USE OF DESCRIPTOR FINGERPRINTS TO SIMILARITY AND CLUSTER ANALISYS OF BIODIESEL FUELS ON THE BASIS OF THEIR COMPOSITION AND PROPERTIES.

INTRODUCTION OF FUZZY DESCRIPTOR FINGERPRINTS.

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ABSTRACT: A novel approach for similarity search of different objects, *fuzzy descriptor fingerprints* has been devised. Each cluster is characterized by a fuzzy descriptor fingerprint which is formed of real values instead of Boolean values *0*=false and *1*=true. A novel similarity index for similarity comparison between Boolean and fuzzy fingerprints, *Fuzzy Factor* (FF) has been introduced. This method was exemplified with similarity and cluster analysis of biodiesel fuels.

Keywords: fingerprints, fuzzy descriptor fingerprints, clustering, Fuzzy Factor (FF), biodiesels.

INTRODUCTION

The present paper introduces a novel chemometric approach of a new type of descriptor fingerprints - *fuzzy descriptor fingerprints* applied to the problem of classification of biodiesel fuels. Descriptor fingerprints approach devised by one of the authors (IB)(1) has been previously successfully applied to the solution of the problem of discrimination between allergens and non-allergens (2) and clustering of biodiesels (3) by using the Butina method (4). With the present introduction of the fuzzy descriptor fingerprints, each cluster is assigned with a fuzzy fingerprint.

Biodiesel fuel is composed by methyl esters of long chain fatty acids (FAME) produced from plant oils, animal fats and other lipids [5-7]. As a "green" fuel biodiesel has a series of advantages over petro-diesel fuels such as their derivation from renewable feed-stock, biodegradability, non-toxic and essentially free of metals, sulfur, carcinogenic aromatics fuel as well as low greenhouse effect and a positive energy balance.

Feed-stock availability for biodiesel production depends on the geography, climate and economics of different countries. At present, the dominant feed-stock (about 80 %) is vegetable oils, namely soy bean oil in USA, rapeseed and sunflower oil in Europe and palm oil in Southeast Asia. Other feed-stock having real or potential commercial interest are animal fats, non-edible and waste oils. Traditional for Bulgaria feed-stock are sunflower and rapeseed oils.

Since biodiesel is a mixture of *F*atty *A*cid *M*ethyl *E*sters (FAME), its properties depend on the chemical structure of the individual FAME and their contents (FAME profile). FAME profiles of biodiesel are influenced by the stocks and origin of the oils used [5,7,8] and can be obtained by chromatographic methods [9-13] providing valuable multi-component information. So, FAME profiles appears to be an instrument for a selection of feed-stock to produce fuels with certain properties [8,14], for investigations [15,16], and for fuel spillage and remedial actions in the environment [17,18].

THE DESCRIPTOR FINGERPRINT APPROACH.

Fingerprints in Chemoinformatics are primarily developed to characterize chemical structures within the various similarity search procedures [19-21]. The latter are usually formed in two ways. In the most popular way an array of structural fragments (structural keys), e.g. 1024 is created. A fingerprint is a string or binary array of Is and Os. The elements of the fragment array are juxtaposed to the fingerprint array elements having one-to-one correspondence between fragments and the array elements (see Figure 1). Each studied structure is further fragmented and analyzed for the presences or absence of fragments from the fragment array. In the case of presence of such a fragment a number (bit) I is put into the corresponding position (element) of the fingerprint string (bit) arrayand vice verse in the case of the absence of the corresponding fragment a O is put into the corresponding location within the fingerprint. It should be mentioned that the Daylight company has developed

another type of fingerprints - *hashed fingerprints*[22].However this approach is out the scope of this work and will not be discussed here.

The fingerprints are usually employed in QSAR/QSPR for similarity search and clustering of structures. (Figure 1). Two chemical structures are compared for similarity by comparing their fingerprints by using any similarity measures available in literature [23,24]. For our further investigation we use the well-known Tanimoto [25] similarity index (TI) having the following form:

$$TI = N_C / (N_A + N_B - N_C) \tag{1}$$

where N_A is the number of *I*s in the first structure fingerprint*A*, N_B -is the corresponding number of the second structure fingerprint*B*, and N_C is the number of *I*s common toboth structure fingerprints, i.e., *I*s being in the same position of the compared fingerprints. This index takes real values between 0.0 and 1.0. The larger is the value the most similar are the two structures. A comprehensive description of Tanimoto index is given in [23,24]. It is clear that the structural fingerprints incorporate Boolean logic, *I*=true and *0*=false.

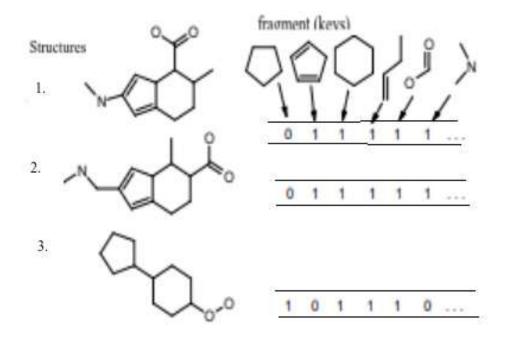


Figure 1. Formation of structural fingerprints for three structures.

Our idea was to employ descriptors instead of structure fragments in the formation of the fingerprints. A *descriptor fingerprint* is created by determination an interval for each descriptor within the fingerprint array and precision of its possible

values, e.g. an initial value (let us call it *initValue*) and ending value (*endValue*) and a precision step (resolution) *resValue*. Hence, for each descriptor its interval is divided into N=(initValue-endValue)/resValue discretefingerprint array elements (sub-intervals). The concatenation of all the descriptor elements forms the *descriptor fingerprint* itself. Further, in the course of descriptor creation for an object the program determines in which element (sub-interval) the current descriptor value falls by putting *I* in this element, the other descriptor elements remaining zeros. The formation of a descriptor fingerprint is illustrated in **Figure 2**.

This approach can be applied both to chemical structures and to various other chemical and non-chemical objects. It has been applied to discrimination between allergen/non-allergen food proteins [2], and to biodiesel fuels in our case. It obviously extends the area of application of the fingerprint method outside the chemical structure description, even outside chemistry, by using any physical, chemical, and biological as well as other user defined properties for descriptors of forming the descriptor fingerprint. In cases of chemical structures the structural fingerprints can also be concatenated to the descriptor fingerprints, thus both the chemical structure and its properties to be characterized by a common fingerprint. Accordingly, it allows the inclusion of all information available to the similarity perception process.

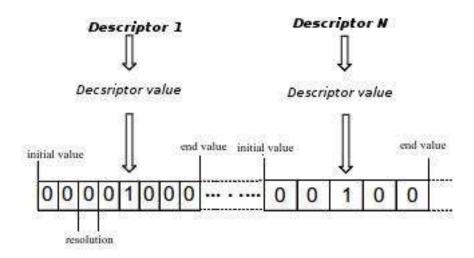


Figure 2. Formation of a descriptor fingerprint.

The descriptors forming a descriptor fingerprint can be both real values or some Boolean values indicating the presence or absence of a feature (any color, presence or absence of a property, chemical group, etc.). These discrete descriptors take one element of the fingerprint array, being either *1* or *0*. A general requirement is the quality of the descriptors to describe uniquely the studied objects and being well discriminating. Here the values of the individual FAME profiles for each biodiesel probe (case)

have been used as descriptors. Two types of descriptors have been used ones having realnumerical values and indicator ones indicating the presence (1) or absence (0) of a property.

INTRODUCTION TO FUZZY DESCRIPTOR FINGERPRINTS.

As mentioned above the fingerprint approach reflects the classical Boolean logic (1=true and 0=false). We shall call these fingerprints Boolean fingerprints. However, in the case of any type of clustering we have in many cases the 1s falling in different positions within adescriptor interval for different objects of the same cluster. Hence, our aim was to reflect this fact by using fuzzy instead of Boolean logic. Fuzzy logic was developed by Zadeh [26]. In place of discrete values 1 and 0, here we have real values between 0.0 and 1.0, say, we can have a value of 0.17 (17%) and respectively 0.83 (83%) instead 0 and 1. Accordingly, at each element of any descriptor interval (as mentioned above the descriptor interval is devided into sub-intervals) we will have real values between 0.0 and 1.0.

For the formation of the fuzzy fingerprints, in our case, we have created clusters as described in the Experimental section. For each such a cluster the program sums all the *I*s of all cluster fingerprints falling in each fingerprint array element (descriptor sub-interval). Let the sum being denoted as S_{el} . In as much as, each descriptor must have value *I* we delete the S_{el} sums of each sub-interval element to the number n_d of all *I*s falling in the descriptor interval. Hence, the fuzzy fingerprint array element values are as follows (see **Figure 3**):

$$s_d = \frac{\sum_{fps} 1s}{n_d}$$

Thus, each separate cluster consisting of a number of *Boolean fingerprints* is represented by one *fuzzy fingerprint*. This approach has an additional advantage in the case of large databases. By using cluster fuzzy descriptor fingerprints the number of the database fingerprints is reduced to the number of the clusters instead to the number of the objects/Boolean fingerprints. Accordingly, the similarity comparison is carried out between one or more query object Boolean fingerprints and the fuzzy fingerprint representing the corresponding clusters. Here, we cannot use the Tanimoto index as a measure of similarity. Hence, we introduce a new *Fuzzy Factor* (*FF*)given with relation (3):

$$FF = 1.0 - \frac{\sum_{d} (1.0 - S_d)}{N_d}$$
 3.

Here S_d are the sums (2) which positions correspond to the positions of the *I*s in the query Boolean fingerprint, divided by the number of the descriptors N_d . Thus, for each query fingerprint we obtain N_{clstr} solutions, where N_{clst} is the number of clusters.

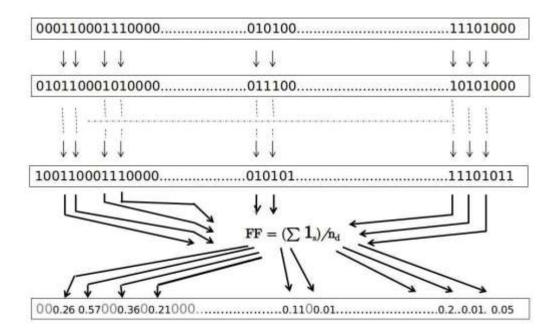


Figure 3. Creation of fuzzy fingerprints.

On can see from the relation 3 that in case of no coincidence of the query fingerprints of value I with fuzzy fingerprint elements of value different from zero all S_d sums will be zero then the FF will be also zero. In case of coincidence of the query fingerprints of value I with fuzzy fingerprint elements of value different from zero all S_d sums will be 1.0 then the FF will be also 1.0. The most probable query object fells in the cluster having the maximal FF value and it is considered the most similar to the associated object having the most similar properties to the corresponding cluster. The formation of fuzzy fingerprints is depicted in **Figure 3** and similarity search in fuzzy clusters is illustrated in **Figure 4**.

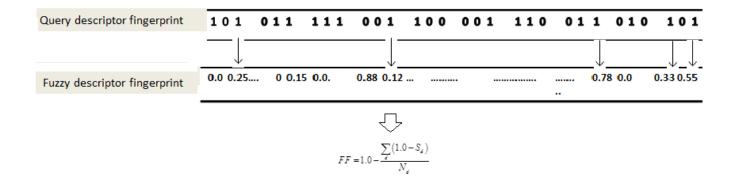


Figure 4. Depiction of the similarity search procedure between a query and a cluster fuzzy fingerprints.

It should be mentioned here one additional advantage of the employment of fuzzy descriptor fingerprints. Their use reduces substantially the representation and search in large databases, as each fuzzy fingerprint representing one and only one

cluster which often consists of a large number of Boolean fingerprints. On the other hand in as much the fuzzy fingerprint values represent the weights of the descriptors (properties) the coincidence of element 1 of the query fingerprints to the corresponding fuzzy descriptor element gives the weight (influence) of this descriptor on the query fingerprint. Each cluster is associated with some query properties, e.g. in the case of biodiesels names of the oils, citane index, color, etc. (In our case they are given as a string), thus the maximal *FF* with a cluster assumes that the query object has also these properties.

EXPERIMENTAL

Aset of 98 biodiesel samples belonging to 6 different classes of biodiesel oils – sunflower, rape, corn, soybean, palm and peanut, as well as samples of oil mixtures of the these classes has been used for our fingerprint analysis The FAME-profile for each sample was created by gas chromatographic (GC) analysis. All GC analyses were performed on a GC system Agilent Technologies 7890A equipped with FID, split/splitless injector and Agilent 7693A automated liquid sampler. The fatty acid methyl esters composition (%) of biodiesels being produced of different vegetable oils (Fatty acid methylesters palmitate (C16:0), palmitoleate (C16:1), stearate (C18:0), oleate (C18:1), linoleate (C18:2), linolenate (C18:3), arachidate (C20:0), cis-11-eicosenoate (C20:1), behenate (C22:0), cis-13-docosanoate (C22:1), tetracosanoate (C24:0), cis-15-tetracosanoate (C24:1). SAT – total esters of saturated acids, MUNS- total esters of monounsaturated acids, PUNS total esters of polyunsaturated acids) was determined and used for descriptors for the fingerprint creation.

The program written in Java consists of four tabs. A descriptor configuration file is created in the first tab. This file describes each descriptor with its *initVal,endVal* and *resVal* values. By using this configuration file and reading the data from a tab-tabulated text file (converted from an Excel file) *fingerprint* (*.fp) and *names* (*.nam) files are generated in the next tab. Any information about the separate objects, consisting of the oil names, some of their properties, is encoded in the *names* file. The values of the cetane number were additionally introduced in the *names* file. Inn the *Clustering* tab the *fingerprint* files are further used for clustering (by using Butina method) and creation of fuzzy descriptor fingerprints. The similarity search is carried out in the next *Similarity Search* tab.

Results and Discussion

We have explored two ways of forming clusters, the first one is the clustering to be carried out in a natural way according to the origin of biodiesel, i.e., one cluster of sunflower oil, one cluster of rape, one cluster of soy bean fingerprints, etc, oils. No clustering procedure was used to this end. Then, the number of the clusters will be 11 (see **Table 1**) and the number of the biodiesels forming this type of clusters is the same as these given in **Table 1**.

The second way of clustering is based on the Tanimoto index similarity of the source file Boolean type descriptor fingerprints by using the method of Butina [4] leading to the creation of two files: a cluster (*.clust) file containing the cluster fingerprints, and an output (*.out) text file of the generated clusters. The clustering procedure is based on an analysis through a

pair-wise comparison of the fingerprints and selection by using a threshold Tanimoto value (TV). All generated pairs having TI

below the threshold value are discarded, the remaining pairs being further sorted in a decreasing order of the TI values.

Table 1.	Number of clusters	formed	from biodiesels of different vegetable origin. (* X means mixtures of unknown or	
partially unknown composition).				

ClusterNo	Name of the biodiesel oil origin	Number of samples
1	sunflower	33
2	rape	19
3	corn	8
4	soybean	18
5	palm	5
6	peanut	6
7	X-mix-rape*	2
8	X-mix-sunflower*	1
9	X-mix-sunflower-soy*	1
10	X-mix-soy-rape*	1
11	X-mix*	2

Two options concerning the threshold value are encoded in this approach. The first one is a user chosen manual input of the threshold value, the second an automatic generation of it. The automatic generation implies an initial pair-wise comparison of all the objects (data-set Boolean fingerprints) at a threshold value equal to zero, subsequent sorting downwards with respect to TI value, and a further step of comparing the names (including types of oils) of the objects. When a difference between the names is encountered the corresponding TI value plus 0.000001 is accepted for the threshold value. Thus, we found automatically the threshold value of 0.5763 in our case.

At the next step, fuzzy descriptor fingerprints characterizing each cluster are generated for both types of clusters according to the methods discussed above.

An internal validation using the Boolean descriptor fingerprints of the 98 biodiesels (here called query fingerprints) against the cluster fuzzy descriptor fingerprints, generated by the first type of clustering, was carried out in the third *Similarity Search* tab and the results for each Boolean fingerprint are sorted in descending order with respect of the *FF* values generated. In **Listing1**in **Appendix 1**all results for the Boolean query 1, and the maximal and second maximal *FF* results for the others are provided.

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Some of the query biodiesel fuels denoted by X are mixtures of partly know composition. One can see from **Listing 1**that except from the first case 98 query **X-mix-soy-rape** being mixture of unknown X and soybean and rape composition which produces low *F*F value, the method accurately recognizes the known oil in all the other cases. The NO MATCH flag is generated by simple string comparison of the names (String type) of biodiesels of the fuzzy cluster and the name of Boolean query fingerprint, e.g., Query name "sunflower" with fuzzy name "sunflower" which implies that the result is correct. Vice verse, comparing the Query name "sunflower" with cluster name "rape" will produce NO MATCH flag. Hence, some of the X-mix-... comparisons, denoted by NO MATCH flag might be correct.

An external validation was performed by separating the test series of 98 biodiesel oils into two groups. The first group (data-set group) was formed with 83 oils belonging to 6 classes of biodiesels (sunflower, rape, corn, soy bean, palm, and peanut) with a known origin. The fuzzy descriptor fingerprints for these clusters were generated. The second query group consists of 15 analytes of both biodiesels of known, partially known and unknown constitution (the two later denoted by X).

The maximal *FF* results of similarity comparison between the 15 Boolean query fingerprints each one with the 6 cluster fuzzy fingerprints are provided in **Figure 5**. One can see that only in one case, the maximal FF fingerprint 98 of X-mix-soy-rape produces corn biodiesel to cluster 3, although the full mixture is not known. The mark NO MATCH is assigned if the names of the biodiesels does not coincide (string comparison) with the oil names of the clusters, which is the case of all X-*** mixtures, although the results look correct. Hence this procedure could be applied as an analytic method for elucidation of any mixture composition. The other cases marked as no matching are unknown mixtures other cases marked as no matching are unknown mixtures other cases strings and mark them with NO MATCH flag if they are not equal. One can see that in all but mixture 98 the method recognizes at least one of the mixture component. However in case 98 the X component is not known.

MAX FF fingerprint Query	23sunflower with CLUSTER 1 sunflower FF=0.52972
MAX FF fingerprint Query	33sunflower with CLUSTER 1 sunflower FF=0.61789
MAX FF fingerprint Query	49 rape with CLUSTER 2 rape FF=0.47511
MAX FF fingerprint Query	50rape with CLUSTER 2 rape FF=0.25882
MAX FF fingerprint Query	53corn with CLUSTER 3 corn FF=0.44762
MAX FF fingerprint Query	78soy bean with CLUSTER 4 soy bean FF=0.67407
MAX FF fingerprint Query	80palm with CLUSTER 5 palm FF=0.77667
MAX FF fingerprint Query	88peanut with CLUSTER 6 peanut FF=0.34667
MAX FF fingerprint Query	92X-mix-rape with CLUSTER 2 rape FF=0.24284> NO MATCH
MAX FF fingerprint Query	93X-mix-sunfl with CLUSTER 1 sunflower FF=0.30344> NO MATCH
MAX FF fingerprint Query	94X-mix-rape with CLUSTER 5 palm FF=0.25333> NO MATCH
MAX FF fingerprint Query	95X-mix with CLUSTER 1 sunflower FF=0.19355> NO MATCH
MAX FF fingerprint Query	96X-mix with CLUSTER 3 corn FF=0.27619> NO MATCH
MAX FF fingerprint Query	97X-mix-sunfl-soy with CLUSTER 4 soy bean FF=0.27037> NO MATCH
MAX FF fingerprint Query	98X-mix-soy-rape with CLUSTER 3 corn FF=0.18095> NO MATCH

Figure 5. Similarity comparison of 15 Boolean query fingerprints with the 6 cluster fuzzy fingerprints generated from 83 Boolean fingerprints.

Next, by using the Butina method for clustering using the Boolean descriptor fingerprints we generated a new set of 18 clusters. They, together with the number of fingerprints in each cluster are depicted in **Table 2**.

Further, from the clusters generated in such a way the fuzzy descriptor fingerprints characterizing each cluster are generated according the method discussed above. Then, an internal validation using the query Boolean descriptor fingerprints of the 98 biodiesels against the cluster fuzzy descriptor fingerprints is carried out and the results for each Boolean fingerprint are sorted in descending order with respect to the FF values generated. Results having maximal FF for each query Boolean descriptor fingerprint, compared to all cluster fuzzy fingerprints are provided in **Listing 2** in **Appendix 1**. The query biodiesel fuels are mixtures of partly know composition. One can see from Figure 5 that except from the first case query 63 soy bean with Cluster 6 the method accurately recognizes the known oil in all the other cases.

CONCLUSIONS

The application of the method of descriptor fingerprints to the problems of clustering of biodiesels indicates that they can be a useful tool to this end. A novel type of *fuzzy descriptor fingerprints* related to each cluster and a new Fuzzy Factor index have been introduced and tested with our set of 98 biodiesels. They were generated both from the 12 clusters shown in Table 1, formed from biodiesels composed of uniform oil types - sunflower, rape, corn, soybean, palm peanut, etc., each cluster being represented by one fuzzy fingerprint.

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Additionally, 18 fuzzy clusters fingerprints generated from the 18 clusters (**Table 2**) obtained by employing the method of Butina, have been treated by using 98 query Boolean descriptor fingerprints. The search and subsequent clustering results, based on the highest FF value for each query fingerprint indicate that the fuzzy fingerprint approach leads to very good discrimination between different biodiesel fuels.

Table 2.Clusters generated by Butina method. and number of biodiesels in each cluster.

Cluster No	biodiesel kind	Nu of biodiesels
1	sunflower	31
2	sunflower	2
3	rape	16
4	rape	2
5	rape	1
6	corn	4
7	corn	2
8	corn	2
9	soy bean	19
10	palm	6
11	peanut	5
12	peanut	1
13-18	X-***	each one x1

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Appendix 1.

PRINT Clusters for Queries

Query 8sunflower with CLUSTER 3 corn FF=0.41944> NO MATCH
MAX FF fingerprint Query 9sunflower with CLUSTER 1 sunflower FF=0.46199
Query 9sunflower with CLUSTER 3 corn FF=0.41111> NO MATCH
MAX FF fingerprint Query 10sunflower with CLUSTER 1 sunflower FF=0.45505
Query 10sunflower with CLUSTER 8 X-mix-sunfl FF=0.43333> NO MATCH
MAX FF fingerprint Query 11sunflower with CLUSTER 1 sunflower FF=0.51566
Query 11sunflower with CLUSTER 8 X-mix-sunfl FF=0.40000> NO MATCH
MAX FF fingerprint Query 12sunflower with CLUSTER 1 sunflower FF=0.52866
Query 12sunflower with CLUSTER 10 X-mix-soy-rape FF=0.46667> NO MATCH
MAX FF fingerprint Query 13sunflower with CLUSTER 1 sunflower FF=0.63081
Query 13sunflower with CLUSTER 3 corn FF=0.27500> NO MATCH
MAX FF fingerprint Query 14sunflower with CLUSTER 1 sunflower FF=0.63169
Query 14sunflower with CLUSTER 3 corn FF=0.30278> NO MATCH
MAX FF fingerprint Query 15sunflower with CLUSTER 1 sunflower FF=0.63169
Query 15sunflower with CLUSTER 3 corn FF=0.30278> NO MATCH
MAX FF fingerprint Query 16sunflower with CLUSTER 1 sunflower FF=0.62765
Query 16sunflower with CLUSTER 3 corn FF=0.33611> NO MATCH
MAX FF fingerprint Query 17sunflower with CLUSTER 1 sunflower FF=0.62563
Query 17sunflower with CLUSTER 3 corn FF=0.30278> NO MATCH
MAX FF fingerprint Query 18sunflower with CLUSTER 1 sunflower FF=0.55492
Query 18sunflower with CLUSTER 4 soy bean FF=0.28070> NO MATCH
MAX FF fingerprint Query 19sunflower with CLUSTER 1 sunflower FF=0.58030
Query 19sunflower with CLUSTER 8 X-mix-sunfl FF=0.33333> NO MATCH
MAX FF fingerprint Query 20sunflower with CLUSTER 1 sunflower FF=0.60947

20 ---sunflower with CLUSTER 4 soy bean FF=0.29474---> NO MATCH Ouerv MAX FF fingerprint Query 21 ---sunflower with CLUSTER 1 sunflower FF=0.62159 Query 21 ---sunflower with CLUSTER 3 corn FF=0.30278---> NO MATCH MAX FF fingerprint Query 22 ---sunflower with CLUSTER 1 sunflower FF=0.60947 Ouery 22 ---sunflower with CLUSTER 4 soy bean FF=0.29123---> NO MATCH MAX FF fingerprint Query 23 ---sunflower with CLUSTER 1 sunflower FF=0.51856 23 ----sunflower with CLUSTER 8 X-mix-sunfl FF=0.40000---> NO MATCH Query 23 ---sunflower with CLUSTER 8 X-mix-sunfl HF=0.40000---> NO MATCH MAX FF fingerprint Query 24 ---sunflower with CLUSTER 1 sunflower FF=0.55492 Query 24 ---sunflower with CLUSTER 10 X-mix-soy-rape FF=0.26667---> NO MATCH MAX FF fingerprint Query 25 ---sunflower with CLUSTER 1 sunflower FF=0.62653 Query 25 ---sunflower with CLUSTER 3 corn FF=0.31944---> NO MATCH MAX FF fingerprint Query 26 ---sunflower with CLUSTER 1 sunflower FF=0.66616 Query 26 ---sunflower with CLUSTER 8 X-mix-sunfl FF=0.26667---> NO MATCH MAX FF fingerprint Query 27 ---sunflower with CLUSTER 1 sunflower FF=0.42649 -sunflower with CLUSTER 8 X-mix-sunfl FF=0.26667---> NO MATCH Query 28 ---sunflower with CLUSTER 9 X-mix-sunfl-soy FF=0.4269 Query 28 ---sunflower with CLUSTER 9 X-mix-sunfl-soy FF=0.33333--> NO MATCH MAX FF fingerprint Query 29 ---sunflower with CLUSTER 1 sunflower FF=0.60947 Query 29 ---sunflower with CLUSTER 8 X-mix-sunfl FF=0.3333--> NO MATCH MAX FF fingerprint Query 30 ---sunflower with CLUSTER 8 X-mix-sunfl FF=0.33333--> NO MATCH Query 30 ---sunitower with CLUSTER 0 Actination in the control of the second se Query 31 ---sunflower with CLUSTER 8 A-mix-sunfl Freq.50000--> INO MATCH MAX FF fingerprint Query 32 ---sunflower with CLUSTER 1 sunflower FF=0.57311 Query 32 ---sunflower with CLUSTER 3 corn FF=0.44444--> NO MATCH MAX FF fingerprint Query 33 ---sunflower with CLUSTER 1 sunflower FF=0.57715 Query 33 ---sunflower with CLUSTER 3 corn FF=0.42718--> NO MATCH MAX FF fingerprint Query 34 ----rape with CLUSTER 2 rape FF=0.41829 Query 34 ----rape with CLUSTER 7 X-mix-rape FF=0.26667---> NO MATCH MAX FF fingerprint Query 35 ---rape with CLUSTER 2 rape FF=0.46109 Query 35 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.33333---> NO MATCH MAX FF fingerprint Query 36 ---rape with CLUSTER 2 rape FF=0.41526 Query 36 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MATCH MAX FF fingerprint Query 37 ---rape with CLUSTER 2 rape Ff=0.2000 ---> NO MATCH MAX FF fingerprint Query 37 ---rape with CLUSTER 2 rape Ff=0.3333--> NO MATCH MAX FF fingerprint Query 38 ---rape with CLUSTER 2 rape FF=0.53056 Query 38 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667--> NO MATCH MAX FF fingerprint Query 39 ---rape with CLUSTER 2 rape FF=0.53647 Query 39 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MATCH MAX FF fingerprint Query 40 ----rape with CLUSTER 2 rape FF=0.47927 40 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.33333---> NO MATCH MAX FF fingerprint Query 41 ---rape with CLUSTER 2 rape FF=0.50427 Query 41 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MATCH MAX FF fingerprint Query 42 ---rape with CLUSTER 2 rape FF=0.49140 Owner 42 ---rape with CLUSTER 2 -> NO MATCH --rape with CLUSTER 7 X-mix-rape FF=0.26667---> NO MATCH MAX FF fingerprint Query 43 ---rape with CLUSTER 2 rape FF=0.48837 Query 43 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MAT NO MATCH Query 44 ----rape with CLUSTER 7 X-mix-rape Vift CLUSTER 2 rape FF=0.51526 Query 45 ---rape with CLUSTER 7 X-mix-rape FF=0.30000---> NO MATCH
 Query
 45
 --rape with CLUSTER /
 A-mix-rape FF-0.50011

 MAX FF fingerprint
 Query
 46
 --rape with CLUSTER 2
 rape FF=0.50011

 Query
 46
 --rape with CLUSTER 9
 X-mix-sunfl-soy FF=0.26667--->
 NO MATCH

 The second s MAX FF fingerprint Query 47 ----rape with CLUSTER 2 rape FF=0.51275 Query 47 ----rape with CLUSTER 7 X-mix-rape FF=0.30000---> NO MATCH MAX FF fingerprint Query 48 ---rape with CLUSTER 2 rape FF=0.44670 Query 48 ---rape with CLUSTER 7 X-mix-rape FF=0.30000---> NO MATCH MAX FF fingerprint Query 49 ---rape with CLUSTER 2 rape FF=0.44078 Query 49 ---rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MATCH MAX FF fingerprint Query 50 ---rape with CLUSTER 2 rape FF=0.20215 Query 50 ---rape with CLUSTER 10 X-mix-soy-rape FF=0.26667---> NO MATCH MAX FF fingerprint Query 51 ---rape with CLUSTER 2 rape FF=0.49419 Query 51 ---rape with CLUSTER 9 X-mix-sumf-soy FF=0.3333--> NO MATCH MAX FF fingerprint Query 52 ---rape with CLUSTER 2 rape FF=0.46677 Query 52 ---rape with CLUSTER 9 X-mix-sumf-soy FF=0.26667---> NO MATCH MAX FF fingerprint Query 53 ---corn with CLUSTER 3 corn FF=0.45556 Query 53 ---com with CLUSTER 4 soy bean FF=0.37544---> NO MATCH MAX FF fingerprint Query 54 ---corn with CLUSTER 3 corn FF=0.53056 Query 54 ---corn with CLUSTER 4 soy bean FF=0.41404---> NO MATCH MAX FF fingerprint Query 55 ---corn with CLUSTER 3 corn FF=0.40278 Query 55 ---com with CLUSTER 4 soy bean FF=0.34737---> NO MATCH MAX FF fingerprint Query 56 --- corn with CLUSTER 3 corn FF=0.47778 ---corn with CLUSTER 4 soy bean FF=0.40702---> NO MATCH MAX FF fingerprint Query 57 ---corn with CLUSTER 3 corn FF=0.58611 ---corn with CLUSTER 4 soy bean FF=0.46667-NO MATCH Query 57 -----Om with CLUSTER 10 X-mix-soy-rape FF=0.40000---> NO MATCH MAX FF fingerprint Query 59 ---corn with CLUSTER 3 corn FF=0.51944 Query 59 ---corn with CLUSTER 4 soy bean FF=0.49474---> NO MATCH Query 60 ---com with CLUSTER 4 soy bean FF=0.40702---> NO MATCH

MAX FF fingerprint Ouery 61 ---soy bean with CLUSTER 4 soy bean FF=0.70526 61 ---soy bean with CLUSTER 3 corn FF=0.46944---> NO MATCH MAX FF fingerprint Query 62 ---soy bean with CLUSTER 4 soy bean FF=0.66316 Query 62 ---soy bean with CLUSTER 3 corn FF=0.41389---> NO MATCH MAX FF fingerprint Query 63 ---soy bean with CLUSTER 4 soy bean FF=0.53333 Query 63 ---soy bean with CLUSTER 3 corn FF=0.41389---> NO MATCH MAX FF fingerprint Query 64 ---soy bean with CLUSTER 4 soy bean FF=0.65263 Query 64 ---soy bean with CLUSTER 3 corn FF=0.41111---> NO MATCH MAX FF fingerprint Query 66 ---soy bean with CLUSTER 4 soy bean FF=0.63509 Query 66 ---soy bean with CLUSTER 3 com FF=0.33889---> NO MATCH MAX FF fingerprint Query 68 ---soy bean with CLUSTER 4 soy bean FF=0.66667 Query 68 ---soy bean with CLUSTER 3 com FF=0.39444---> NO MATCH Query 69 ---soy bean with CLUSTER 3 corn FF=0.45278---> NO MATCH soy bean FF=0.62105 MAX FF fingerprint Query 70 ---soy bean with CLUSTER 4 soy bean FF=0.51579 Query 70 ---soy bean with CLUSTER 3 corn FF=0.35556---> NO MATCH MAX FF fingerprint Query 71 --- soy bean with CLUSTER 4 soy bean FF=0.61404 71 ---soy bean with CLUSTER 3 corn FF=0.38056---> NO MATCH WAX FF fingerprint Query 72 ---soy bean with CLUSTER 1 sunflower FF=0.42563---> NO MATCH MAX FF fingerprint Query 74 ----soy bean with CLUSTER 4 soy bean FF=0.65965 Query 74 ---soy bean with CLUSTER 3 corn FF=0.43056---> NO MATCH MAX FF fingerprint Query 75 --- soy bean with CLUSTER 4 soy bean FF=0.67018 -soy bean with CLUSTER 3 com FF=0.45278---> NO MATCH Query 76 ----soy bean with CLUSTER 4 soy bean FF=0.71930 Query 76 ----soy bean with CLUSTER 3 corn FF=0.46944---> NO MATCH MAX FF fingerprint Query 77 ---soy bean with CLUSTER 4 soy bean FF=0.69474 ---soy bean with CLUSTER 3 corn FF=0.43611 NO MATCH Query 78 ---soy bean with CLUSTER 3 corn FF=0.48611---> NO MATCH Query 78 ---soy bean with CLUSTER 3 corn FF=0.48611---> NO MATCH MAX FF fingerprint Query 79 ---soy bean with CLUSTER 4 Query 79 ---soy bean with CLUSTER 3 corn FF=0.41944---> N 4 soy bean FF=0.63158 NO MATCH MAX FF fingerprint Query 80 ---palm with CLUSTER 5 Query 80 ---palm with CLUSTER 4 soy bean FF=0.37895---> palm FF=0.76667 NO MATCH palm FF=0.73333 MAX FF fingerprint Query 81 ---palm with CLUSTER 5 Query 81 ---palm with CLUSTER 4 soy bean FF=0.31228---> NO MATCH MAX FF fingerprint Query 82 ---palm with CLUSTER 5 Query 82 ---palm with CLUSTER 1 sunflower FF=0.26667-palm FF=0.71111 NO MATCH MAX FF fingerprint Query 83 ---palm with CLUSTER 5 Ouery 83 ---palm with CLUSTER 4 soy bean FF=0.29825---palm FF=0.58889 NO MATCH palm FF=0.73333 MAX FF fingerprint Query 86 ---peanut with CLUSTER 6 peanut FF=0.48889 Query 86 ---peanut with CLUSTER 3 corn FF=0.20000---> NO MATCH MAX FF fingerprint Query 87 --- peanut with CLUSTER 6 peanut FF=0.62222 87 --- peanut with CLUSTER 3 corn FF=0.25833---> NO MATCH MAX FF fingerprint Query 89 ---peanut with CLUSTER 6 peanut FF=0.68333 Query 89 ---peanut with CLUSTER 3 corn FF=0.25833---> NO MATCH MAX FF fingerprint Query 90 ---peanut with CLUSTER 6 peanut FF=0.62778 ---peanut with CLUSTER 3 corn FF=0.21667-NO MATCH
 Query
 91
 ---peanut with CLUSTER 3
 corn FF=0.22500--->
 NO MATCH

 MAX FF fingerprint
 Query
 92
 ---X-mix-rape with CLUSTER 7
 X-mix-rape FF=0.63333

 Query
 92
 ---X-mix-rape with CLUSTER 7
 X-mix-rape FF=0.63333

 Query
 92
 ---X-mix-rape with CLUSTER 7
 X-mix-rape FF=0.63333

 Query
 92
 ---X-mix-rape with CLUSTER 8
 X-mix-sunf FF=0.63333

 Query
 92
 ---X-mix-rape with CLUSTER 2
 rape FF=0.20/95--->
 NO BIALCH

 MAX FF fingerprint
 Query
 93
 ---X-mix-sunfl with CLUSTER 8
 X-mix-sunfl FF=0.63333

 Query
 93
 ---X-mix-sunfl with CLUSTER 1
 sunflower FF=0.36774--->
 NO MATCH

 Cuery
 93
 ---X-mix-sunfl with CLUSTER 1
 sunflower FF=0.36774--->
 NO MATCH
 MAX FF fingerprint Query 94 ---X-mix-rape with CLUSTER 7 X-mix-rape FF=0.66667 Query 94 ---X-mix-rape with CLUSTER 8 X-mix-sunfl FF=0.30000---> NO MATCH MAX FF fingerprint Query 95 ---X-mix with CLUSTER 9 X-mix-sunfl-soy FF=0.40000--NO MATCH Query 95 ---X-mix with CLUSTER 8 X-mix-sunfl FF=0.36060/---> NU MAX CLUSTER 10 X-mix-soy-rape FF=0.46667---> MAX FF fingerprint Query 96 ---X-mix with CLUSTER 10 X-mix-soy-rape FF=0.46667---> NO MATCH Query 96 --- X-mix with CLUSTER 3 corn FF=0.35278---> NO MATCH MAX FF fingerprint Query 97 ---X-mix-sunfl-soy with CLUSTER 9 X-mix-sunfl-soy FF=1.00000 97 ----X-mix-sunfl-soy with CLUSTER 8 X-mix-sunfl FF=0.63333---> NO MATCH Query MAX FF fingerprint Query 98 ---X-mix-soy-rape with CLUSTER 10 X-mix-soy-rape FF=1.00000

Query 98 ---X-mix-soy-rape with CLUSTER 9 X-mix-sunfl-soy FF=0.26667---> NO MATCH

Listing 1.Results from internal validation of the 98 fingerprints versus all 11 fuzzy cluster descriptor fingerprints, generated by the 11 clusters. The full results are presented onlyfor the 1st query fingerprint, the maximal and second maximal FF results provided for the other query fingerprints.

PRINT Clusters for Queries

 MAX FF fingerprint
 Query
 1
 ---sunflower with CLUSTER 1
 sunflower FF=0.49735

 Query
 1
 ---sunflower with CLUSTER 2
 sunflower FF=0.33333
 guery
 1
 ---sunflower with CLUSTER 14
 X-mix-sunfl FF=0.26667--->
 NO MATCH

 Query
 1
 ---sunflower with CLUSTER 14
 X-mix-sunfl FF=0.26667--->
 NO MATCH

Query	1	sunflower with CLUSTER 6	corn FF=0.23333> NO MATCH
Query	1	sunflower with CLUSTER 7	corn FF=0.23333> NO MATCH
Query	1	sunflower with CLUSTER 10	palm FF=0.22222> NO MATCH
Duerv	1	sunflower with CLUSTER 8	corn FE=0.20000> NO MATCH

Ç

Query 1sunflower with CLUSTER 13 X-mix-rape FF=0.20000> NO MATCH	MAX FF fingerprint Query 45 rape with CLUSTER 3 rape FF=0.59306
Query 1	MAX FF fingerprint Query 46rape with CLUSTER 3 rape FF=0.56806
Query 1	MAX FF fingerprint Query 47 rape with CLUSTER 3 rape FF=0.56250
Query 1sunflower with CLUSTER 9 soy bean FF=0.14035> NO MATCH	MAX FF fingerprint Query 48 rape with CLUSTER 4 rape FF=0.56667
Query 1	MAX FF fingerprint Query 49 rape with CLUSTER 3 rape FF=0.49583
Query 1	MAX FF fingerprint Query 50 rape with CLUSTER 5 rape FF=0.73333
Query 1	MAX FF fingerprint Query 51rape with CLUSTER 3 rape FF=0.56389
Query 1	MAX FF fingerprint Query 52rape with CLUSTER 3 rape FF=0.54306
Query 1sunflower with CLUSTER 5 rape FF=0.06667> NO MATCH	MAX FF fingerprint Query 53corn with CLUSTER 6 corn FF=0.65000
Query 1sunflower with CLUSTER 15 X-mix-rape FF=0.06667> NO MATCH	MAX FF fingerprint Query 54corn with CLUSTER 6 corn FF=0.73333
	MAX FF fingerprint Query 55corn with CLUSTER 7 corn FF=0.70000
MAX FF fingerprint Query 2sunflower with CLUSTER 1 sunflower FF=0.49735	MAX FF fingerprint Query 56corn with CLUSTER 8 corn FF=0.76667
MAX FF fingerprint Query 3sunflower with CLUSTER 2 sunflower FF=0.63333	MAX FF fingerprint Query 57corn with CLUSTER 6 corn FF=0.68333
MAX FF fingerprint Query 4sunflower with CLUSTER 2 sunflower FF=0.63333	MAX FF fingerprint Query 58corn with CLUSTER 6 corn FF=0.63333
MAX FF fingerprint Query 5sunflower with CLUSTER 1 sunflower FF=0.62724	MAX FF fingerprint Query 59corn with CLUSTER 7 corn FF=0.70000
MAX FF fingerprint Query 6sunflower with CLUSTER 1 sunflower FF=0.62079	MAX FF fingerprint Query 60corn with CLUSTER 8 corn FF=0.76667
MAX FF fingerprint Query 7sunflower with CLUSTER 2 sunflower FF=0.63333	MAX FF Ingerprint Query 60cont with CLUSTER 8 contrep-0.70007 MAX FF fingerprint Query 61soy bean with CLUSTER 9 soy bean FF=0.70526
MAX FF fingerprint Query 8sunflower with CLUSTER 1 sunflower FF=0.55842	MAX FF fingerprint Query 62soy bean with CLUSTER 9 soy bean FF=0.66316
MAX FF fingerprint Query 9sunflower with CLUSTER 2 sunflower FF=0.73333	MAX FF fingerprint Query 63soy bean with CLUSTER 6 corn FF=0.55000> NO MATCH
MAX FF fingerprint Query 10sunflower with CLUSTER 14 X-mix-sunfl FF=0.53333> NO	MAX FF ingerprint Query 64soy bean with CLUSTER 9 soy bean FF=0.65263
MAX FF inigeiphine Query 10sumiowei with CLOSTER 14 X-inix-sumi FF=0.55555> NO MATCH	
MAX FF fingerprint Query 11sunflower with CLUSTER 2 sunflower FF=0.56667 MAX FF fingerprint Query 12sunflower with CLUSTER 2 sunflower FF=0.53333	MAX FF fingerprint Query 66soy bean with CLUSTER 9 soy bean FF=0.63509 MAX FF fingerprint Query 67soy bean with CLUSTER 9 soy bean FF=0.68772
MAX FF fingerprint Query 14sunflower with CLUSTER 1 sunflower FF=0.64229	MAX FF fingerprint Query 69soy bean with CLUSTER 9 soy bean FF=0.62105
MAX FF fingerprint Query 15sunflower with CLUSTER 1 sunflower FF=0.64229	MAX FF fingerprint Query 70soy bean with CLUSTER 9 soy bean FF=0.51579
MAX FF fingerprint Query 16sunflower with CLUSTER 1 sunflower FF=0.63584	MAX FF fingerprint Query 71soy bean with CLUSTER 9 soy bean FF=0.61404
MAX FF fingerprint Query 17sunflower with CLUSTER 1 sunflower FF=0.63584	MAX FF fingerprint Query 72soy bean with CLUSTER 9 soy bean FF=0.47368
MAX FF fingerprint Query 18sunflower with CLUSTER 1 sunflower FF=0.56057	MAX FF fingerprint Query 73soy bean with CLUSTER 9 soy bean FF=0.59298
MAX FF fingerprint Query 19sunflower with CLUSTER 1 sunflower FF=0.59627	MAX FF fingerprint Query 74soy bean with CLUSTER 9 soy bean FF=0.65965
MAX FF fingerprint Query 20sunflower with CLUSTER 1 sunflower FF=0.61864	MAX FF fingerprint Query 75soy bean with CLUSTER 9 soy bean FF=0.67018
MAX FF fingerprint Query 21sunflower with CLUSTER 1 sunflower FF=0.63154	MAX FF fingerprint Query 76soy bean with CLUSTER 9 soy bean FF=0.71930
MAX FF fingerprint Query 22sunflower with CLUSTER 1 sunflower FF=0.61864	MAX FF fingerprint Query 77soy bean with CLUSTER 9 soy bean FF=0.69474
MAX FF fingerprint Query 23sunflower with CLUSTER 2 sunflower FF=0.73333	MAX FF fingerprint Query 78soy bean with CLUSTER 9 soy bean FF=0.68070
MAX FF fingerprint Query 24sunflower with CLUSTER 1 sunflower FF=0.56057	MAX FF fingerprint Query 79soy bean with CLUSTER 9 soy bean FF=0.63158
MAX FF fingerprint Query 25sunflower with CLUSTER 1 sunflower FF=0.63584	MAX FF fingerprint Query 80palm with CLUSTER 10 palm FF=0.76667
MAX FF fingerprint Query 26sunflower with CLUSTER 1 sunflower FF=0.57907	MAX FF fingerprint Query 81palm with CLUSTER 10 palm FF=0.73333
MAX FF fingerprint Query 27sunflower with CLUSTER 1 sunflower FF=0.47749	MAX FF fingerprint Query 82palm with CLUSTER 10 palm FF=0.71111
MAX FF fingerprint Query 28sunflower with CLUSTER 1 sunflower FF=0.47749	MAX FF fingerprint Query 83palm with CLUSTER 10 palm FF=0.58889
MAX FF fingerprint Query 29sunflower with CLUSTER 1 sunflower FF=0.62294	MAX FF fingerprint Query 84palm with CLUSTER 10 palm FF=0.73333
MAX FF fingerprint Query 30sunflower with CLUSTER 1 sunflower FF=0.50760	MAX FF fingerprint Query 85palm with CLUSTER 10 palm FF=0.73333
MAX FF fingerprint Query 31sunflower with CLUSTER 2 sunflower FF=0.50000	MAX FF fingerprint Query 86peanut with CLUSTER 11 peanut FF=0.52889
MAX FF fingerprint Query 32sunflower with CLUSTER 2 sunflower FF=0.66667	MAX FF fingerprint Query 87peanut with CLUSTER 11 peanut FF=0.67556
MAX FF fingerprint Query 33sunflower with CLUSTER 2 sunflower FF=0.60000	MAX FF fingerprint Query 88peanut with CLUSTER 12 peanut FF=0.86667
MAX FF fingerprint Query 34rape with CLUSTER 3 rape FF=0.48889	MAX FF fingerprint Query 89peanut with CLUSTER 11 peanut FF=0.74667
MAX FF fingerprint Query 35rape with CLUSTER 4 rape FF=0.83333	MAX FF fingerprint Query 90peanut with CLUSTER 11 peanut FF=0.68000
MAX FF fingerprint Query 36rape with CLUSTER 3 rape FF=0.47639	MAX FF fingerprint Query 91peanut with CLUSTER 11 peanut FF=0.76000
MAX FF fingerprint Query 37rape with CLUSTER 3 rape FF=0.60972	MAX FF fingerprint Query 92X-mix-rape with CLUSTER 13 X-mix-rape FF=0.86667
MAX FF fingerprint Query 38rape with CLUSTER 3 rape FF=0.60972	MAX FF fingerprint Query 93X-mix-sunfl with CLUSTER 14 X-mix-sunfl FF=1.00000
MAX FF fingerprint Query 39rape with CLUSTER 3 rape FF=0.62222	MAX FF fingerprint Query 94X-mix-rape with CLUSTER 15 X-mix-rape FF=1.00000
MAX FF fingerprint Query 40rape with CLUSTER 4 rape FF=0.83333	MAX FF fingerprint Query 95X-mix with CLUSTER 16 X-mix FF=1.00000
MAX FF fingerprint Query 41rape with CLUSTER 3 rape FF=0.57917	MAX FF fingerprint Query 96X-mix with CLUSTER 17 X-mix FF=1.00000
MAX FF fingerprint Query 42rape with CLUSTER 4 rape FF=0.70000	MAX FF fingerprint Query 97X-mix-sunfl-soy with CLUSTER 18 X-mix-sunfl-soy
MAX FF fingerprint Query 43rape with CLUSTER 4 rape FF=0.70000	FF=1.00000
MAX FF fingerprint Query 44rape with CLUSTER 3 rape FF=0.63889	
MAX FF fingerprint Query 98X-mix-soy-rape with CLUSTER 17 X-mix FF=0.46667> NO MATCH	

Listing 2. Internal validation by comparing the 98 Boolean query fingerprints with fuzzy fingerprints of the 18 clusters generated by the Butina method. The first query is presented to all 18 fuzzy fingerprints, the other queries with maximal **FF**.