

Progetto FIRB LIBI

MTA

USER GUIDE



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1. Introduction

This document is intended as a description of main functionalities and user interface of the MTA system. It aims to facilitate the MTA usage in biomedical literature mining tasks.

1.1. Generalities

MeSH Term Associator (MTA) is a data mining tool able to discover association rules on biomedical text corpora. It imports both some MeSH¹ (Medical Subject Headings) taxonomies and a set of abstracts published on Medline and discovers associations at different levels of abstraction (generalized association rules). Both automatic and semiautomatic approaches can be applied to structure the set of discovered rules and filter out uninteresting ones. In the automatic approach user domain knowledge is exploited to strongly guide the exploration of the set of discovered rules. Discovered association rules can be imported/exported in PMML. Similarities between discovered association rules can be visually explored through a multidimensional analysis technique. MTA integrates the IBM Web Services for Life Sciences² which allow to directly query the PubMed remote database (http://www.ncbi.nlm.nih.gov/entrez/query.fcgi) and to obtain a set of abstracts of interest for the task at hand. It includes two data mining algorithms for generalized association rules.

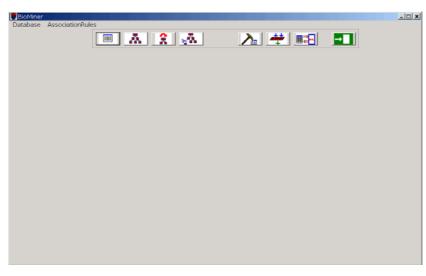


Fig. 1 MTA initial window

1.2. System requirements

- Microsoft® Windows® 2000
- 256 MB of available RAM is needed
- 640 MB of space on hard disk. User has to take into account that the space on hard disk depends on input data size and the size of discovered association rules as well.

¹<u>http://www.nlm.nih.gov/mesh/</u>

² Weil, N. *BioIT World*, URL: <u>http://www.bio-itworld.com/news/042203_report2381.html</u>

2. Installing MTA

MTA requires a DataBase connection to store input text corpora, to perform mining processes and to access discovered knowledge for filtering and visualization steps.

MTA interfaces Microsoft Access (97 or 2000) DataBase Management Systems (DBMS). It requires two different databases, one for input data and mining results and another to manage taxonomical knowledge used during the mining process.

3. Using MTA

MTA supports the following tasks:

- access to input data ;
- creating new input data source ;
- selecting taxonomical knowledge;
- loading and restoring taxonomical knowledge;
- mining generalized association rules;
- filtering mined association rules;
- importing/exporting association rules from/to a representation model in PMML standard language.

A

4. Access input data

This version of MTA complies the connection to a database only by means of Microsoft Jet Engine that resorts to the DAO access, namely only the Microsoft® Access ® version XX.XX DBMS.

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			🧮 Apri in sola lettura	1	

Fig. 2 Database configuration.

In order to select a data source, user should select the menu item AssociationRules > ExtractRules

or to press the button **Solution**. From the next new dialog window by pressing the button *Open Database* the user can access and connect to Microsoft Access target database (Fig. 2).

BioMiner					<u> </u>
Database	AssociationRules	2 .A			
	Tables in Database terms_1 terms_3 terms_4 terms_5 terms_6 terms_6 terms_6 terms_6 terms_6 terms/6	Input data : Minimun Support 0.05 Minimun Confidence 0.5 Generalizing Rules	C Extracted Rules		
	Neurons Brain Cholinesterase Inhibitors Cell Membrane Structures Pharmaceutical Preparations	Open Database	Selecting taxonomies da Cerea in: Speimentationi	tabase :	? × ⊡▼
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		Close		LaxDB	xmlrule:
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Fig. 3 Input data selection.

Then, table names (dataset) of the selected database is showed in the list window *Tables in Database*: the user can select the target dataset and field names are showed in list window *Fields in database table* (Fig. 3).

5. Create new data source

This functionality allows to create a new data source having to contain target database. More precisely, the input data originally consists of a set of tagged files representing a set of biomedical

scientific paper abstracts. By selecting the menu item *Database> Create MeshTerm DB* or by pressing the button the window reported in Fig. 4 is showed.

BioMiner Database	AssociationRules			_ 🗆 🗙
Database		<u>a 2 a</u>	▶ 🗮 📰	
		BioMiner: Creating Mesh-Terms DB	×	
			Choose Query Files	
			Create DB	
			Close	
				1

Fig.4 Text data preparation.

This operation allows the user to select the original tagged files (by pressing button *Choose Query Files*) and, subsequently, create a corresponding new Microsoft Access database (by pressing button *Create DB*, see Fig.5).

BioMiner Database Associa	ationRules	<u>8</u> .A			LO X
	BioMiner: Cres	iting Mesh-Terms DB	_	×	
	Selecting query files Ceca in @ Rehverativ 8 11695244 9 11695244 9 117551903 9 117562751 9 118772538 9 11877274 4 Nome Re. Too file:	Image: 11877298 I 11877298 I 11877436 I 11877436 I 11892322 I 11893252 I 11893252 I 11943869 I 11943869	■ 119536	core Query Files Create DS Clore	

Fig.5 Text corpora DB creation.

6. Select taxonomy of terms

The taxonomical knowledge exploited in MTA consists of a vocabulary composed by a set of "is-a" taxonomies that the user can browse by selecting the menu item *Database > Select Taxonomies* or

by pressing the button

All existing taxonomies	Pruned hierarchies in upward direction	Pruned hierarchies in downward direction
Chemicals and Drugs Chemicals and Drugs Chemicals and Drugs Chemical Sciences Chemical Sciences Comparison of the Comparison of th		Health Cocupations

Fig. 6 Taxonomy navigation.

This step allows the user to select concept hierarchies that will play the role of taxonomical knowledge in the mining process. From the window showed in Fig.6 the selection of portions to be pruned is enabled by pressing the Prune buttons; the pruning process starts by pressing button Execute.

7. Load and Restore taxonomies

Taxonomical knowledge is loaded (Fig. 7) in the database by selecting Database > Load

and subsequently, by selecting an XML file *Taxonomies* or by pressing the button representing. The XML file is given in input to a parser and concept hierarchies and attributes are selected and preserved in the database interfaced by MTA. A previously pruned taxonomy can be completely restored by selecting the *Database* > *Restore Taxonomies* operation or by pressing the





BioMiner Database AssociationRules	<u>- 🗆 x</u>
Execute Close	
Selecting taxonomies database : 2 🗶 Cerca in: 🔄 Sperimentacioni 💽 🛩 🗈 👉 🖽 🔻	
Results Inforules0105	
□ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■	
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Tipo file: Annulla	

Fig. 7 Taxonomy load/restoration.

8. Mining Generalized Association Rules

MTA includes two algorithms for generalized association rule mining, namely the standard Apriori algorithm³ and the DELIS (DEscending Levels Increasing Size) algorithm, which allows to discover non-redundant association rules resorting to the concept of closed item sets⁴. To start up the mining process the following steps should be performed:

- 1. selection of the AssociationRules >Extract Rules option or click on the
- 2. selection of database storing the taxonomical knowledge (Fig. 8);
- 3. selection of the input data source, selection of the mining method, setting of the input parameters (*minimum support, minimum confidence*) (Fig. 9);
- 4. specification of the database name that will store discovered rules (Fig. 10);
- 5. discovered rules can be roughly browsed by the interface (Fig. 11).

³ Agrawal, R., and Srikant, R., "Fast Algorithms for Mining Association Rules", *Proc. of the Twentieth Int.Conf. Very Large Databases*: Santiago, Cile,1994.

⁴ Pasquier, N., Bastide, Y., Taouil, R., and Lakhal, L.. "Discovering Frequent Closed Itemsets for Association Rules", *Proc. of the 7th Int. Conference on Database theory*. C. Beeri and P. Buneman, Eds. Lecture Notes In Computer Science, vol. 1540. Springer-Verlag, London, 398-416, 1999.

	2 J. S.	▶ 🗯 🖃	
BioMiner: Extracting Rules		- Extracted Rules	- I X
Tables in Database	Input data :	Extracted Rules	
terms_2 terms_3	Minimun Support		
terms_4 terms 5	0.05		
terms_51 terms_52			
terms_6	Minimun Confidence		
	0.5		
Fields in database table			
Therapeutic Equivalency Amyloid Neuropathies	Generalizing Rules		
Tacrine Rats, Wistar			
Neurons Brain Cholinesterase Inhibitors	Open Database		
Cell Membrane Structures			
Pharmaceutical Preparations	Extract with APRIORI		
	Extraxt with DELIS		
	Close		
		Ľ	

Fig. 9 Window to set input for the mining process.

BioMiner		>
Database Association		
	BioMiner:Restoring Taxonomies	
	Execute Close	
	Selecting taxonomies database :	
	Cerca in: 🔁 Sperimentazioni 💽 🔶 🖄 🖽 🗸	
	□Results ■Inforules0105	
	솀Dataset	
	⊠Inforules_53_70	
	Inforules_53_70P ■ mesh4 ■ Sperime	
	Inforules0104 ❷rules_53_70 ❷taxDB	
	Nome file: mesh4	
	Nome file: mesh4	

BioMiner: Extracting Rules	2 .A			_ = ×
Tables in Database Tables in Database torms_1 torms_4 terms_5 terms_5 terms_52 terms_52 terms_6	Input data : Minimun Support 0.7 Minimun Confidence 0.5	Extracted Rules		
Fields in database table terms_2: Alzheimer Disease terms_2: Therapeutic Equivalency terms_2: Tarrine terms_2: Tarrine terms_2: Rats, Wistar terms_2: Rats, Wistar terms_2: Cholinesterase Inhibitor terms_2: Colinesterase Inhibitor	Saving extracted rule Savajr Results DExp1P11 DExp1P12 DExp1P13 DExp1P21 DExp1P22 DExp1P23		? ▼ ● Exp3P2 ● Exp3P2 ● Exp3P2 ● Exp4P1 ● Exp4P1 ● Exp4P2	
Completed!!	E E×p1P23 E×p2P12 ▲ Nome file: Salga come:	enexp3P12 휍Exp3P13	Exp4P2 Exp4P2	

Fig. 8 Taxonomy selection.

Fig. 10 Mining result storage.

BioMiner			<u>- 🗆 X</u>
Database AssociationRules	Input data : 0.7	Extracted Rules Extracted Rules Brain Diseases => Mental Disorders Mental Disorders => Dementia Nervous System Diseases => Mental Disorders	
Fields in database table Fields in database table terms_2: Alzheimer Disease terms_2: Anyioid Neuropathies terms_2: Anyioid Neuropathies terms_2: Ration terms_2: Review terms_2: Review terms_2: Review terms_2: Colliesterase Inhibitor terms_2: Cell Membrane Structur ¥	Minimun Confidence 0.5 Image: Constraint of the second se	Mental Disorders => Nervous System Disease: Central Nervous System Diseases => Mental E Mental Disorders => Central Nervous System I Dementia => Derain Diseases Brain Diseases => Dementia Delirium, Dermentia, Amnestic, Cognitive Disordi Brain Diseases => Delirium, Dementia, Amnes Dementia => Dementia Dementia => Dementia Nervous System Diseases => Dementi Dementia => Nervous System Diseases Central Nervous System Diseases Central Nervous System Diseases Delirium, Dementia, Amnestic, Cognitive Disordi	
Completed!!	Extraxt with DELIS Close	Dementia => Delirium, Dementia, Amnestic, C Nervous System Diseases => Delirium, Demert Delirium, Dementa, Amnestic, Cognitive Disord Central Nervous System Diseases => Delirium Delirium, Dementia, Amnestic, Cognitive Disorders => Central	Nervous System Diseases

Fig. 11 Window showing the completion of a mining task.

9. Filter Mined Association Rules

As the number of discovered rules can be very high, MTA supports some functionalities for rule filtering with the aim to browse among them looking for interesting ones.

Four modalities have been implemented in MTA:

- 1. *Template*, where the user can specify the kind of rules of interest;
- 2. *Cover*, where the rules are synthesized in order to identify the most concise ones;
- 3. Rating, interesting rules are identified on the basis of their statistical behaviour;

4. *Specificity*, where user can explore the rules by means of rule subspaces.

The task is started by selecting the menu item *AssociationRules* > *Filter Rules* or by clicking the ++

button that loads the window showed in Fig. 12 which allows the user to select the database of rules to be analysed (*Load Rules* button).

ent Rules			Using Template	Load Rules
			Using Cover	Tables List in Rules Databa:
			Using Rating	
			Using Specificity	Current Rules Table
			Cascade Filtering	Rules Number
				Input data used :
Loading extracted r		? X		Min Support Value :
Cerca in: 🔁 Results	Exp2P12	1 🕈 🖬 ▼ 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		Min Confidence Value :
Exp1P12 Exp1P13	 Exp2P13 Exp2P21 Exp2P21 	 ▲Exp3P1 ▲Exp3P2 ▲Exp3P2 		Database taxonomies used
윈Exp1P21 윈Exp1P22 윈Exp1P23	⑧Exp2P22 옌Exp2P23 옌Exp3P11	셸Exp3P2 셸Exp3P2 셸Exp4P1		
•			Close	
Nome file: Exp1P11		Apri		
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Fig.12 Window for rule filtering operations: rule database selection.

By selecting the table containing rules of interest (*Table List in Rules Database* frame), the system loads rules and some information describing the rules set are provided (number of rules, minimum support and confidence values, employed taxonomies (Fig.13). Then, the filtering technique can be selected and the result is showed to the user in the *Current Rules* frame (Fig.14). An option to combine different filtering techniques in a single filtering workflow that operates in a cascade mode is also provided.

BioMiner: Filtering Rules Current Rules Using Cover Using Rating Using Specificity Current Rules Table	- ×
Using Template Load Rules Using Cover Using Rating Using Rating	ase
Using Cover Using Rating Using Rating	ase
Using Rating	ase
Using Rating	ase
Using Rating	
Using Specificity	
Using Specificity Current Rules Table	
Using Specificity Current Rules Table	
Table Name	
Rules Number ()	
Cascade Filtering	
Input data used :	
Min Support Value :	0.6
Phil support value -	
Min Confidence Value :	0.7
Min Confidence Value :	· · ·
Database taxonomies used	
Analytical, Diagnostic and Th	rape .
Anatomy Anthropology, Education, Soc	iolog-
Biological Sciences Chemicals and Drugs	
Close Diseases	
Geographic Locations Health Care	
Health Care	
Information Science	_
Organisms Persons	
Persons Physical Sciences	-

Fig.13 Window for rule filtering operations: rule loading and filtering method selection.

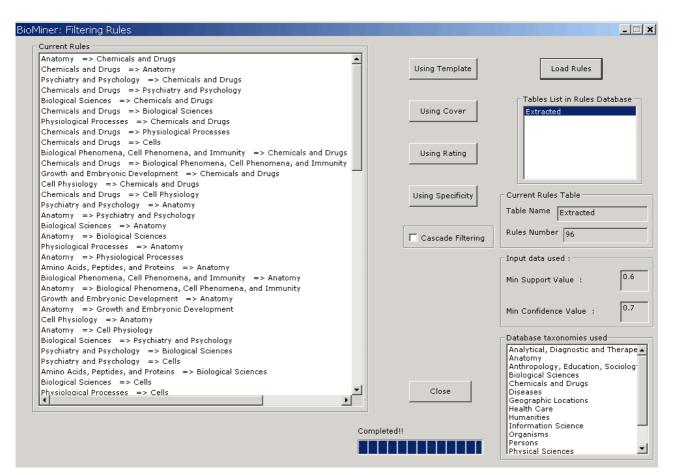


Fig.14 Window for rule filtering operations: example of a filtering task.

9.1 Template Filtering

The Template method allows users to specify the notion of interesting and not-interesting rules. By means of the scroll controls (Items, Taxonomies Classes, Cardinality) the user can specify the criteria that resulting rules should meet (*Inclusive Template*) and/or do not have to meet (*Restrictive Template*), see Fig.15. The resulting rules are ordered on the basis of support values (or confidence values), see Fig.16. Filtered rules can be saved (*Save Rules* button) in the same repository of analysed rules.

BioMiner: Filtering Rules: Using Template		
Antecedent Specific : Items Taxonomy Classes Cardinality ADD Taxonomy Classes Cardinality ADD	Consequent Specific : Items ADD Taxonomy Classes Cardinality ADD ADD	Filtered rules
Antecedent template features Image: state state state Image: state Im	Consequent template features	
Restrictive Template Restrictive Template Add Template Reset All	Seve ru/es Close	

Fig.15 Template filtering set up.

BioMiner: Filtering Rules: Using Template		
Antecedent Specific :	Consequent Specific :	Filtered rules
Items ADD	Items ADD	Chemicals and Drugs => Biological Sciences Chemicals and Drugs => Anatomy Chemicals and Drugs => Cells Chemicals and Drugs => Anatomy AND Biological Scien
Taxonomy Classes Cardinality	Taxonomy Classes Cardinality	Chemicals and Drugs => Anatomy AND biological Science Chemicals and Drugs => Biological Sciences AND Cells Chemicals and Drugs => Physiological Processes Chemicals and Drugs => Biological Phenomena, Cell Ph
Antecedent template features		Chemicals and Drugs => Cell Physiology Chemicals and Drugs => Anatomy AND Physiological Phn Chemicals and Drugs => Anatomy AND Biological Phenc Chemicals and Drugs => Anatomy AND Cell Physiology
T	T	Chemicals and Drugs => Psychiatry and Psychology Amino Acids, Peptides, and Proteins => Biological Sciences
C Inclusive Template	Order by © Decreasing Support © Decreasing Confidence	Amino Acids, Peptides, and Proteins => Anatomy Amino Acids, Peptides, and Proteins => Cells
Chemicals and Drugs+ => Any		
Restrictive Template		
Add Template Reset All Filter Ordering filtered rul		۲

Fig.16 Template filtering results.

9.2 Cover Filtering

The Cover method allows to specify criteria to identify the most concise and non-redundant rules (Fig.17). Covers can be extracted both on the antecedent part and the consequent part of the rules (*Algorithm direction* frame). Moreover, covers can be combined with a clustering method (*Cover algorithm type* frame) and matching rules can be showed in two different modalities (*Order by* frame). Filtered rules can be saved as well (*Save Rules* button).

Cover algorithm type	Filtered rules
• with Cover set	Biological Sciences => Chemicals and Drugs
	Chemicals and Drugs => Biological Sciences Biological Sciences => Anatomy
with Cover set and Clustering	Anatomy => Biological Sciences
	Biological Sciences => Cells
	Anatomy => Chemicals and Drugs
Algorithm direction	Chemicals and Drugs => Anatomy
C Fixed Antecedent	Chemicals and Drugs => Cells
C The Anceceden	Anatomy AND Biological Sciences => Chemicals and Drugs =
Fixed Consequent	Chemicals and Drugs AND Biological Sciences => Anatomy
	Chemicals and Drugs AND Biological Sciences -/ Anatomy Chemicals and Drugs AND Anatomy => Biological Sciences
	Biological Sciences => Chemicals and Drugs AND Anatomy
Order by	Anatomy => Chemicals and Drugs AND Biological Sciences
Decreasing Support	Chemicals and Drugs => Anatomy AND Biological Sciences
	Biological Sciences AND Cells => Chemicals and Drugs
C Decreasing Confidence	Chemicals and Drugs AND Cells => Biological Sciences
	Chemicals and Drugs AND Biological Sciences => Cells
	Biological Sciences => Chemicals and Drugs AND Cells
	Chemicals and Drugs => Biological Sciences AND Cells
Filter	Physiological Processes => Anatomy
	Anatomy => Physiological Processes
	Biological Phenomena, Cell Phenomena, and Immunity => Anatomy
Save rules	Anatomy => Biological Phenomena, Cell Phenomena, and Immunity
537574855	Cell Physiology => Anatomy
	Anatomy => Cell Physiology
Reset All	Physiological Processes => Cells
11000(11)	Biological Phenomena, Cell Phenomena, and Immunity => Cells
	Cell Physiology => Cells
	Biological Sciences => Psychiatry and Psychology
Close	Psychiatry and Psychology => Biological Sciences
	Physiological Processes => Chemicals and Drugs
	Chemicals and Drugs => Physiological Processes
mpleted!!	Biological Phenomena. Cell Phenomena. and Immunity => Chemicals a

Fig.17 Cover filtering: setting and results.

9.3 Rating Filtering

This method allows to detect interesting rules on the basis of their values with respect to a statistical property. More precisely, the resulting rules are detected on the basis of their "estimated statistical behaviour" (*Statistical behaviour* buttons) with respect to a selected (*Statistical viewpoint* button) statistical measure (see Fig. 18). In particular, a minimum threshold value should be specified for the property Dependency. Filtered rules can be saved as well (*Save Rules* button).

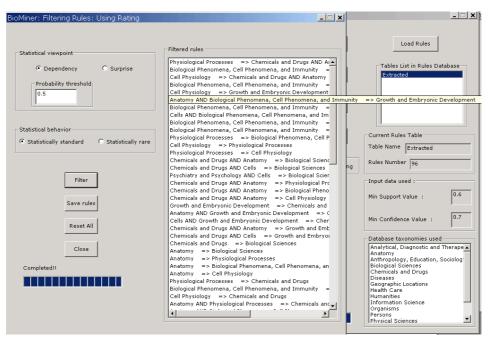


Fig.18 Rating filtering setting and results.

9.4 Specificity Filtering

This method allows to select subspaces of rules satisfying user interest and to explore more and more specific sets of rules. In particular, the user can browse towards subspaces that are the specialization of one of the two sides of a selected rule (that is the representative rule of a certain subspace). Subspaces of interest are identified by defining one or more nodes of the taxonomy (i.e., biomedical concepts) that are relevant for the user (*Ground Items* scroll control) and by selecting preferences on rule parts to be explored (*Antecedent/Consequent* radio button), see Fig.19. Once the initial subspace is obtained, the user pursues his exploration by choosing a single rule (by means of the *Filtered Rules* frame), then the next subspaces are generated by specializing one side (*More specific* button) as well as by specializing the other side (*Enhance other side* button), see Fig.20.

BioMiner: Filtering rules: Using Specificity	
BioMiner: Filtering rules: Using Specificity Ground Items Anatomy ADD Chemicals and Drugs Chemicals and Drugs Con Antecedent Con Consequent Order by Con Consequent Order by Conceasing Support Conceasing Confidence More Specific Enhance other side Filter Reset All Save rules Close	Filtered rules Filtered rules
Close Completed!!	×

Fig.19 Specificity filtering method: setting and results.

Ground Items	Filtered rules
Anatomy 💌	Biological Sciences => Chemicals and Drugs Biological Sciences => Chemicals and Drugs AND Anatomy
	Biological Sciences => Chemicals and Drugs AND Anatomy Biological Sciences => Chemicals and Drugs AND Cells
ADD	- Anatomy => Chemicals and Drugs
Chemicals and Drugs	 Physiological Processes => Chemicals and Drugs Biological Phenomena, Cell Phenomena, and Immunity => Chemicals and D
	Cell Physiology => Chemicals and Drugs
I F	— Psychiatry and Psychology => Chemicals and Drugs
O On Antecedent	Growth and Embryonic Development => Chemicals and Drugs
Off Antecedenic	
On Consequent	
Order by	
Decreasing Support	
C Decreasing Confidence	
C Decreasing Confidence	
More Specific	
Enhance other side	
1	
Filter	
Reset All	
Save rules	
Close	
Completed!!	

Fig.20 Specificity filtering method: subspace browsing.

10. Import/Export Association Rules

MTA supports the importing/exporting of association rules from/to a data-mining description model compliant with the PMML language⁵. This functionality is accessible by clicking on the \square

button or by selecting the menu item *Association Rules*> *Import/Export Rules*. In order to export rules, the user should select the data source (button *Select Database*) containing rules stored as results of previous mining sessions (see Fig. 22). Then, from the list shown in the *Rules Tables in Database* box, a rule set should be selected. The export step is accomplished by specifying the name of target XML file (see Fig. 23), the database storing the taxonomical knowledge and by pressing the button *Export*.

To import rules, the user should select the source XML file (*Select XML file* button). The import step is accomplished by specifying the database storing the taxonomical knowledge, pressing the button *Import* and by specifying the name of database that will store the imported rules.

BioMiner: Importing/Exporting Rules	
Importing rules from xml file to database	Exporting rules from database to xml file
Rules Database	Rules Tables in Database Select Database Extracted Filtered_17_12_20_36_35 Export Export
	Close

Fig.22 Rule Import/Export: selection of rules.

⁵ <u>http://www.oasis-open.org/cover/pmml.html</u>

👮 BioMiner					<u> </u>
Database A	ssociationRules				
	BioMiner: Importing/Exporting Ru	lles			
	Importing rules from xml file to databas	e	Exporting rules from database	to xml file	
	Rules Table in Database	Select XML file	Rules Tables in Database Extracted Filtered_17_12_20_36_35 Export		
	Cerca in:	n I rules file : Sperimentazioni			
	2) taxDB ⊉ TAXDB ⊉ XmIS3_7 @ XmIRules @ xmIrules @ xmIrules @ xmIrules Nome file: Tipo file:	₽ <mark>×</mark> 70 s 0104	mirules01505		

Fig.23 Rule Import/Export: selection of xml file.