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Water Contamination with Pharmaceuticals: Data Availability and Evaluation Approach with Hasse Diagram Technique and METEOR

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Abstract:

The occurrence and fate of pharmaceuticals entering the aquatic environment has become an increasing concern for researchers and regulators in the past decade, and recent research has focused on pharmaceutical contamination from point sources, such as wastewater treatment facility outfalls. As an important initial step we are going to analyze 75 recent publications concerning the information on 12 selected drugs belonging to different groups of pharmaceuticals. Hence we cope with an initial data-matrix of the dimension 12x75. Thus, the object set contains 12 chemicals, the information base *IB* 75 attributes. This 12x75-data-matrix is evaluated by the Hasse Diagram Technique, a method derived from discrete mathematics. As this initial step leads to a diagram with many incomparabilities a data-reduction method on the attribute side is performed as the second step. Aggregation procedures of the data-matrix will be performed by applying METEOR (Method of Evaluation by Order Theory). Different weighting schemes are performed. In all approaches EES = Estinyl Estradiol is in a maximal position whereas FEN: Fenofibrate is a minimal object. This means that EES is the best scrutinized pharmaceutical and FEN the least analysed one within this information base *IB*.

1 Contamination of Water and Soil with Pharmaceuticals

Achieving sustainable development in the environmental and health sector it is absolutely necessary to keep the drinking water free of contaminants. Unfortunately several chemicals are detected in the media water: surface water, wastewater, groundwater, drinking water, sediments and soil.

The quality and availability of drinking water are essential for survival and the reality of life on earth. Problems related to water resources are often associated with developing countries only. However, water is a limited resource even in Europe.

Pharmaceuticals, hormones and endocrine disruptors have become major issues in environmental chemistry, due to their presence in environmental waters (following incomplete removal in wastewater treatment or point-source contaminations) and concern about possible estrogenic and other effects, both on wildlife and humans [Richardson, 2003] [Rooklidge 2004]. The occurrence and fate of pharmaceutically active compounds (PhACs) in the aquatic environment has been recognized as one of the emerging issues in environmental chemistry. More than 80 PhACs from various prescription classes have been detected in the µg/l-level in sewage, surface and groundwater. A systematic investigation of how effectively drinking water treatment technologies remove pharmaceutical products has found that the technologies being used in Germany appear to do a good job [Ternes 2002]. However, some of the technologies used elsewhere in the world may be letting pharmaceuticals back into drinking water. Although research shows that pharmaceutically active products are found in surface waters throughout the United States [Kolpin 2002] and Europe, there is as yet very little information on how effectively different drinking water treatment technologies remove these pharmaceutical residues. Ternes's work [Ternes 2002], which represents the most comprehensive assessment published to date also aimed at evaluating the ability of advanced wastewater treatment technologies like membranes and source separation to reduce the volume of pharmaceuticals being discharged into EU waters.

Being aware of the manifoldness of sub-topics of the contamination of environmental media with pharmaceuticals like wastewater technologies, the development of new pharmaceuticals, and the appearance of (unexpected) metabolites due to the purification process we believe that the data situation on this contamination issue should be further scrutinized.

As an important initial step we are going to analyze recent publications concerning the information on several selected drugs.

Drugs which have been detected so far belong to the following groups of pharmaceuticals:

1. Lipid regulators (Bezafibrate, Chlofibric acid, Fenofibrate)
2. Antiphlogostics (Diclofenac, Ibuprofen, Phenazone)
3. Beta blocker (Metoprolol)
4. Psychiatric drugs (Diazepam)
5. Antiepileptic (Carbamazepine)
6. Antibiotics (Roxithromycine, Sulfamethoxazole)
7. Estrogens (Ethinylestradiol)
8. Contrast media
9. Cytostatic drugs

We consider all major drug classes with the exception of contrast media and cytostatic drugs. We are analyzing the pharmaceuticals in a study of 75 recent publications. Most of the papers were published in the year 2003, a small number in 2004 since we started evaluating the situation in February 2004. Table 1 summarizes the trade names, the acronyms (ACR) and the drug groups.

Table 1: Drugs to be evaluated

Name of Drug	**ACR.**	**Drug group**
Bezafibrate	BEZ	Lipid regulator
Carbamazepine	CAR	Antiepileptic
Clofibric acid	CLO	Lipid regulator
Diclofenac	DIC	Anti rheumatic, anti-inflammatory, Antiphlogistic
Diazepam	DAP	Psychiatric drug
Ethinyl Estradiol	EES	Sex hormones, Steroid
Fenofibrate, Fenofibric Acid	FEN	Lipid regulator
Ibuprofen	IBU	Analgetic, Antiphlogistic
Metoprolol	MET	Beta blocker
Phenazone	PHE	Analgetic, Antiphlogistic
Roxithomycine	ROX	Antibiotic
Sulfamethoxazole	SUL	Antibiotic, sulfonamide

The appearance and non-appearance of drugs in any publication is coded by 1 (available) or 0 (not-available). Thus the order relation $x<y$ means that the drug y encompasses those publications which contain information about drug x. The corresponding table is given in the appendix.

As Figure 1 shows, the flood of information increases remarkably. The number of pharmaceuticals investigated in the publications ranges from 1 to 76. Most authors scrutinized the range from 5 to 10 drugs. In only five publications more than 40 pharmaceuticals were investigated. Therefore we analyze the information by means of mathematical techniques. In this first approach we are only interested in an evaluation of the 12 drugs (Table 1) with respect to their appearance in the different journals.

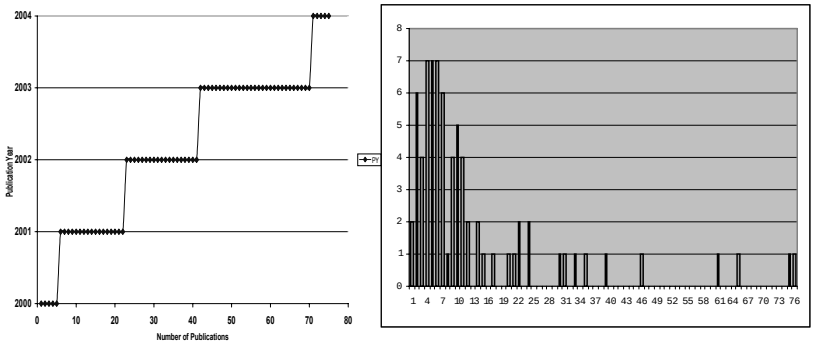

Figure 1: Number of publications on "Pharmaceuticals in Environmental Media". Publications from 2000-2004 (left), Number of Pharmaceuticals in 75 Different publications (right)

2 Mathematical Evaluation Methods

2.1 Hasse Diagram Technique (HDT)

The Hasse Diagram Technique is well explained in a variety of different environmental and chemical as well as statistical journals. In environmental chemistry Hasse Diagrams were introduced by Halfon & Reggiani [Halfon 1986]. A rather comprehensive description can be found in [Brüggemann 2001a]. A comparison of the Hasse Diagram Technique with multivariate statistical methods is given by Voigt [Voigt 2004 in press]. Therefore only some aspects are picked out, which will be useful in the subsequent application.

Consider two objects, then we say $y > x$ (with respect to the m properties of interest) if $q(x,j) \leq q(y,j)$ for all $j = 1, 2, .., m$ and there is at least one j , for which $q(x,j) < q(y,j)$ (because of the demand "for all" this definition is denoted as "generality principle").

If $q(x,j) \leq q(y,j)$ or $q(y,j) \leq q(x,j)$ for all $j=1,..,m$ then the objects x and y are comparable. The mere fact that x is comparable with y is often denoted as $x \perp y$.

Often however one finds

$q(x,j) < q(y,j)$ for one index set I' and

$q(x,j) > q(y,j)$ for another index set I'' with $I' \cap I'' = \varnothing$.

In that case, the objects x and y are incomparable and one writes: $x \parallel y$.

The order relation defined here is known as product order. There are, however many other ways to define order relations, see e.g. the publication by Ivanciuc and Klein [Ivanciuc, 2004].

The main frame of HDT can thus be formulated as the “four-point-program”:

1. Selecting a set of elements E of interest which are to be compared. The so-called ground set.
2. Selecting a set of properties IB, by which the comparison is performed, called the information base.
3. Find a common orientation for all properties; according to the criteria they are assigned.
4. Analysing $x,y \in E$ whether one of the following relations is valid:
    - $x \sim y$ (equivalence, we call the corresponding equivalence relation R, the equality of two tuples $\mathbf{q}(x)$, $\mathbf{q}(y)$),i.e. $q(x,j) = q(y,j)$ for all $j = 1,...,m$.
    - $x \leq y$ or $x \geq y$ (comparability, often called a comparability relation)
    - $x \| y$ (there is an incomparability in the data of x and y”).

A set E equipped with an order relation $\leq$ is said to be an ordered set (or partially ordered set) or briefly "poset" and is denoted as $(E, \leq)$. Because the $\leq$-comparison depends on the selection of the information base (and of the data representation (classified or not, rounded, etc.) we also write (E, IB) to denote this important influence of the IB for any rankings [Brüggemann 2002].

Sometimes it is useful to refer to the quotient set, which is induced by the equivalence relation of equality, R (see for details: Brüggemann [Brüggemann 1999]). As usual we write E/R for the quotient set, and $(E/R, IB)$ for the partially ordered quotient set.

If disjoint subsets of E, E_{i1}, E_{i2} can be found such that for $x \in E_{i1}$, $y \in E_{i2}$ no $x \perp y$ can be found then these subsets with the inherited order relation are called (isolated) hierarchies or -if only one object (one equivalence class) constitutes a part of the Hasse Diagram - an isolated element. Different hierarchies indicate quite specific data structures.

In order to interpret a Hasse Diagram some further terms concerning its structure have to be introduced:

A chain is a set of mutually comparable objects. An antichain is a set of mutually incomparable objects. An articulation point is an element of $E/\mathcal{H}$ whose elimination would increase the number of hierarchies. If there are articulation points, then the Hasse diagram can almost be separated in hierarchies. This means that the identification of articulation points helps to discover specific data structures within the data matrix. [Voigt et al. Journal Analytical and Bioanalytical Chemistry, 2004]. Levels: a first screening and a partitioning of

set E according to increasing values of the attributes. They are defined by the longest chain within the Hasse Diagram (see below). Not unique from the point of view of order theory, but uniquely defined, if additional rules are introduced (for example: conservativity, i.e. if HDT objects are assigned to the highest possible level). The set of levels together with the $\leq$ -relation forms a new poset $(L, \leq)$, which represents a chain over all objects of L, i.e. a total order. Both, the empirical poset $(E, \leq)$ and $(L, \leq)$ are related by an order preserving map. A rather important tool is the so-called W-Matrix. It is a measure of dissimilarity of different posets. For details see Brüggemann et al. [Brüggemann 2001a], [Brüggemann 2002], [Brüggemann 1999].

The WHasse program is developed, improved and updated by Rainer Brüggemann (a brief technical information about the WHasse-program, written in DELPHI, can be found in Brüggemann et al. [Brüggemann 1999]) and is available for non-commercial use from the second author. For commercial applications it is recommended to contact the company Criterion – Evaluation and Information Management [Criterion 2004].

2.2 METEOR (Method of Evaluation by Order Theory)

Aggregation procedures of the data-matrix will be performed by applying METEOR (Method of Evaluation by Order Theory). The basic idea is that subsets of IB can be combined by weighted sums; see Brüggemann et al. [Brüggemann 2001b]. Therefore the columns of the data-matrix (rows: the elements, columns the attributes) must be considered as vectors of a linear space. In order to combine them freely, a common scaling level must be assumed. Formally an embedding onto an appropriate metric space must be performed, which, however, needs a careful analysis of the scale level of the attributes. Each positive monotonous combination of, say, two attributes, leading to a "superattribute" corresponds order theoretically to an order preserving map. One may see this as "climbing up" a hierarchy of criteria: Basically a very detailed study is possible by means of a large set of indicators. Often indicators can be grouped as for example toxicities of different species may be aggregated to an ecotoxic potential. This conceptual grouping has its counterpart by numerical aggregation of indicators. Here the weighted sum is selected as aggregation procedure. Usually the aggregation is done step by step, therefore the role of weighting can be traced back, when the final result, a linear order, is obtained. Furthermore, checking the local incomparability of any element $x \in E/R$, i.e.

$$U(x) := \text{card}\ \{y: y \parallel x\ ,\ y,x \in E/R\}$$

it is possible to identify weight-sensible and weight-insensible elements of the ground set *E* and *E/R*, resp., see Brüggemann et al. [Brüggemann 2001a]. If the attributes of a set of objects are considered as entries of a data-matrix then it might be useful to briefly discuss possible aggregations (often just linear combinations) of the entries q(x,j) of the matrix.
There are three possibilities, which are discussed in Table 2:

Table 2: Combination of the entries of the data-matrix

$\lambda_{j1} \cdot q(x, j1) + \lambda_{j2} \cdot q(x, j2) + \ldots$	Combination of attributes	METEOR, hierarchy of indicators, different scale level might be combined
$\mu_x \cdot q(x, j) + \mu_y \cdot q(y, j) + \ldots$	Combination of objects, leading for example to "pseudo-objects"	PREPROCESSING, for example by object reduction processes. For example classification as discussed by Brüggemann, Bartel, 1999. Not needed in many applications of HDT
$f(q(x, j1), q(x, j2), q(y, j1), q(y, j2))$	Combination of both	PREPROCESSING, for example Cluster analysis based on distances, see for example Luther et al., 2000

q = attribute or indicator
x,y = objects
j1,j2 = indicate specific indicators or attributes of *IB*
μ,λ = scalars

3 Application of the Hasse Diagram Technique on the 12x75 Data-matrix

12 pharmaceuticals (objects) are evaluated with 75 publications (attributes) applying the data-driven evaluation method, HDT. It was found that the pharmaceuticals CAR, CLO, DIC, SUL, ROX and IBU show optimal results, i.e. they are the most often represented ones in publications. These objects are proper maximal objects that means they have lower neighbours but no higher ones. FEN shows bad results in comparison to all other pharmaceuticals. It is a minimal object. The pharmaceuticals BEZ, DAP, EES and PHE are so-called isolated objects. They cannot be compared to any other object. Hence six proper maximal, one proper minimal and four isolated objects are found in the diagram.

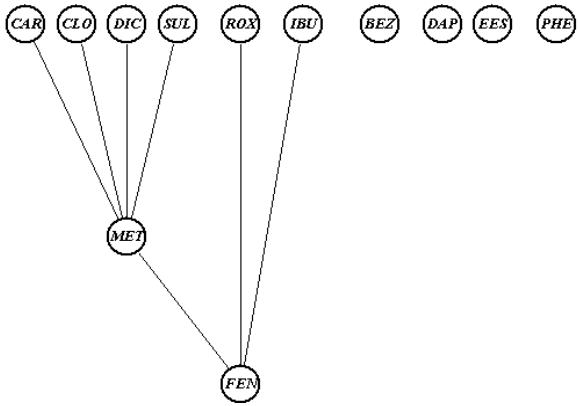

Figure 2: Hasse Diagram of 12x75 Data-matrix

Differences concerning the numbers of successors can be detected in the diagram, e.g. the maximal objects CAR, CLO, DIC, and SUL are connected and hence comparable with two other objects, namely MET and FEN, whereas the maximal objects ROX and IBU are connected with only one other object, namely FEN. Applying an order preserving map φ: $(E/R, IB) \rightarrow$ {Level} we find:

Level 1: {CAR, CLO, DIC, SUL, ROX, IBU}

Level 2: {MET}

Level 3: {FEN}

Level 1 < Level 2 <Level 3

"good" "bad"

Furthermore for example FEN is the only articulation point. By elimination of the object FEN two additional isolated elements would appear. All in all the Hasse Diagram has only a poor structure, i.e. the number of comparabilitiy relations is low. The next logical step is therefore to perform data reduction procedures e.g. logical aggregations of attributes.

4 Application of METEOR

4.1 Weighting schemes

The original data-matrix of 12 pharmaceuticals (objects) and 75 parameters (attributes) will be subject to several logical aggregation steps. The aim of the aggregation procedure which can be performed by applying the Hasse Diagram Technique Program [Brüggemann 2002] is

to get after a series of enriched partial orders finally a unique prioritisation scheme. Note that the attributes are now considered as continuous variables with a range [0, 1].

Several different weighting procedures are considered and performed (Figure 3).

1. Aggregation to get three super indicators concerning analytical journals (ANAL), the scientific journal Environmental Science and Technology (ESTE), and miscellaneous journals (MISC) (Section 4.2.1)
2. W-Matrix: 1 attribute is left out, all other 74 attributes are kept. Based on this finding, the remaining 74 attributes are equally weighted, whereas the weight of the omitted attribute is formally considered as 0. This is an example of an extreme case of weighting (Section 4.2.2)
3. Two different weightings, normalization to 1, n=75 (Section 4.2.3)

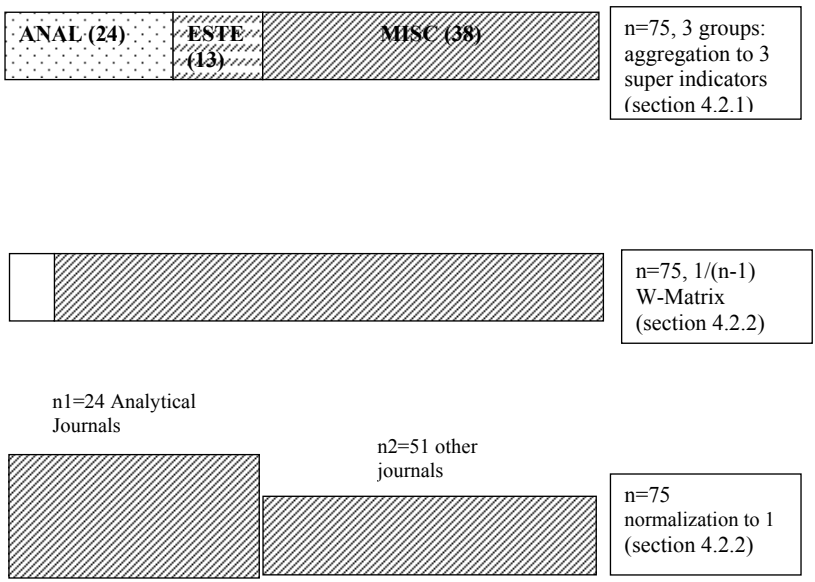

Figure 3: Different Weighting Schemes

4.2 Results from Different Weightings

4.2.1 Equal Weights of Analytical and Environmental Journals

The aggregation of the data-matrix will be performed and the results presented by the application of METEOR . The attributes encompass scientific journals which have different focuses. We aggregate the three main analytical journals: Analytical Chemistry, Journal of Chromatography A and Trends in Analytical Chemistry into one super indicator, named ANAL. The second one is given by the journal Environmental Science and Technology (ESTE) whereas the third super indicator encompasses all the other journals (MISC). Hence we cope with three aggregation groups; where each of the following super indicators "ANAL", "ESTE", and "MISC" are calculated by a sum with equal weights. For example:

$$ANAL = \sum_{j=1}^{j=24} w_j \cdot q_j \quad q_j \in IB_{AnalyticalJournals} \quad w_j = 1/24$$

$$IB_{AnalyticalJournals} = \{P03, P07, ..., P32\ \} \subset IB$$

Analogously:

$$ESTE = \sum_{j=1}^{j=13} w_j \cdot q_j \quad q_j \in IB_{ESTE} \quad w_j = 1/13$$

and

$$MISC = \sum_{j=1}^{j=38} w_j \cdot q_j \quad q_j \in IB_{MISC} \quad w_j = 1/38$$

Thus 75 attributes were grouped to

- 24 publications in analytical journals: ANAL
- 13 publications in Environ. Sci. Tech.: ESTE
- 38 publications in miscellaneous journals: MISC

and we get a new information base, consisting of three “superattributes”, called IB_3.

A lot of visible changes took place comparing the original Hasse Diagram of the 12x75 data-matrix (Figure 2) with the reduced 12x3 data-matrix (Figure 4). The enhancement of the levels (corresponding to a maximal chain of 7 objects (FEN < MET < PHE < SUL < CAR < IBU < DIC (or EES)) and of comparabilities is enormous (a drastic enrichment of partial order!). Now no isolated object is found in this diagram. The former isolated object EES is a maximal object now and has 9 successors. Obviously the isolation of EES under the original *IB* might be interpreted as an effect of appearance or non-appearance of journals in the same

group and thus might be regarded as of minor importance. The other two maximal objects also encompass many successors. DIC has also nine successors whereas CLO has 8 ones. The maximal chain FEN< MET < … < DIC may be striking. Taking a look on Table 1 one sees that this chain contains different types of drugs. Thus, one may ask what is in common for these objects: The common property is its poor representation in the journal ESTE. Obviously these drugs are of more interest for journals with analytical background or of general environmental concern.

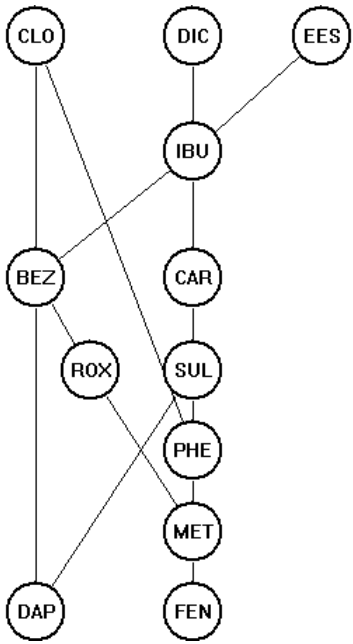

Figure 4: Hasse Diagram of IB_3= {ANAL, ESTE, MISC}, 12x3 Data-Matrix

4.2.2 Aggregation by Different Weights, Normalisation to 1

The so-called W-matrix describes the influence of the attributes on the Hasse Diagram. For further reading we recommend a recent article of Brüggemann et al [Brüggemann 2002]. The W-matrix is calculated for all objects given in the original diagram in Figure 2. It reveals that the attribute 48 (publication Ternes et al., Ozonation: A Tools for Removal of Pharmaceuticals, Contrast Media and Musk Fragrances from Wastewater, Water Research 37, 1976-1982, 2003) is the most important attribute in this approach. The reason is that the

author analyses all chosen pharmaceuticals with the exception of EES. Ethinyl Estradiol is considered to be of major importance by most other authors of the regarded publications. Four changes take place leaving out this attribute (diagram not shown).

After leaving out attribute No. 48 (P48) the next logical step might be the aggregation of all remaining 74 attributes 1/74 = 0,01351 and the setting of P48 = 0. The linear order Hasse Diagram is given in Figure 5, left hand side.

Another step towards a linear order is to combine the attributes of *IB* by different weighting schemes: One might for example be more interested in analytical journals than in environmental ones or verse visa. In order to do this the "ESTE" and "MISC" are put together as "ENVI" journals with the same weights. Thus the problem is reduced to weight 75 attributes as follows:

One group, belonging to ANAL and consisting of n1 = 24 journals gets the weight w1, and the other group “ENVI” and consisting of n2 = 51 journals gets another weight, namely w2.

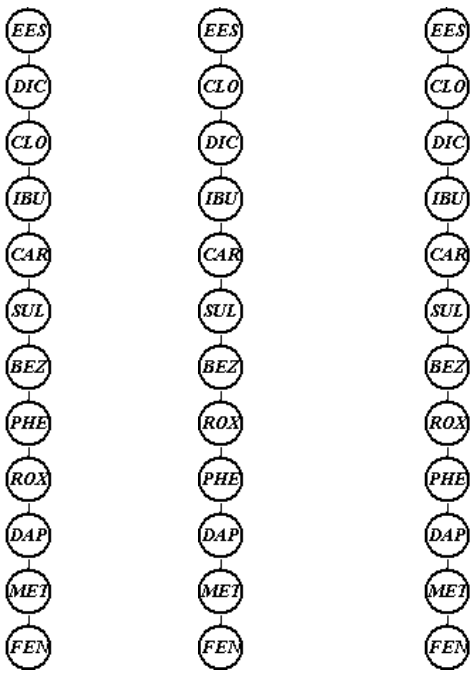

Figure 5: Hasse Diagram P48=0 and all other 74 objects 1/74 (left), middle and right: Analytical and Environmental journals aggregated with different Weights (see text)

The preference among the two journal's subsets will be expressed by g12.
Therefore:

$$w1 = g12 \cdot w2$$

If, for example, g12 = 2, then the weight of the first group is twice the weight of the other group.
At this stage, the weight on the level of attributes is still unknown. Let now be n1 the number of attributes in the first, and n2 that of the second subset (the subsets are disjoint and their union equals *IB*) and assume the same weights for the attributes within each subset of *IB*.
Demanding:

$$n1 \cdot w1 + n2 \cdot w2 = 1$$

and together with the preference equation, we arrive at the following expressions:

$$w1 = \frac{g12}{n1 \cdot g12 + n2} \qquad w2 = \frac{1}{n1 \cdot g12 + n2}$$

Let us consider within the first exercise the Analytical journals to be more important than the Environmental journals, g12 must be selected > 1. For g12, arbitrarily the value 2 is given, then:

g12 = 2
n_1 = 24 Analytical Journals
n_2 = 51 Environmental Journals

w_1 = (weight of Analytical Journals) = 0.02020
w_2 = (weight of Environmental Journals) = 0.01010
The corresponding Hasse Diagram is given in the Figure 5 in the middle section.

Alternatively we weight the environmental journals double with respect to the analytical journals, i.e. g12=0.5.

g12 = 0.5

Then, evaluating the same formulas, but taking into regard the modified preference g12 we arrive at:

w1 = (weight of Analytical Journals) = 0.0079

w2 = (weight of Environmental Journals) = 0.0159

The corresponding Hasse Diagram is given in the Figure 5, right hand side.

The ranking of the objects EES>IBU>BEZ>ROX>MET>FEN of the 12x3 data-matrix (partial order) is also kept in the linear order diagrams, which clearly demonstrates the main advantage of METEOR: It is systematically based on a sequence of order preserving maps, which can be graphically displayed as Figure 6 shows:

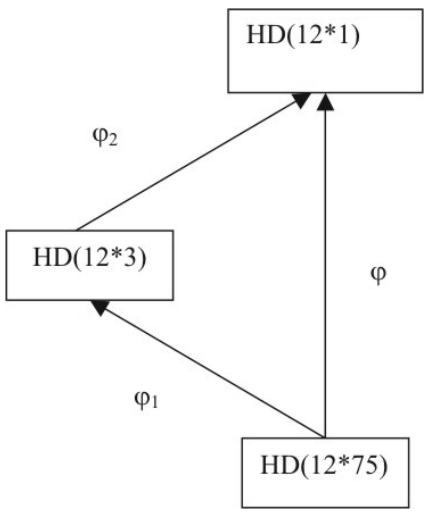

Figure 6: Composition of Order Preserving Mappings must be Consistent. The steps to and from the intermediate state "HD(12*3)" must be consistent with the aggregation in one step. The notation HD(12*k), k=1,3,75 refers to the corresponding data matrices.

4.3 Summary of Main Results

Several differences can be seen when reducing the initial 12x75 data-matrix applying the METEOR method. In our examples we reduced the data-matrix by different weighting methods. The Hasse diagram of the original 12x75 data-matrix (Figure 2) shows only 3 levels and a huge number of incomparabilities and a small number of comparabilities. The diagram of the 12x3 data-matrix in Figure 4 (equal weighting procedure aggregation of the 75 attributes to three super-attributes) is well structured into 7 levels and gives more comparabilities than incomparabilities.

The aggregation by different weights, normalisation to 1, implies linear order diagrams. It is striking that the two Hasse diagrams with different weights show the same linear orders. There is no difference if we weight the analytical journals twice than the environmental journals or the other way round. With respect to the presence of pharmaceuticals in environmental media this does not make any difference. This means that all journals treat the same pharmaceuticals only different aspects of the topic, the analytical journals go more into depth in the analytical methods whereas the environmental journals take a look at the monitoring side or biodegradation side of the issue.

In the diagram in which the object P48=0 (Figure 5 l.h.s.) two changes in positions DIC-CLO and PHE-ROX are detected. EES = Estinyl Estradiol is always in a maximal position whereas FEN: Fenofibrate is always a minimal object. This means that EES is the best scrutinized pharmaceutical and FEN the least analysed one within this information base *IB*.

5 Discussion and Outlook

A main drawback of HDT is that quite often the order relations are very poor. This is due to the fact that no compensation among attribute values is allowed. That means a “good” value with respect to one attribute cannot compensate a “bad” value with respect to another attribute. However, quite often attributes can conceptually be grouped with each other because they have a similar meaning. Thus it makes sense to define “super attributes” which neglect differences on a very detailed level of consideration and which correspond to a higher point of view in the hierarchy of the criteria. If the algorithmic aggregation to superattributes is done by a positive monotonous function (keeping the orientation of the attributes), then the results are to be considered as images of an order preserving map. Thus a step by step aggregation allows a systematical analysis along the hierarchy of criteria. In this paper the chemistry of pharmaceuticals is of interest as the occurrence of drugs becomes more and more

important in environmental media. This fact has its counterpart in the publishing activity and here the question is answered how pharmaceuticals can be evaluated just by the occurrence in different journals. The Hasse diagram with 12 objects (pharmaceuticals) and 75 attributes (publications) is rather poorly structured. Only few order relations are found which make evident that it is not very probable that the occurrence of one drug in one publication implies the occurrence of another drug in the same publication.

If, however, the journals are grouped then a drastic enrichment of order relations occur which is clear from a mathematical point of view but which also shows that there are common interests on pharmaceuticals either from an analytical point of view, or from a theoretical point of view or from a general environmental point of view. According to different weighting schemes one finally ends up in a linear order that is a member of the set of linear extensions. Thus the study of linear extensions becomes an important topic and will be followed in our future research within this data-matrix. The topic of linear extensions is treated in other publications of this specific issue of *MATCH Communications in Mathematical and in Computer Chemistry*.

Additionally we will focus on the content concerning pharmaceuticals of the journal articles in future evaluation approaches. The occurrence in different environmental media like surface water, groundwater, drinking water, sewage sludge, soil etc. will be looked upon. Although the contamination of water with pharmaceuticals is considered to be an extremely important topic for the future of our drinking water, little is done to purify the water from these pharmaceuticals. A recent study conducted by the US Geological Survey and the Centers for Disease Control and Prevention, 24 water samples were collected at selected locations within a drinking-water-treatment (DWT) facility and from the two streams that serve the facility to evaluate the potential for wastewater-related organic contaminants to survive a conventional treatment process and persist in potable-water supplies [Stackelberg 2004]. Further research is urgently needed and should be initiated also by evaluation approaches with environmetrical and chemometrical methods as for example performed in this paper.

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Appendix: 12*75 data matrix used in this evaluation study

Publ.\Pha	BEZ	CAR	CLO	DIC	DAP	EES	FEN	IBU	MET	PHE	ROX	SUL
P01	0	0	0	1	0	0	0	0	0	0	0	0
P02	1	1	1	1	0	0	0	1	0	0	0	0
P03	0	1	0	1	1	1	0	1	0	0	0	1
P04	0	0	0	0	0	1	0	0	0	0	0	0
P05	0	0	0	0	0	1	0	0	0	0	0	0
P06	0	0	0	0	0	1	0	0	0	0	0	0
P07	0	0	0	0	0	0	0	0	0	0	0	1
P08	1	1	1	1	1	1	1	1	1	1	1	1
P09	1	1	1	1	0	0	1	1	1	1	1	1
P10	0	0	1	1	0	0	0	1	0	0	0	0
P11	0	1	0	0	0	0	0	0	0	0	0	0
P12	0	0	0	0	0	1	0	0	0	0	0	0
P13	0	0	1	1	0	0	0	1	0	0	0	0
P14	0	0	0	0	0	0	0	0	0	0	1	1
P15	1	1	1	1	0	0	0	1	0	0	0	0
P16	0	0	0	1	0	0	0	1	0	0	0	0
P17	0	0	0	0	0	1	0	0	0	0	0	0
P18	0	0	0	0	0	1	0	0	0	0	0	0
P19	0	0	0	0	0	1	0	0	0	0	0	0
P20	0	0	0	0	1	0	0	0	0	0	0	0
P21	0	0	0	0	0	0	0	0	0	0	0	0
P22	0	0	1	1	0	0	0	1	0	1	0	0
P23	0	0	0	0	0	1	0	0	0	0	0	0
P24	0	0	0	0	0	1	0	0	0	0	0	0
P25	0	0	0	0	0	0	0	0	0	0	0	0
P26	0	1	1	1	0	1	0	1	0	1	0	1
P27	0	0	0	0	0	0	0	0	0	0	0	0
P28	0	1	0	0	0	0	0	0	0	0	0	0
P29	0	1	1	1	0	0	0	0	0	0	0	0
P30	1	0	1	1	0	0	0	1	0	0	0	0
P31	0	0	0	0	0	0	0	0	0	0	0	0
P32	0	0	0	0	0	1	0	0	0	0	0	0
P33	0	0	0	0	0	1	0	0	0	0	0	0
P34	0	0	0	0	0	0	0	0	0	0	0	0
P35	0	0	0	0	0	0	0	0	0	0	0	0
P36	0	0	0	0	0	0	0	0	0	1	0	0
P37	1	1	1	1	1	1	1	1	1	1	1	1
P38	1	1	1	1	1	1	0	1	0	1	1	0
P39	0	0	0	0	0	0	0	1	0	0	0	0
P40	0	0	0	0	0	1	0	0	0	0	0	0
P41	0	0	0	0	0	0	0	0	0	0	0	0
P42	0	0	0	0	0	0	0	0	0	0	0	0
P43	0	0	0	0	0	1	0	0	0	0	0	0

P44	0	0	0	0	0	0	0	0	0	0	1	0
P45	1	1	1	1	0	1	0	0	1	1	1	1
P46	1	1	0	1	1	1	0	1	0	0	1	1
P47	0	0	1	0	0	0	0	0	0	0	0	0
P48	0	1	1	1	0	0	1	1	1	0	1	1
P49	0	0	0	0	0	0	0	0	0	0	0	1
P50	0	0	1	0	0	1	0	1	0	0	0	0
P51	1	1	1	1	1	0	1	1	1	1	1	1
P52	0	0	0	0	0	1	0	1	0	0	1	1
P53	0	0	0	0	0	1	0	0	0	0	0	1
P54	0	0	1	0	0	0	0	0	0	0	0	0
P55	1	0	1	0	1	0	0	0	0	0	0	1
P56	0	0	1	1	0	0	0	0	0	0	0	0
P57	0	0	0	0	0	1	0	0	0	0	0	0
P58	0	0	0	0	0	1	0	0	0	0	0	0
P59	1	1	1	1	0	0	0	0	0	0	0	0
P60	0	0	0	1	0	0	0	0	0	0	0	0
P61	0	0	0	0	0	1	0	0	0	0	0	0
P62	0	1	1	1	0	0	0	1	0	0	0	0
P63	0	0	0	0	0	1	0	0	0	0	0	0
P64	0	0	0	0	0	0	0	0	0	0	0	0
P65	0	0	0	0	0	0	0	0	0	0	0	0
P66	0	1	1	1	0	0	0	0	0	0	0	0
P67	0	0	0	1	0	0	0	1	0	0	0	0
P68	0	0	0	0	0	1	0	0	0	0	0	0
P69	1	0	1	0	1	0	0	1	0	0	0	0
P70	0	0	0	0	0	1	0	0	0	0	0	0
P71	0	0	0	0	0	0	0	0	0	0	0	0
P72	0	0	0	0	0	0	0	0	0	0	0	0
P73	0	1	1	1	0	0	0	1	0	1	0	0
P74	1	1	1	1	0	1	0	0	1	1	0	1
P75	0	0	0	0	0	0	0	0	0	0	0	0

Explanation of abbreviations: Publ: Publication, Phar. = Pharmaceutical, P = Publication