text and chemical structures using both line and area densities. As a result, we obtained high extraction accuracy for both the CLiDE (89%) and textbook (96%) data sets. The large number of successful extractions in our system suggests that Otsu's

method is effective. Figures 4 and 5 show examples of images for which extraction failed. In our system using the density of lines, we suggest that extraction failure is caused by a drastic decrease in the density of the chemical structure images. In Figure 4, because H is connected to the lower left side of the compound with a low-density line, H is not recognized as an element in the compound. Similarly, in Figure 5, the low-density area depicted by the dashed line divides the chemical structure image into several parts. We surmise that the decrease in recognition rate of the CLiDE images originates from a misunderstanding of the bond length or number of elements in complex structures. For the extraction of images, we found that the proposed system is effective given the success rate of 90% obtained when applied to a total of 450 sample images.

Next, using the nomenclature of the extracted image, the correct recognition rate for the CLiDE and textbook data sets was about 50%. On the basis of the kind and number of elements in the Molfiles obtained by MolConvert, we identified possible reasons for failed recognition. We compared the numbers of elements in the Molfiles obtained from the original chemical images and those obtained from the extracted chemical images. We also counted the number of images for which the number of elements was equivalent in the two groups of Molfiles. The results are shown in Figures 6 and 7.



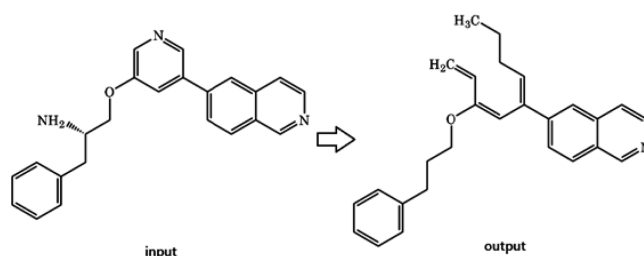
**Figure 6.** Correct answer rates for CLiDE data set (Elements with low correct answer rates are H, C, N, and O.).



**Figure 7.** Correct answer rates for textbook data set (Elements with low correct answer rates are H and C.).

From these graphs, we can see that the numbers of N, O, and Cl elements have a high probability of agreement in the textbook data set. Moreover, we also observe that the numbers of B, F, and Na elements are highly likely to match in the CLiDE data set. In particular, although many CLiDE images were used, the numbers of elements for B, Na, and P agree

perfectly. Thus, assuming that problems do not arise easily in elements with high correct answer rates, we focused on elements such as H, C, N, and O. Comparison of samples before and after the experiments shows that the number of images with increases in H is equal to that with decreases in O. Similarly, there are some images where the number of increases in H is equal to the number of decreases in N; this shows that both O and N were mistaken for H. Considering the characteristics of O and H, the end of the O on either side is thick, while the central circumference is thin; we believe that the edges on the right and left sides of the O are mistaken for the vertical bar in the H. For the characters n and h, recognition depends on whether the line segment that connects the vertical bar on either side is level or slanted and whether the system believes that recognition has been affected. An example of an original image in which the chemical structure was not correctly extracted is shown in Figure 8. In this figure, one of the bonds



**Figure 8.** Incorrectly extracted image.

of the pyridine-ring disappeared owing to misrecognition. Moreover, both the N of the isoquinoline-ring and that of the amino group connecting benzene and pyridine were misread as C.

The prototype system has been tested by eight subjects, including three totally blind individuals. Evaluation of the use of CLeArS by the three totally blind subjects (one in his 30s, one in his 40s, and one in his 60s, two of whom are authors of this paper) is particularly important. Additional details of these three subjects are given below. Mr. Suzuki, mentioned in the acknowledgments, is an engineer developing audio equipment, while Mr. Morii, who is one of the coauthors, is an Information Technology engineer. Both these individuals, who were educated in Japan and have a high school chemistry degree, can understand simple chemical names and structures. The third subject, Kamijo, who is the corresponding author, is a researcher and teacher of chemistry at a junior college. The other five subjects, who studied chemistry at a Japanese high school, are nondisabled students at a university or graduate school. The results show that the names of compounds can be recognized immediately and that the system's usefulness is not dependent on tactile graphics; instead, information is obtained by listening only.

## CONCLUSION

As supporting technology in the education of chemistry students with visual disabilities, we constructed CLeArS, which depends only on hearing, and is not dependent on tactile sensations. CLeArS can extract chemical images from documents containing chemical structures and can read aloud the chemical structure name conforming to IUPAC rules. Using CLeArS, we presented experimental results of correct extraction and conversion rates of the nomenclature for both CLiDE and

textbook images. According to these results, a recognition rate of about 90% was achieved for images in each group. Investigation of the density in the vertical direction is necessary to improve the extraction rate.

Nomenclature experiments were carried out using both the same and different fonts. Images with the same fonts achieved a recognition rate of 56%, while different fonts resulted in a decreased recognition rate of 48%. The reason that the correct answer rates for C and H decreased could be that the number of elements was not recognized correctly because C and H are generally omitted in chemical structures.

We are in the process of carrying out further experiments to collect additional evaluation data and identify improvements to the system.

Although this research and the resulting prototype system have been validated by only a small number of subjects, we have presented a first step in the creation of a method (like CLArS) to access text without resorting to tactile methods. Moreover, text containing chemical structures can easily be read aloud by the verified screen reader.

We have developed our software specifically for use by those with visual disabilities. However, because we intend information to be shared between those with and without disabilities, we do not expect the use of our software to be limited to the former group. We would like to believe that our software will have a ripple effect in various fields. For example, our software could be used in elementary educational programs or systems for beginner classes. On the other hand, it could provide an effective means for studying the development of teaching materials and searching for references by individuals in higher education.

As future work, we need to reconstruct the algorithm for image recognition and improve the system for reading aloud chemical information.

Because the use of databases will become even more important in the future, reading aloud several kinds of image files will allow those with visual disabilities to use information on various Web sites. Moreover, by increasing the extent of this research, there is the possibility that our research will be useful in the improvement of environments for those learning or working with visual disabilities.

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### Notes

The authors declare no competing financial interest.

## ACKNOWLEDGMENTS

The authors would like to thank Prof. Dr. Masaaki Tsuda of the University of Toyama, and Dr. Junya Suzuki from Sony Co. Ltd., for their insightful discussions. This study was made possible by the staff of the Hirobayashi Laboratory in the Department of Intellectual Information Systems Engineering, Faculty of Engineering, University of Toyama. Haruo Kamijo received a Grant-in-Aid for Scientific Research (KAKENHI) from the Japanese Society for the Promotion of Science (JSPS) (2013–2015, Grant-in-Aid for Exploratory Research, subject number 25590293), and is a scholarship student at the College Women's Association of Japan (CWAJ) 2013 (scholarship for the visually impaired to study in Japan).

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