R. R. Ernst has shown that the SNR improvement of white noise in a single scan performed in a total time, T_t , is equal to the SNR improvement achieved through time averaging of a signal response n times in the same total performance time; that is, $T_t = nt_s$ where t_s is the scan time of the signal averaging process. This SNR improvement over a single scan performed in time t_s is proportional to $T_1^{1/2}$. In the least squares filter proposed here, the total performance time can be thought of in terms of the number of points, N_h , in the filter function, h(t). Gated detection uses only some portion of the total signal waveform available in the given signal response cycle, whereas the least-squares filter uses the entire N_h points available to determine the signal value. Thus, the SNR improvement of the least-squares filter over gated detection is given by $(N_h/N_g)^{1/2}$, where N_g is the number of points averaged in the gated detection scheme. The gated detector employed in these experiments used a total of six points to determine the signal value. The maximum number of points used by the leastsquares filter was 512, which gives a theoretical SNR improvement of 9.2. This is in good agreement with the actual SNR improvement measured to be 10.0. A plot was also made of the SNR of each GC run vs. the number of points used in the filter-function waveform. The plot was linear, meaning better SNR is obtained by using more data points in the filter function. The limiting factor in the number of points used is

the speed with which the computer can perform the necessary operations.

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Comparison of Manual and Online Searches of Chemical Abstracts

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Manual and online searches of Chemical Abstracts on five selected topics were conducted to compare the cost effectiveness, relevance factor, and search characteristics of the two methods. It was found that the online search was more expensive when the cost calculation was based on the part-timer's salary while it was less expensive when it was based on the professional worker's salary. A universal equation to evaluate the overall cost effectiveness of the search was proposed. The equation takes into consideration such factors as relevance factor, recall factor, cost factor and time factor and gives a value of "1" when the search is most cost effective. The actual application of this equation for the five selected topics gave 0.778 for the online search and 0.736 for the manual search, which indicates that the online search is a little more cost effective than the manual search. Each method of searching has its own merits and demerits, and a practice of using a single method of searching sometimes gives an incomplete search result.

INTRODUCTION

Chemical Abstracts (CA), founded in 1907 by the American Chemical Society, is now the largest and oldest abstract journal in the field of chemistry. It deals not only with the area of pure chemistry but also with the surrounding areas of chemistry such as biochemistry, applied chemistry, and so on. It is surprising to note that a high proportion of articles dealt with by CA is rather biology oriented than chemistry oriented. A considerable number of articles can be retrieved by using biology-oriented questions.

This means that CA has become more a comprehensive information source than before and that its scope of usefulness has been expanded. It means, at the same time, that it has become more complicated than before and that it has become more difficult to search and retrieve appropriate articles.

Online information search and retrieval is widely accepted in various areas of sciences, and its usefulness and cost effectiveness as an alternative to manual searching have been examined from different points of view.1-8 A small but focused study conducted by Michaels compared the comprehensiveness of searches performed by using CA Condensates online with that of the manual searches in keyword indexes of CA.9 The results were not conclusive, but she pointed out the subject and vocabulary problems that are specific to each mode of searching.

The cost involvement of online retrieval can be discussed on such aspects as computer connect time, telephone fee, staff's salary, equipment cost, etc. There can be attempted to manipulate those variables to establish a universal formula that can be used to calculate the total online cost. A cost of the manual search should be formulated as well. And when those two types of proper formulas are established, the true comparison of the two methods of information retrieval can be done. But whether or not the establishment of those formulas is meaningful is yet to be discussed. Anyhow, what is worth being done at this moment is to obtain as many results of comparative studies as possible. A project was initiated to perform online and manual searchings using Chemical Abstracts to compare the two searchings.

METHODOLOGY

Types of Questions Used. Considering the fact that a

Table I. Search Topics

no.	search topic	abbreviation
1	blood concentration of phenobarbital	PB-B
2	blood concentration of phenytoin	PH-B
3	morphine dependency	MO-D
4	carcinogenesis of saccharin	SA-C
5	metabolism of phenobarbital	PB-M

	(Nanua)	Search)	Time Spent		(Online	Search)	Time Spent
Index	K.W.I.	C.S.I.	G.S.I.			8 204		
Search Tenn	phenobar :	246(/H,»H	Blood	/ 5	Search LogIc	S pheno S blood C 1 * 2 T 3/6/	•	70
Ab- stract Number (Re- trleve	\$	111161	111[68	40 mln	Ab- stract Number (Re- trleve			# Inira.
Ab- stroct Number (HIt)	1	:		<i>70</i> nin,	Ab- stract Number (IIIt)			55 mln.

K.W.L.:Keyword Index C.S.L.:Chemical Substance Index G.S.L.:General Subject Index

Figure 1. A filled-in report form for search results.

considerable number of biology-oriented articles are cumulated in *Chemical Abstracts* and that the searchers are pharmacy students, the following drug-related sample questions were chosen (Table I).

- (1) Search any literature that has something to do with blood concentration of phenobarbital (abbreviated as PB-B).
- (2) Search any literature that has something to do with blood concentration of phenytoin (abbreviated as PH-B).
- (3) Search any literature that reports morphine dependency (abbreviated as MO-D).
- (4) Search any literature that reports carcinogenicity of saccharin (abbreviated as SA-C).
- (5) Search any literature that reports metabolism of phenobarbital (abbreviated as PB-M).

Searching in General. Both kinds of searches were performed by fourth year pharmacy students, 134 in total. The students were divided into five groups, and one of the above-mentioned five questions was assigned to each group. They were given a 1-h lecture on the outline of the principle of online information retrieval and another 1-h lecture on Chemical Abstracts. None of the students had had any knowledge of the online information retrieval before the lecture was given. On the day when the students actually performed searching, a 1-h prelaboratory lecture was given on Dialog searching. As far as typing speed is concerned, all of the students were regarded as beginners. For the manual searching, a 1-h prelaboratory lecture was given pointing out the characteristics of each index in an illustrative way so that he/she would be able to utilize it easily. Search results of the students were averaged for each group and analyzed for the

- (A) Online Searching. Each student constructed a search equation for Ontap CA Search training file, DIALOG File 107, after the prelaboratory lecture with some help from the instructor. Then, he/she keyed in the search equation through an online terminal.
- (B) Manual Searching. Each student filled in his/her own search procedure, which is shown in Figure 1. He/she then searched for the given question by using each index. The indexes they had to use were the Keyword Index, General Subject Index, Chemical Substance Index, and Formula In-

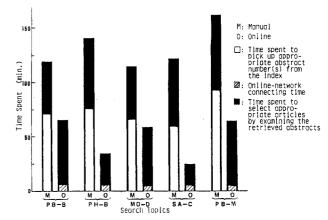


Figure 2. Comparison of manual and online retrievals in terms of time spent.

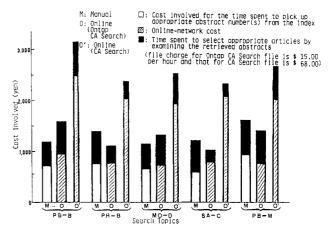


Figure 3. Comparison of manual and online retrievals in terms of cost involved [man power cost: 600 yen/h (\$2.40/h)].

dex. The search range was No. 15 and No. 16 of Vol. 87, which are the issues covered by the Ontap CA Search file. The time spent for search was measured at each step indicated in the search procedure format.

RESULTS AND DISCUSSION

The times spent for online and manual searches were compared and shown in Figure 2. The result indicates that the online search, in this particular instance, was accomplished in a time 50-100 min less than the manual search. When the time spent for the manual search was divided into two portions, one for picking up appropriate abstracts that are assumed to be relevant (or hit) not by reading the content of abstracts but by simply searching through index terms of each index used and the other for selecting relevant (or hit) articles by reading the entire content of the picked abstracts, the amount of time spent by one portion is about the same as the other portion. In these divided two portions, the first portion can be treated as a preliminary search and the second a final search because some of the abstracts picked up in the first portion can be judged to be irrelevant (not hit) when the entire content of the abstract is read.

One of the factors in which the manual search requires more time than the online search in this instance can be explained by the fact that the time required to pick up appropriate abstracts from the index is much greater than the online connect time during which the actual computer search is conducted. Another way of saying this is that cutting down the time spent, by searching quickly for example, to pick up appropriate abstracts from the index (a preliminary search)

Table II. Online Search Results

no.a	search topic	no. of postings	no. of relevant (hit) records	relevance factor (%)
1	PB-B	11	5	45.5
2	PH-B	8	5	62.5
3	MO-D	14	11	78.6
4	SA-C	2	2	100.0
5	PB-M	14	6	42.9
		49 ^b	29 ^b	59.2^{b}

^aSearch equations: (1) (Phenobarbital or RN=50-06-6) and Blood? or Concentration?); (2) (Phenytoin or Diphenylhydantoin or RN=57-41-0) and (Blood? or Concentration?); (3) Morphin? or RN=57-27-2) and (Dependence? or Addiction?); (4) (Saccharin or RN=81-07-2) and (Carcinogen? or Neoplasm or Cancer); (5) (Phenobarbital or RN=50-06-6) and (Metabol? or Enzyme). ^b Total.

shortens considerably the total time spent for the manual search.

The cost involvement was compared also between the online and manual searches and shown in Figure 3. There is no rule to apply as to what scale should be used for the calculation of man power rate. As the first trial, a scale for a part-time worker, who is paid 600 yen (\$2.40)/h and nothing else, was applied. A part-time worker is usually a housewife or a student who strictly works on part-time basis and whose pay is usually much lower than that of the full-time worker. The manual search cost was further divided into two portions, one for picking up appropriate abstract number(s) from each index used and the other for selecting appropriate articles by examining the retrieved abstract(s). The online search cost was also divided into two portions: one for the machine cost including the file usage and telephone network fees and the other for man power cost for the entire time spent. The fee for the file usage (Ontap CA Search) was \$15/h. The man power cost scale used was 600 yen (or \$2.40)/h, the same scale as in the manual search. In a real, comprehensive online search, the Ontap CA Search cannot be used because this file is designed strictly for educational purpose only. Therefore, the cost that would have been attributed if the regular CA Search file had been used was calculated by multiplying the time spent for the Ontap CA Search by the regular CA Search usage cost. When the manual search cost was compared with the online cost of Ontap CA Search, there is no significant difference between the two in the case of the part-time worker as shown in Figure 3. On the other hand, when compared with the online cost of CA Search, it was shown that the online search costs twice as much as the manual search, also shown in Figure 3. Since the use of Ontap CA Search is limited due to the limited volume coverage, only the comparison with the CA Search has reality.

For the cost comparison, the part-time worker's scale, 600 yen (\$2.40)/h, was used as the first evaluation trial. However, it is not realistic to assume that the type of person who performs a scientific literature search is a part-time worker. The types of persons who engage in the literature search will be a professor, a scientific researcher, a student, a secretary, a librarian, and so on. It would be reasonable to assume that

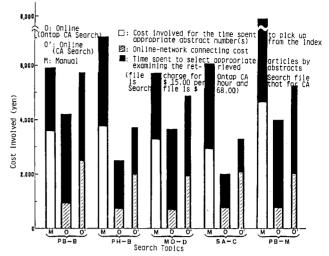


Figure 4. Comparison of manual and online retrievals in terms of cost involved [man power cost: 3000 yen/h (\$12.00/h)].

the majority of them are semiprofessional such as a librarian. a technical secretary, and so on or professional such as a medical doctor, a professor, a scientific researcher, and so on. Therefore, a man power scale of 3000 yen (\$12.00)/h, which is considered to be the hourly pay rate of the semiprofessional, was used, and the results are shown in Figure 4. Now the situation was turned around. It came out that the manual search is more expensive than the online search. Needless to say, if the search was performed by the professional people, the difference of the cost between the two cases would become more. The manual search seems to be free of charge because of the fact that the man power cost is likely to be neglected. The truth is that it is a very expensive operation, especially when it is done by the person whose hourly pay rate is high.

The online relevance factor is also examined and shown in Table II. It ranges from 42.9 to 100%, giving an average of 64.3%. To discuss the reasons why so-called noise is generated when searching has often been a topic of online search. It is mutually correlated with the so-called "drop off", which is "the failure of retrieving some of the relevant articles". The noise ratio of 50% or less should be considered as an acceptable one, especially when the ratio of "drop off" is 50% or less.

The number of retrieved relevant records varied greatly depending on which index was used. Percents of relevant records retrieved manually with various types of CA indexes, when a number of relevant records retrieved online is considered as 100%, are shown in Table III. The use of the General Subject Index was least effective and the Chemical Substance Index most. Although which index should be used is often determined by the type of search topic, it is by all means advisable to use at least three indexes listed here. In case of question 3, the result demonstrated, in particular, that the use of only the Chemical Substance Index leads to an incomplete recall of the records.

When searching CA online, there is some advantage over the manual search (Table IV). First, it is possible to search

Table III. Comparison of Search Results between the Online without Restriction and the Manual with the Index-Restricted Search

no.							ma	nual ^a			
	search		Key	word Index		Chemical tance Index		General vject Index		total	
	topic	a	b	b/a (%)	b	b/a (%)	b	b/a (%)	b	b/a (%)	
1	PB-B	5	4	80	4	80	1	20	4	80	
2	PH-B	5	4	80	5	100	2	40	5	100	
3	MO-D	11	7	64	8	73	0	0	10	91	
4	SA-C	2	2	100	2	100	2	100	2	100	
5	PB-M	6	2	33	6	100	2	33	6	100	

a, number of relevant (hit) records retrieved by the online search; b, number of relevant (hit) records retrieved by the manual search.

Table IV. Characteristics of Online and Manual Search

	online search	manual search
title search	possible	not possible
direct search for "subdivision" and "modification" terms	possible	not possible
CA Registry No. direct search	possible	not possible
systematic name search	possible	possible
types of search terms	fixed more or less	would be expanded while searching
time needed for search expenses	short	long
when searched by part-time worker (\$2.50/h) when searched by semiprofessional (\$12.50/h)	somewhat expensive reasonable	somewhat reasonable expensive

title words directly while in the manual search it cannot be done unless the title words appear in the *Keyword Index*. Second, it is possible to search words in the index subdivisions and/or modifications without referring to each index heading. Third, CA registry numbers can be used directly.

On the other hand, advantages of the CA manual search over the online search are generally considered to be as follows. It is possible to pick up better search words as the searching proceeds because the examination of the nature and scope of the index terms appearing in each index will help a searcher to select more suitable search terms than before. That is, the human flexibility of the thinking process during the manual search contributes to the betterness of searching in the manual search, and this is especially true when the structure and term list of indexes is complicated as seen in CA. Although this type of flexible search practice can be accomplished while performing online search, it is less probable to achieve a good result in this practice of online because of such factors as the limited search time, the restricted types of output, and the routinely operated mechanics.

There are several important factors involved in the literature search such as relevance factor, recall factor, search cost factor, and so on, and those factors are mutually correlated. Each factor can be represented by numerical value ranging from 0 (worst case) to 1 (best case). When we compare the two search techniques, online and manual, it is very convenient if there is a useful equation model to evaluate the cost effectiveness of each search trial. Such an equation is thus proposed and it is primarily an addition of each factor involved in the search:

$$X = (W_1A + W_2B + W_3C + W_4D)/4$$

X is a cost-effective factor of a search. A is relevance factor, which is given as

$$A = R/L$$

where R is the number of relevant records retrieved and L is

the number of retrieved records. B is recall factor, which is given as

$$B = R/T$$

where T is the total number of relevant records in the database. C is cost factor, which is given as

$$1 - \frac{\text{cost of the search in question}}{\text{most expensive cost}} \times 0.5$$

D is time factor, which is given as

$$1 - \frac{\text{time spent in the search in question}}{\text{longest time spent}} \times 0.5$$

 W_n is the weight of each factor and can be varied depending upon how important each factor is evaluated. In the cost and time factors, C and D, the cost or time ratio of the search in question is multiplied by 0.5. This is to avoid producing zero in this component, and it also has an effect to give the component the minimum value of 0.5. The further variation would be obtained by changing the weight value.

This equation was applied for the above-mentioned five instances, and the result is shown in Table V. The recall factor is calculated by considering the number of relevant records retrieved online to be the total number of relevant records in the data base. The reason for this is that dumping out all the records in the data base by means of drug name and its registry number proved that the number of the relevant records retrieved online seems to be the same as the total number of relevant records in the data base. The fact that a number of records covered by Ontap CA Search at the time of experiment was small (it contained only issues 15 and 16 of Vol. 87) gave indirect support to this hypothesis. When the weight factor of each component is set 1, which would be a reasonable value to start with, the average of the online search gave the value of 0.778, while that of the manual search was 0.736. It was then demonstrated that the online search should be a little more beneficial or cost effective than the manual search by the factor of 0.042, which may not be so significant. In case of search topic 4, the value for online search, 0.906, is significantly greater than that for manual search, 0.750. Depending on what values are used for the weight factor, it would lead to different results. The types of questions, needs of search requestor, circumstances of searching operation, and other miscellaneous factors would determine the weight value.

SUMMARY

A model equation to evaluate a cost-effectiveness of literature search was proposed. This equation was actually applied for manual and online searches of CA, where five drug-related search topics were used for the search by students. The calculation by the model equation of cost-effectiveness factors showed that the online search is a little more cost effective than the manual search, although the result may vary depending upon the values of weight factors, the salary basis of the

Table V. Cost Effectiveness of Online and Manual Searches of Chemical Abstracts (Ontap CA Search)

search topic no.	A^a		B^a		C^{a}		D^a		(A+B+C+D)/4	
	online	manual	online	manual	online	manual	online	manual	online	manual
1	0.455	1	1	0.80	0.517	0.5	0.727	0.5	0.675	0.700
2	0.625	1	1	1.00	0.732	0.5	0.876	0.5	0.808	0.750
3	0.786	1	1	0.91	0.576	0.5	0.743	0.5	0.776	0.728
4	1.000	1	1	1.00	0.727	0.5	0.898	0.5	0.906	0.750
5	0.429	1	1	1.00	0.676	0.5	0.789	0.5	0.724	0.750
									0.778^{b}	0.736^{b}

^a A, relevance factor; B, recall factor; C, cost factor; D, time factor. ^b Average.

searchers, the types of search topics, and so on.

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IDC Inorganic Chemicals Data Base. 2. Utilization of Chemical Abstracts Service Data Bases for the IDC Inorganic Chemistry Documentation System

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IDC (Internationale Dokumentationsgesellschaft fuer Chemie m.b.H., Sulzbach, Federal Republic of Germany) makes use of machine-readable data provided by Chemical Abstracts Service (CAS) for supplementing its inorganic chemistry documentation system. Data from CAS (formerly CASIA and CACON and now offered as CA Search) are brought into the format of the IDC documentation system by machine procedures and can be corrected, supplemented, or deleted intellectually if necessary. The procedures involved in this process are described. In addition to the IDC inorganic data base containing bibliographic data, inorganic compounds, their reactions, and nonstructural index terms (concepts), supplementation of the IDC GREMAS file, which correlates CA Registry Numbers with encodings used for inorganic or organic compounds, is carried out by IDC. This file enables IDC to encode a compound once only at its first appearance in the system. Furthermore, CA Concept Headings are transferred intellectually only at their first appearance into Alpha Numbers of the IDC inorganic chemistry documentation system and on further appearances are generated by computer procedures.

Since 1973, the IDC (Internationale Dokumentationsgesellschaft für Chemie m.b.H.) has made use of a special documentation system for inorganic chemistry, the construction of which was described in Part 1 of this series. 1 At the beginning, only patent information was searchable in the data base. This deficiency was criticized by many users. After the economical alternatives for extending the IDC Inorganic Chemicals System were examined, it was decided to supplement the inorganic data base by existing machine-readable versions of data bases of Chemical Abstracts Service (CAS). CAS data bases are made available for evaluation to IDC by an agreement concluded with CAS in 1975. It was the aim to employ the CAS data bases in a manner that would allow, in the final result, the searching in and construction of an inorganic chemicals data base build up analogously to that of the patent data base for inorganic chemicals.

The intellectual effort in supplementing the inorganic chemicals data base as well as the cost for additional work (keyboarding, data processing) was to be kept at a minimum. The unequivocal characterization of chemical substances in the CAS system by CA Registry Numbers made it possible that each chemical substance had to be encoded intellectually only once at the time of its first appearance and could subsequently be found in the data file. This single encoding of inorganic substances was to be supplied in the desired format to the GREMAS Register of IDC (see BMFT Research report of Schwier² and Jungblut³ on the usage of "Data of the Chemical Abstracts Service (CAS). Structural Data Base." 1979).

In order to examine the extent to which the CAS data base could be employed in creating a data base for the IDC search system, a study was conducted with the CAS tape service CA Subject Index Alert (CASIA), containing all entries necessary for constructing a semiannual CA index. In this study, only those entries were examined that had been made within a certain period for CA Section 49 (Industrial Inorganic Chemicals). The study showed that about one-third of the substance and concept information considered to be important for storage in the inorganic chemicals data base was to be found in the CA data base. Intellectual evaluation of the texts belonging to Registry Numbers or Concept Headings furnished a further third of information. The remaining information was taken from the corresponding CA abstracts.

It was concluded that CASIA was suited for supplementing the inorganic data base but not without additional intellectual evaluation of CA abstracts. Some major reasons for this are as follows:

- (1) In general, there are no CA index entries for reactants in inorganic synthesis, even when mentioned in CA abstracts. Since this information is asked for by the users of the IDC inorganic data base, it has to be added to the file. In many cases, reaction products with fractional indexes have no index entries (no own Registry Numbers) in the CA system and thus have to be added to the IDC inorganic file intellectually.
- (2) The encodings of solid solutions and mercury alloys are just two further examples for differences between the CA and IDC systems, making supplementations necessary in constructing the IDC inorganic data base. Solid solutions of