

# Milano Chemometrics and QSAR Research Group

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# Tournament tables, Power-Weakness Ratio and Hasse diagrams: an informative combination for multi-criteria decision-making.

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# Prologue

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The starting points of this work are our two previous papers published in 2015:

R. Todeschini, F. Grisoni, S. Nembri, (2015)  
Weighted power-weakness ratio for multi-criteria decision making.  
*Chemometrics and Intelligent Laboratory Systems*, 146, 329-336.

F. Grisoni, V. Consonni, S. Nembri, R. Todeschini (2015)  
How to weight Hasse diagrams and reduce incomparabilities.  
*Chemometrics and Intelligent Laboratory Systems*, 147, 95-104.

# Tournament table



The results of a Round Robin tournament of N players can be conveniently expressed by mean of a tournament table (**dominance matrix**) as:

	P1	P2	P3	...	...	PN
P1	0	$t_{12}$	$t_{13}$	...	...	$t_{1N}$
P2	$t_{21}$	0	$t_{23}$	...	...	$t_{2N}$
P3	$t_{31}$	$t_{32}$	0	...	...	$t_{3N}$
...	...	...	...	...	...	
...	...	...	...	...	...	...
PN	$t_{N1}$	$t_{N2}$	$t_{N3}$	...	...	0

$$t_{ij} + t_{ji} = 1$$

H.A. David (1971)

Ranking the Players in a Round Robin Tournament.

*Review of the International Statistical Institute*, 39, 137-147.

# Tournament table



The results of a Round Robin tournament of N players can be conveniently expressed by mean of a tournament table (**dominance matrix**) as:

	P1	P2	P3	...	...	PN
P1	0	<b>1</b>	$t_{13}$	...	...	$t_{1N}$
P2	<b>0</b>	0	$t_{23}$	...	...	$t_{2N}$
P3	$t_{31}$	$t_{32}$	0	...	...	$t_{3N}$
...	...	...	...	...	...	
...	...	...	...	...	...	...
PN	$t_{N1}$	$t_{N2}$	$t_{N3}$	...	...	0

$$t_{ij} + t_{ji} = 1$$

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# Tournament table



Tournament table  $T_1$ . For each  $t_{ij}$ : 1 if the  $P_i$  player won over  $P_j$ , 0 if  $P_j$  won, 0.5 if they drew the match.

$T_1$	P1	P2	P3	P4	P5
P1	0	1	1	0.5	0
P2	0	0	1	0.5	0.5
P3	0	0	0	1	1
P4	0.5	0.5	0	0	0.5
P5	1	0.5	0	0.5	0

$$t_{ij} + t_{ji} = 1$$

Sometimes, some conflicting rings arise:

- 1) Ranking cannot be decided
- 2) Transitivity property is lost

$$P1 > P3 > P5 > P1$$

The row sum (**Copeland score**) can be used for ranking:

$$P1: 2.5$$

$$P2 = P3 = P5 = 2$$

$$P4 = 1.5$$

... but the ranking power can be low!

# Tournament table



A tournament table can be derived from any data matrix  $\mathbf{X}$  ( $N, p$ ), where  $N$  is the number of objects and  $p$  the number of variables, i.e. the considered criteria.

$$\mathbf{X} \rightarrow \mathbf{T}_w$$

The **general expression** for this transform is defined by comparing objects pairwise:

$$t_{ij}^w = \sum_{k=1}^p w_k \cdot \delta_{ij,k} \quad \text{where} \quad \delta_{ij,k} = \begin{cases} 1 & \text{if } x_{ik} \triangleright x_{jk} \\ 0.5 & \text{if } x_{ik} \triangleq x_{jk} \\ 0 & \text{if } x_{ik} \triangleleft x_{jk} \end{cases} \quad \text{and} \quad \sum_{k=1}^p w_k = 1$$

... where the **main differences** with respect to the Hasse approach are ...

# Tournament table



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A set of thresholds are also derived from the tournament table:

$$\mathbf{X} \rightarrow \mathbf{T}_w \rightarrow \{t_1, t_2, \dots, t_k\}$$



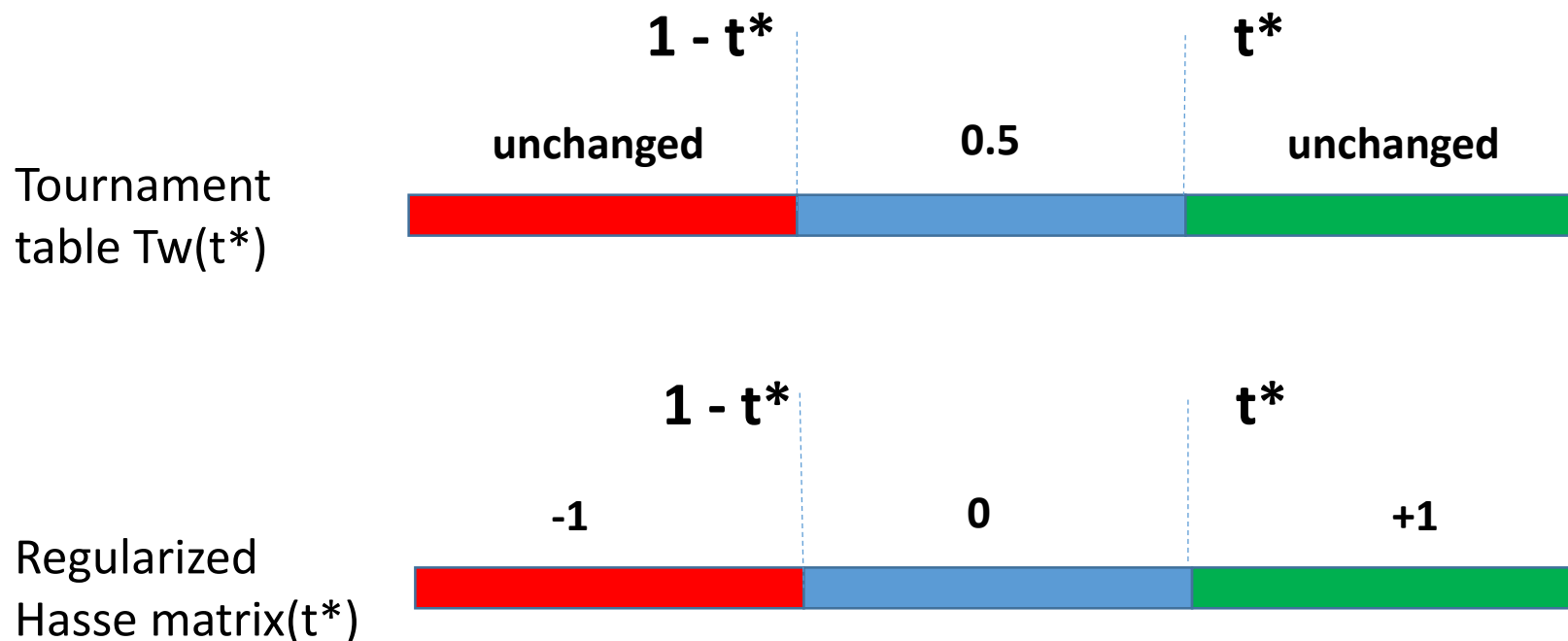
# Tournament table



Analyzing thresholds of the tournament table

$$0.5 \leq t^* \leq 1$$

The following transforms are performed



# Power-Weakness Ratio



For any squared asymmetrical matrix, the **Perron-Frobenius theorem** guarantees the existence of a positive eigenvalue associated with an eigenvector  $\mathbf{e}$  having positive values.

## Tournament table $\mathbf{T}_w$

Kendall (1955) proposed to use the **eigenvector values** to rank the objects, thus also removing possible lost of transitivity:

$$\mathbf{T}_w \rightarrow \mathbf{e}$$

Ramanujacharyulu (1964) proposed to use also the eigenvector values calculated on the transpose of  $\mathbf{T}_w$ :

$$\mathbf{T}_w^T \rightarrow \mathbf{e}^*$$

# Power-Weakness Ratio

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... then the **PWR** of the  $i$ -th object was defined as:

$$PWR_i = \frac{e_i}{e_i^*}$$

Indeed, the first eigenvector awards good players able to win with other good players, while the second eigenvector characterizes bad players which loss with other bad players.

# Power-Weakness Ratio



Tournament table  $\mathbf{T}_1$ . For each  $t_{ij}$ : 1 if the  $P_i$  player won over  $P_j$ , 0 if  $P_j$  won, 0.5 if they drew the match.

$\mathbf{T}_1$	P1	P2	P3	P4	P5
P1	0	1	1	0.5	0
P2	0	0	1	0.5	0.5
P3	0	0	0	1	1
P4	0.5	0.5	0	0	0.5
P5	1	0.5	0	0.5	0

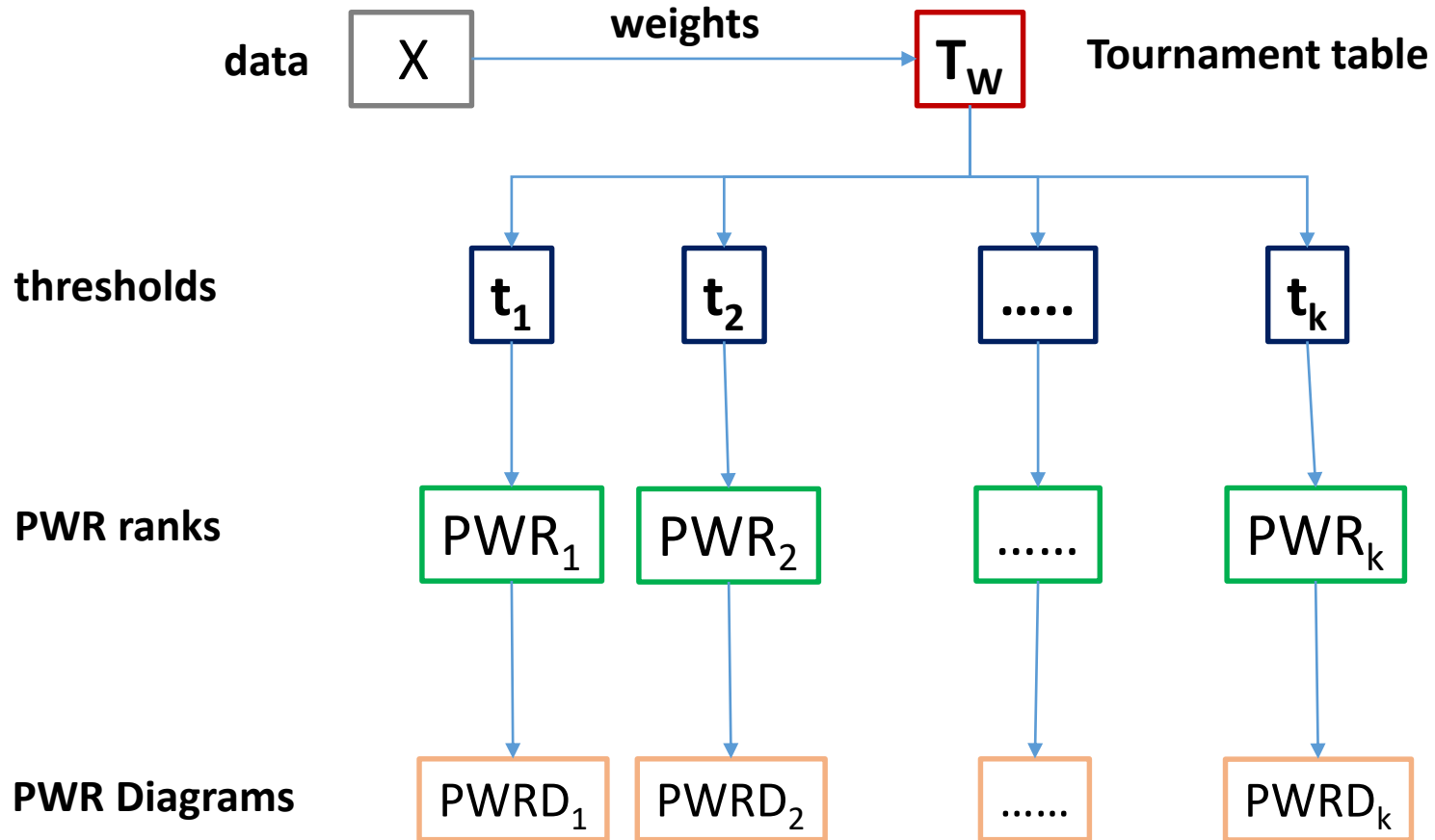
Results of PWR scoring on table  $\mathbf{T}_1$ . Entries of the Perron–Frobenius eigenvector calculated on tournament table ( $\mathbf{e}_{PF}$ ) and on its transpose ( $\mathbf{e}_{PF}^*$ ) for each player are also reported.

Players	$e_{PF}$	$e_{PF}^*$	PWR	RS
P1	0.529	0.370	1.368	2.5
P2	0.430	0.442	0.976	2.0
P3	0.426	0.414	1.025	2.0
P4	0.364	0.535	0.714	1.5
P5	0.471	0.459	1.023	2.0

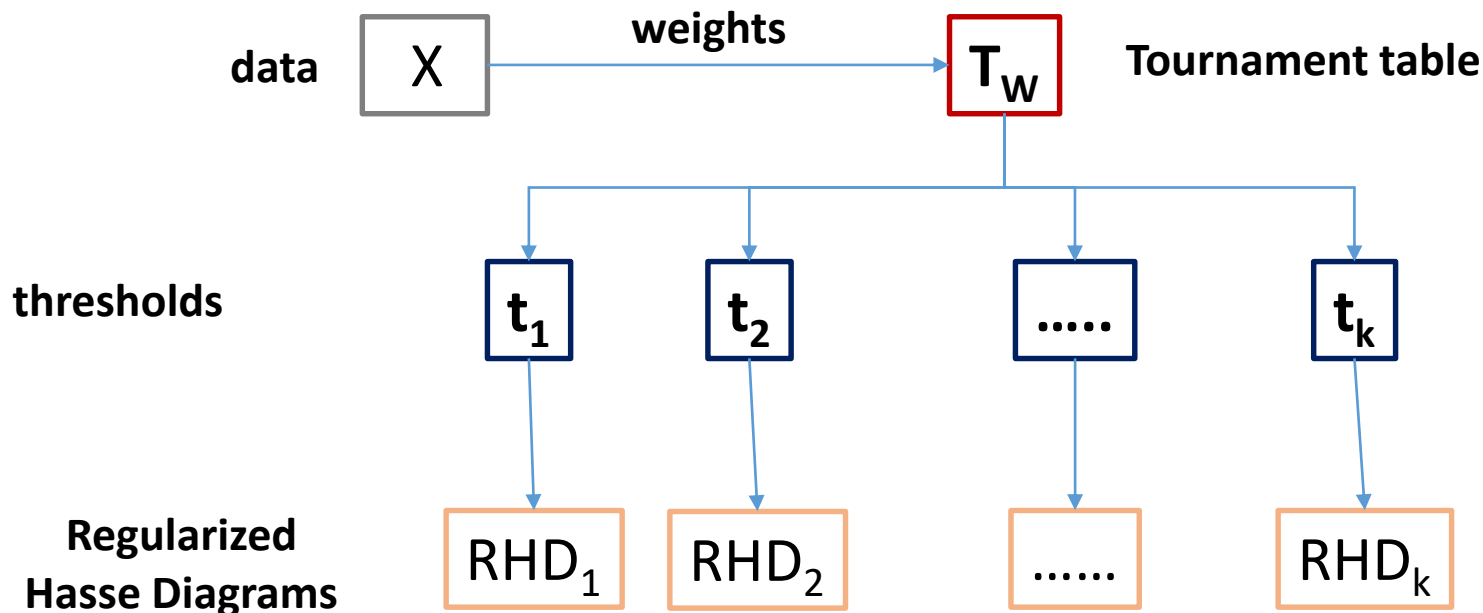
Eigenvector ( $T_w$ )

Eigenvector ( $T_w^T$ )

# Tw transform

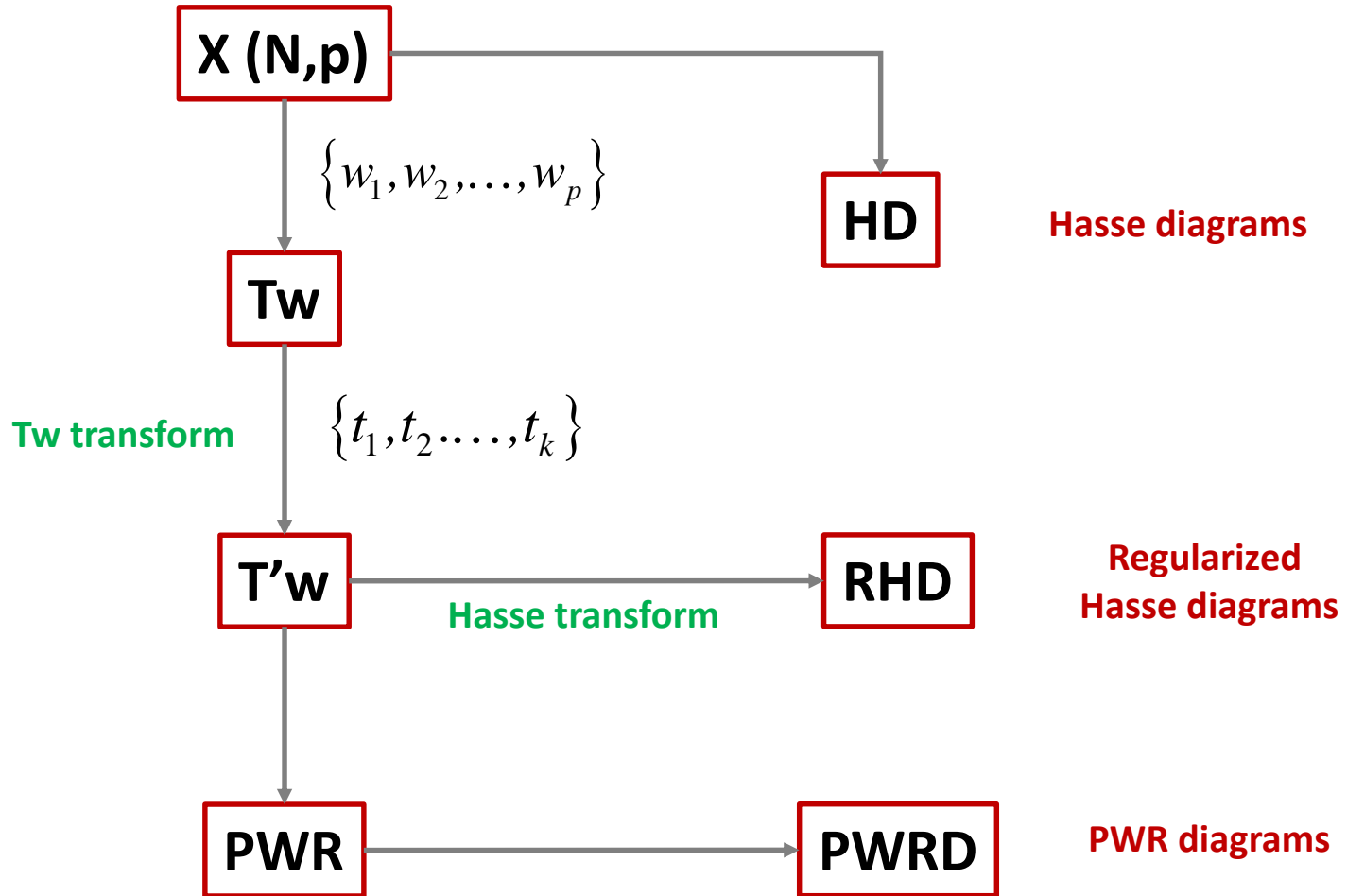


# Hasse transform



$$\left[ \mathbf{H}^R(t^*) \right]_{ij} = \begin{cases} +1 & \text{if } t_{ij}^W \geq t^* \\ -1 & \text{if } t_{ij}^W \leq 1 - t^* \\ 0 & \text{otherwise} \end{cases} \quad 0.50 < t^* \leq 1$$

# Summary



# Comparisons of classification methods



- 32 data sets
- Validation procedure: leave-one-out
- Parameter: Non-Error-Rate (NER%)

## 10 CLASSIFIERS

**N3**

**BNN**

**KNN**

**LDA**

**QDA**

**PLS-DA**

**CAIMAN**

**CART**

**SVM/LIN**

**SVM/RBF**



# Comparisons of classification methods

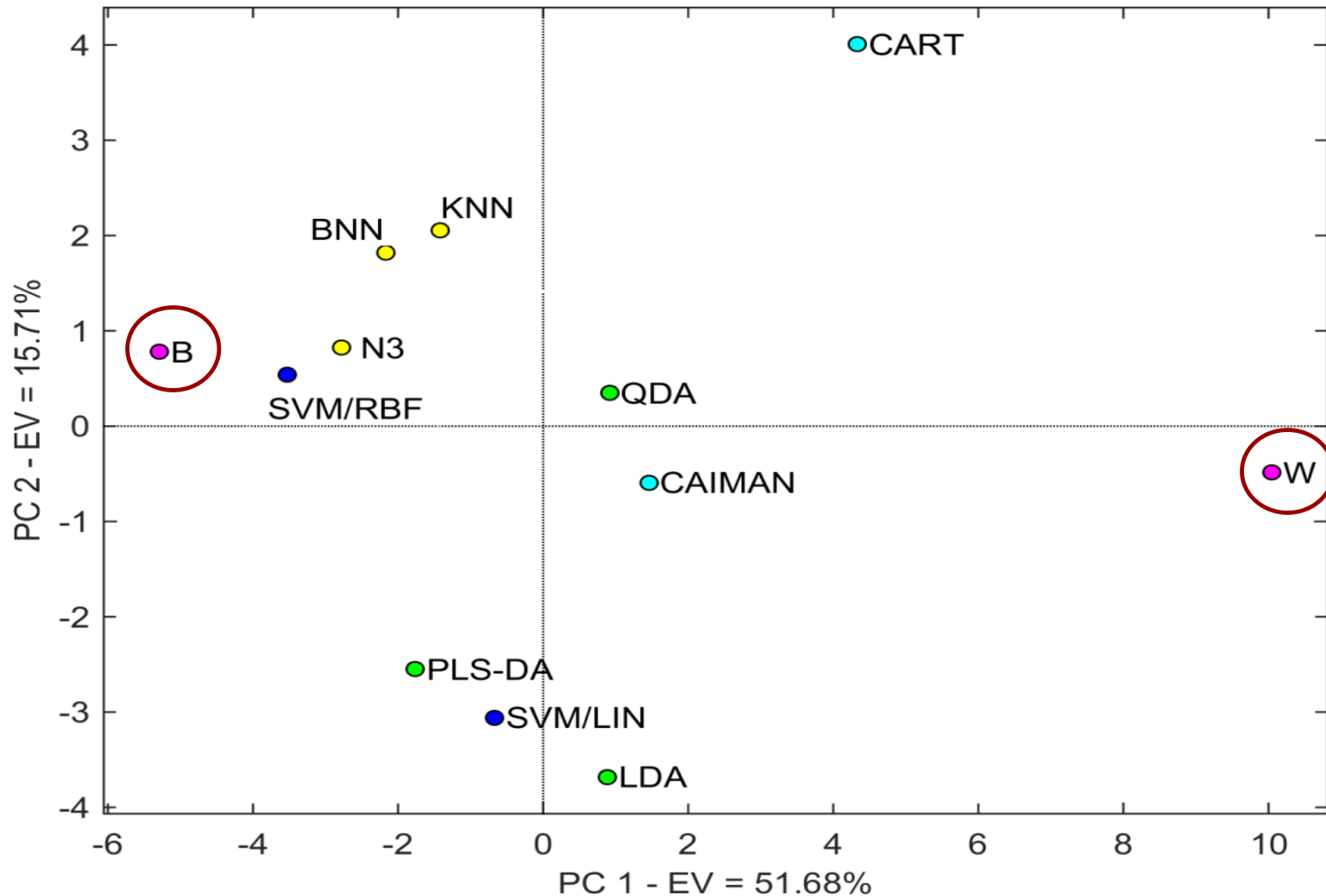


Id	Data set	N3	BNN	KNN	LDA	QDA	PLSDA	CART	CAIMAN	SVM /LIN	SVM /RBF
1	IRIS	96.0	96.7	96.7	<b>98.0</b>	97.3	90.2	94.0	<b>98.0</b>	97.3	97.3
2	WINES	96.2	98.6	97.7	99.1	<b>99.5</b>	<b>99.5</b>	86.2	98.7	99.1	<b>99.5</b>
3	PERPOT	99.0	99.0	99.0	85.0	92.0	86.0	97.0	97.0	87.0	<b>100.0</b>
4	ITAOILS	<b>96.2</b>	95.2	94.7	94.7	95.9	95.9	87.2	82.8	94.7	95.9
5	SULFA	77.4	73.8	73.8	45.2	69.4	74.0	81.5	58.7	50.0	<b>88.7</b>
6	DIABETES	73.6	71.1	70.5	72.7	69.6	<b>75.1</b>	68.8	73.5	72.3	72.8
7	BLOOD	67.9	62.2	62.3	53.7	54.5	<b>68.7</b>	62.1	59.3	50.0	64.1
8	VERTEBRAL	80.8	81.6	80.2	80.7	84.0	82.1	76.9	56.0	83.3	<b>84.3</b>
9	SEDIMENTS	88.9	88.9	<b>89.9</b>	66.9	69.4	79.4	84.3	61.1	50.5	69.9
10	BIODEG	84.5	85.3	<b>85.4</b>	77.0	78.6	79.9	79.6	65.6	81.5	83.8
11	DIGITS	74.2	72.3	73.6	74.0	68.6	41.0	65.2	<b>77.3</b>	74.9	74.5
12	APPLE	94.0	92.3	91.9	91.9	87.6	<b>95.4</b>	92.1	83.9	94.4	92.3
13	TOBACCO	92.3	92.3	92.3	84.6	80.8	88.5	<b>96.2</b>	92.3	92.3	92.3
14	SCHOOL	95.3	<b>96.6</b>	96.2	90.8	95.2	89.4	86.8	95.0	94.0	96.4
15	BANK	86.9	<b>91.2</b>	86.9	86.5	88.5	84.9	86.5	88.5	88.5	88.9
16	HIRSUTISM	88.3	90.1	90.0	55.4	81.4	84.1	70.5	52.9	72.7	<b>93.8</b>
17	THIOPHENE	83.3	83.3	83.3	79.2	79.2	<b>90.5</b>	58.3	83.3	83.3	83.3
18	SUNFLOWERS	92.3	90.4	91.2	87.8	90.8	92.7	82.1	88.9	90.8	<b>96.9</b>
19	VINAGRES	<b>100.0</b>	91.7	95.8	<b>100.0</b>	87.5	<b>100.0</b>	67.3	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>
20	CHEESE	76.1	78.3	78.1	78.8	82.9	84.7	63.9	77.5	76.2	<b>85.6</b>
21	ORUJOS	98.2	<b>98.4</b>	98.2	92.6	94.1	93.9	88.4	62.5	95.7	98.2
22	MEMBRANE	94.4	94.4	94.4	88.9	94.4	<b>96.7</b>	91.7	94.4	91.7	94.4
23	METHACYCLINE	82.5	<b>86.7</b>	82.5	45.8	81.7	55.8	65.8	80.0	54.2	82.5
24	SIMUL4	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	28.1	<b>100.0</b>	46.9	90.6	93.8	34.4	<b>100.0</b>
25	VEGOIL	99.0	<b>100.0</b>	99.0	98.0	82.2	99.0	99.3	89.9	99.3	<b>100.0</b>
26	CRUDEOIL	89.2	84.8	87.9	85.2	73.6	<b>89.7</b>	64.9	78.4	85.3	84.8
27	SAND	93.9	<b>94.9</b>	93.9	93.9	93.9	93.9	81.9	93.9	<b>94.9</b>	<b>94.9</b>
28	HEMOPHILIA	85.6	85.6	82.8	85.6	83.9	85.6	78.9	<b>86.7</b>	<b>86.7</b>	85.6
29	COFFEE	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	92.9	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>	<b>100.0</b>
30	OLITOS	89.1	73.6	70.4	83.1	80.0	<b>94.0</b>	58.0	77.2	87.6	87.6
31	FISH	92.6	92.9	92.9	96.4	85.2	<b>100.0</b>	88.7	89.0	<b>100.0</b>	<b>100.0</b>
32	HEARTH DISEASE	<b>69.9</b>	65.2	63.2	68.8	66.2	69.7	66.1	67.3	68.0	68.0

# Comparisons of classification methods



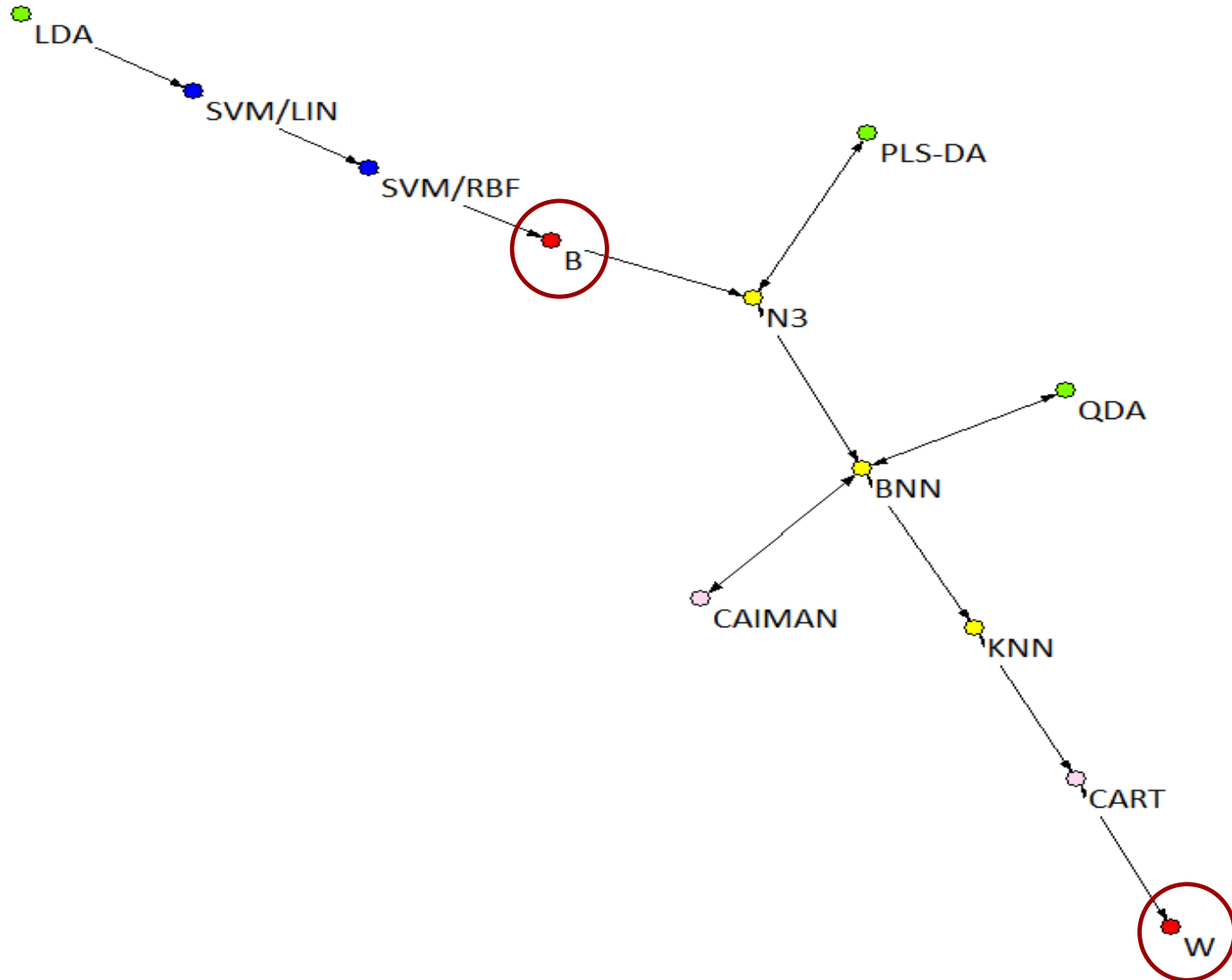
## Principal Component Analysis



# Comparisons of classification methods



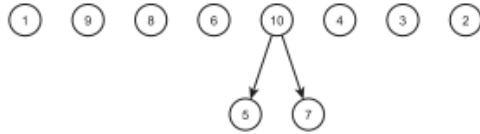
## Minimum Spanning Tree



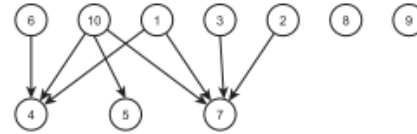
# Regularized Hasse diagrams



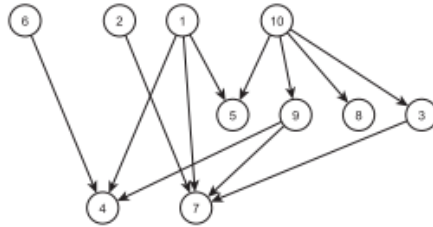
$t^* = 0.92$



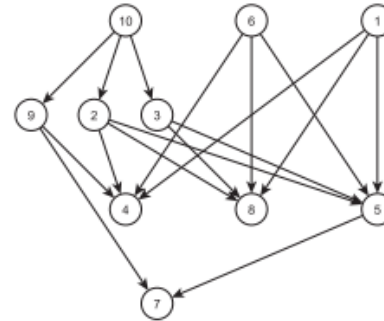
$t^* = 0.81$



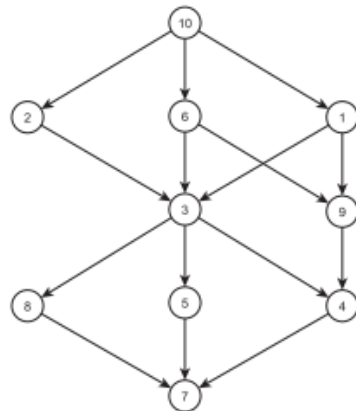
$t^* = 0.73$



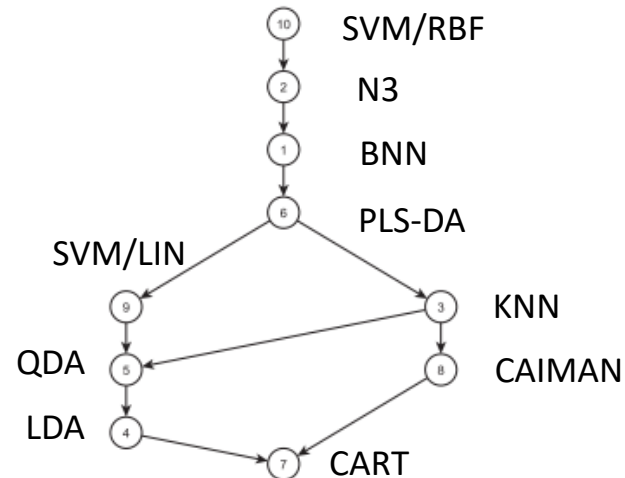
$t^* = 0.64$



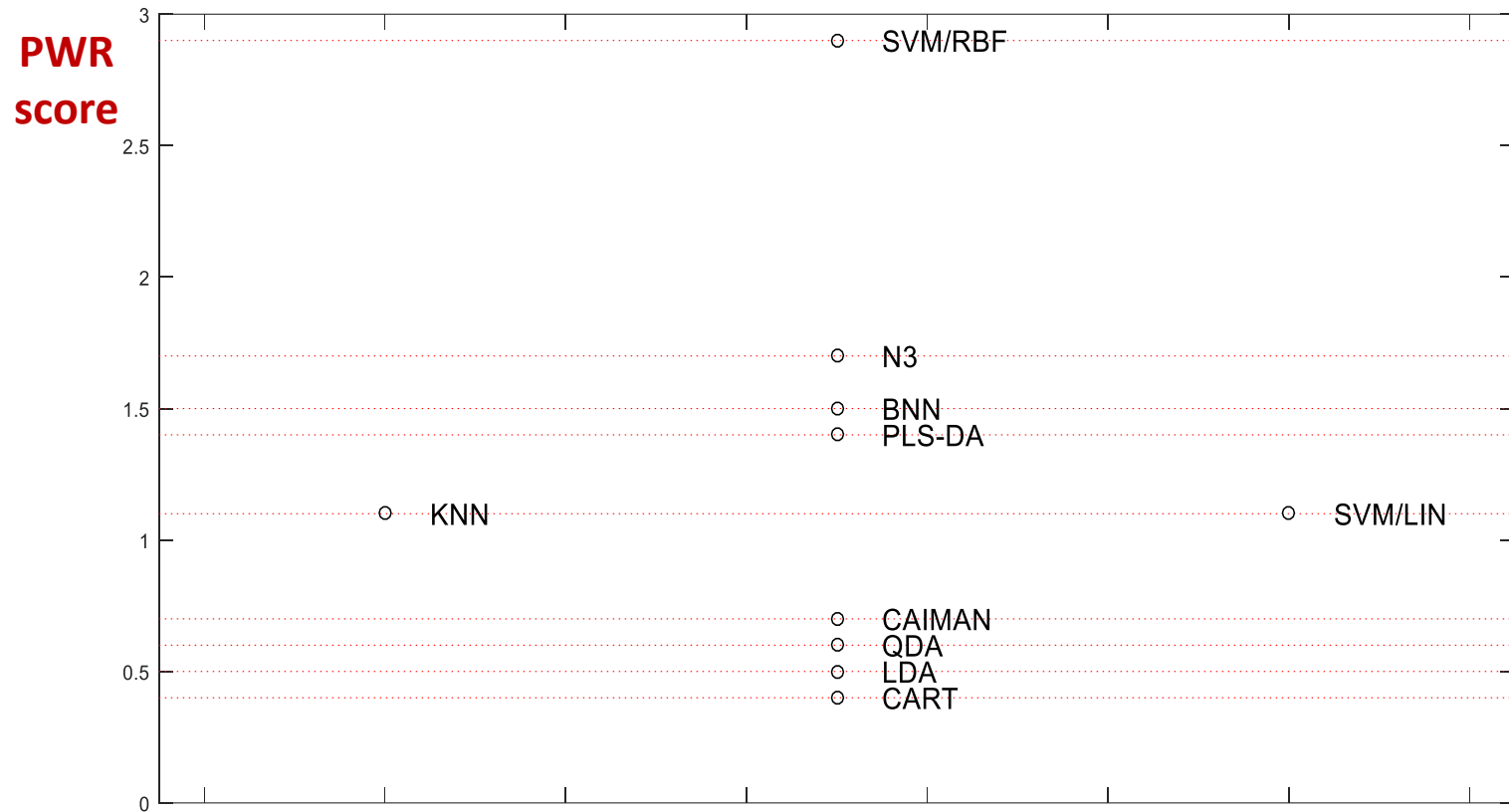
$t^* = 0.58$



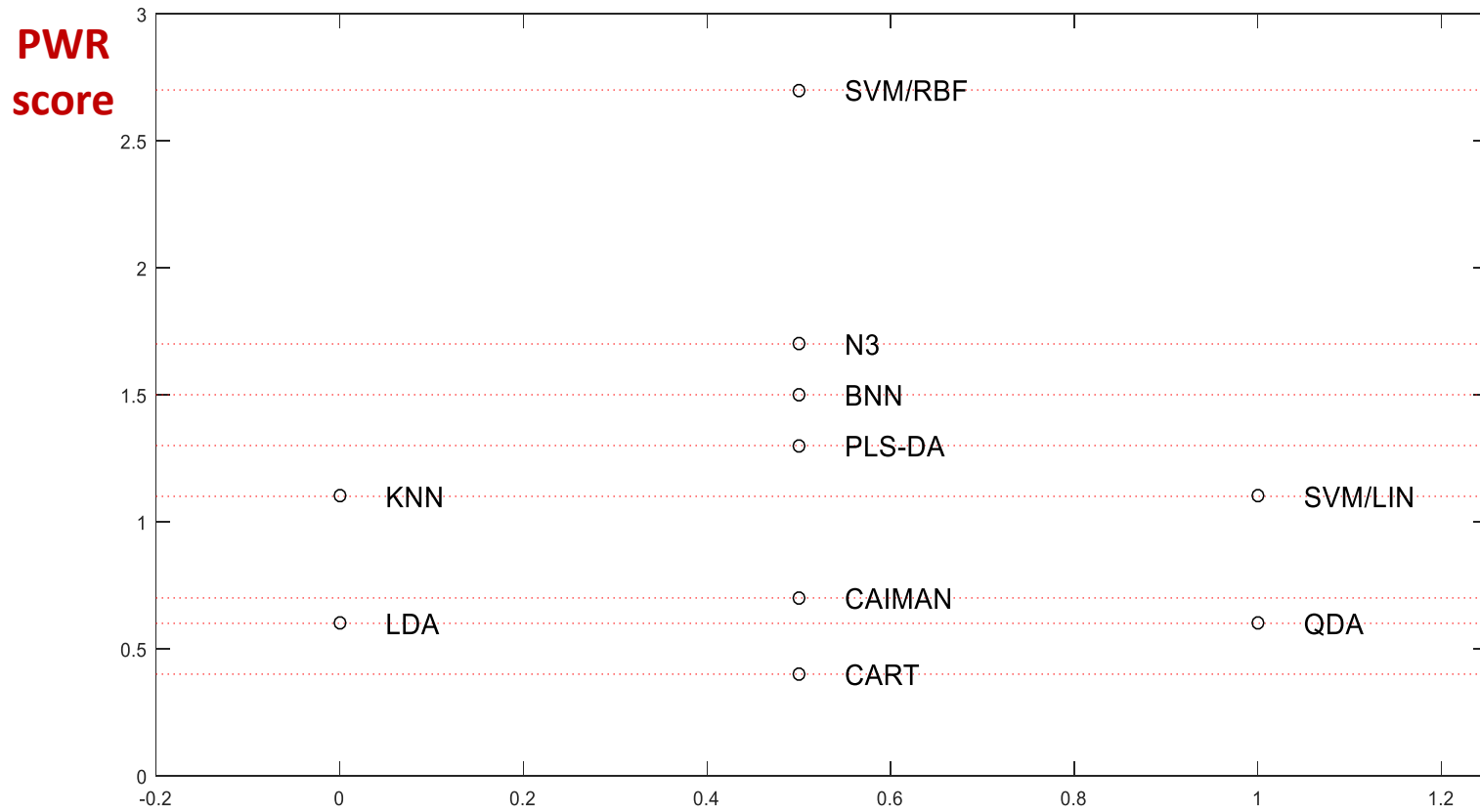
$t^* = 0.55$



# PWR diagrams ( $t^* = 0.5$ )



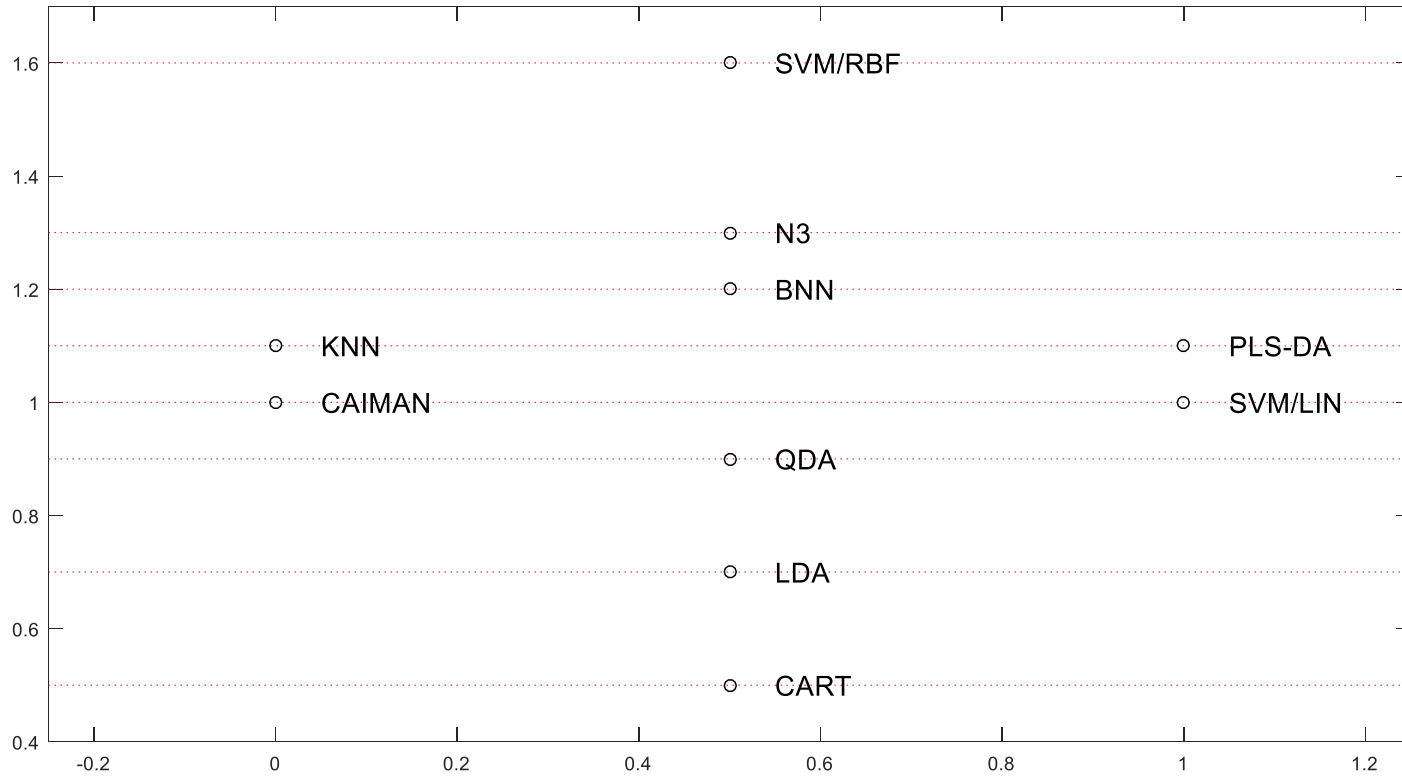
# PWR diagrams ( $t^* = 0.6$ )



# PWR diagrams ( $t^* = 0.8$ )



**PWR  
score**



# Anilines data set



45 anilines described by 4 criteria:

1. log Kow (octanole-water partition coeff.)
2. log VP (vapor pressure)
3. Biodegradability (1: yes; 2: no)
4. PNEC (Predicted No-Effect Concentration)

Study focused on:

1. Hasse diagram (HD)
2. From HD to MonteCarlo ranking
3. From HD to Average ranking

L. Carlsen (2006), A combined QSAR and partial order ranking approach to risk assessment, *SAR and QSAR in Environmental Research*, 17, 133-146.



# Anilines Hasse diagrams

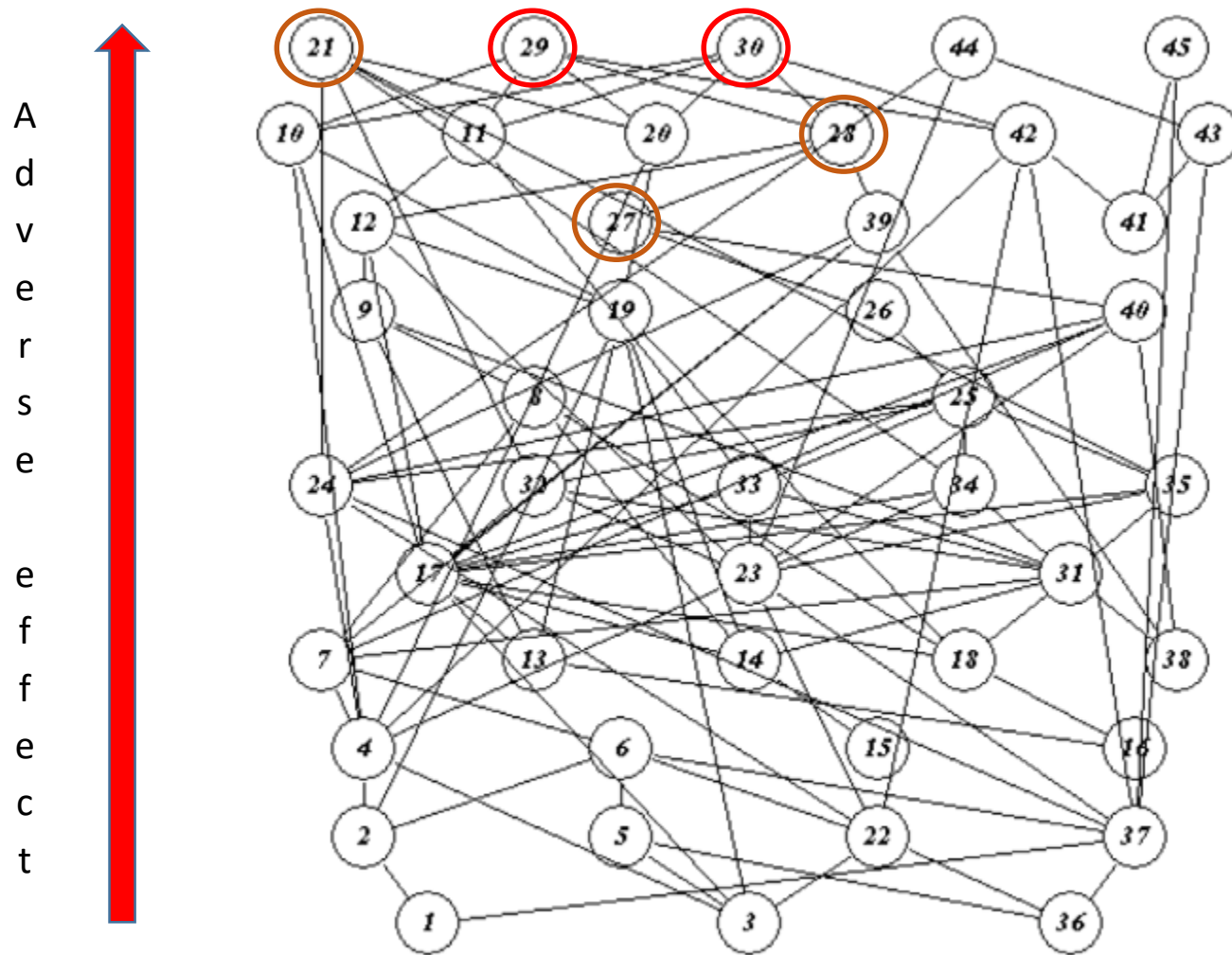
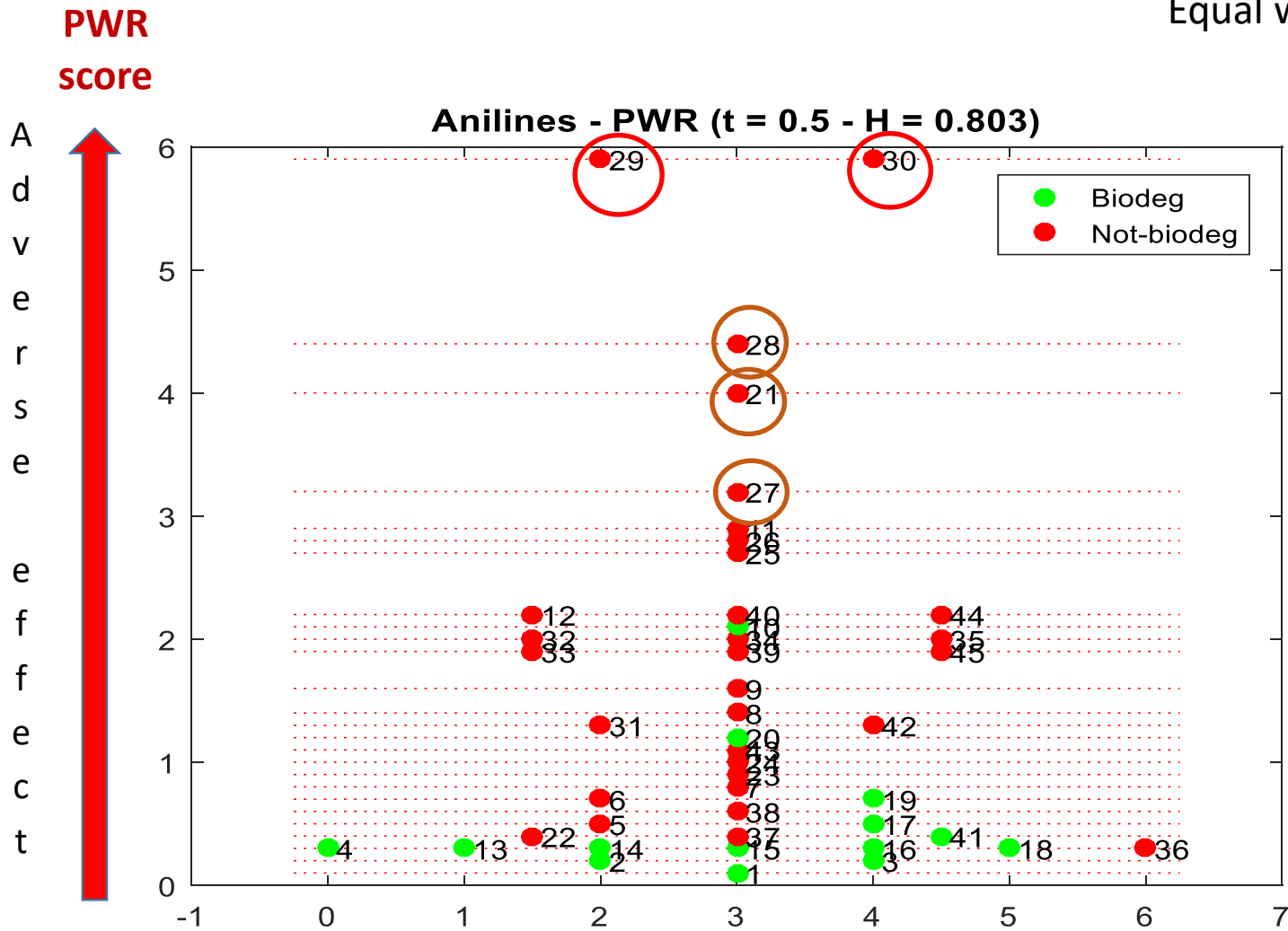


Figure 3. Hasse diagram of the 45 anilines based on the 4 descriptors given in table 2. The single compounds are identified through their ID (cf. table 2).

# Anilines: PWR diagram ( $t^* = 0.5$ )



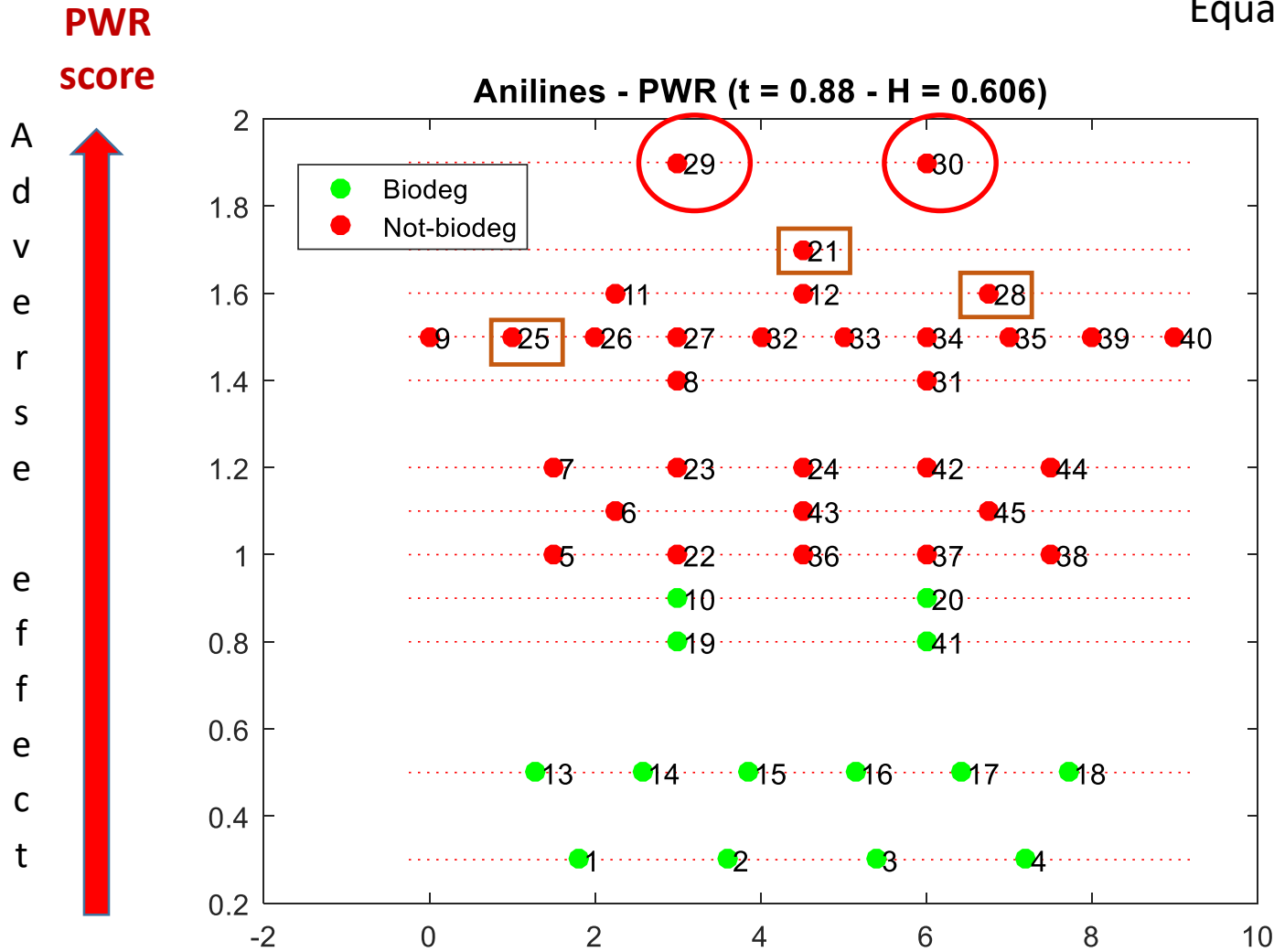
Equal weights



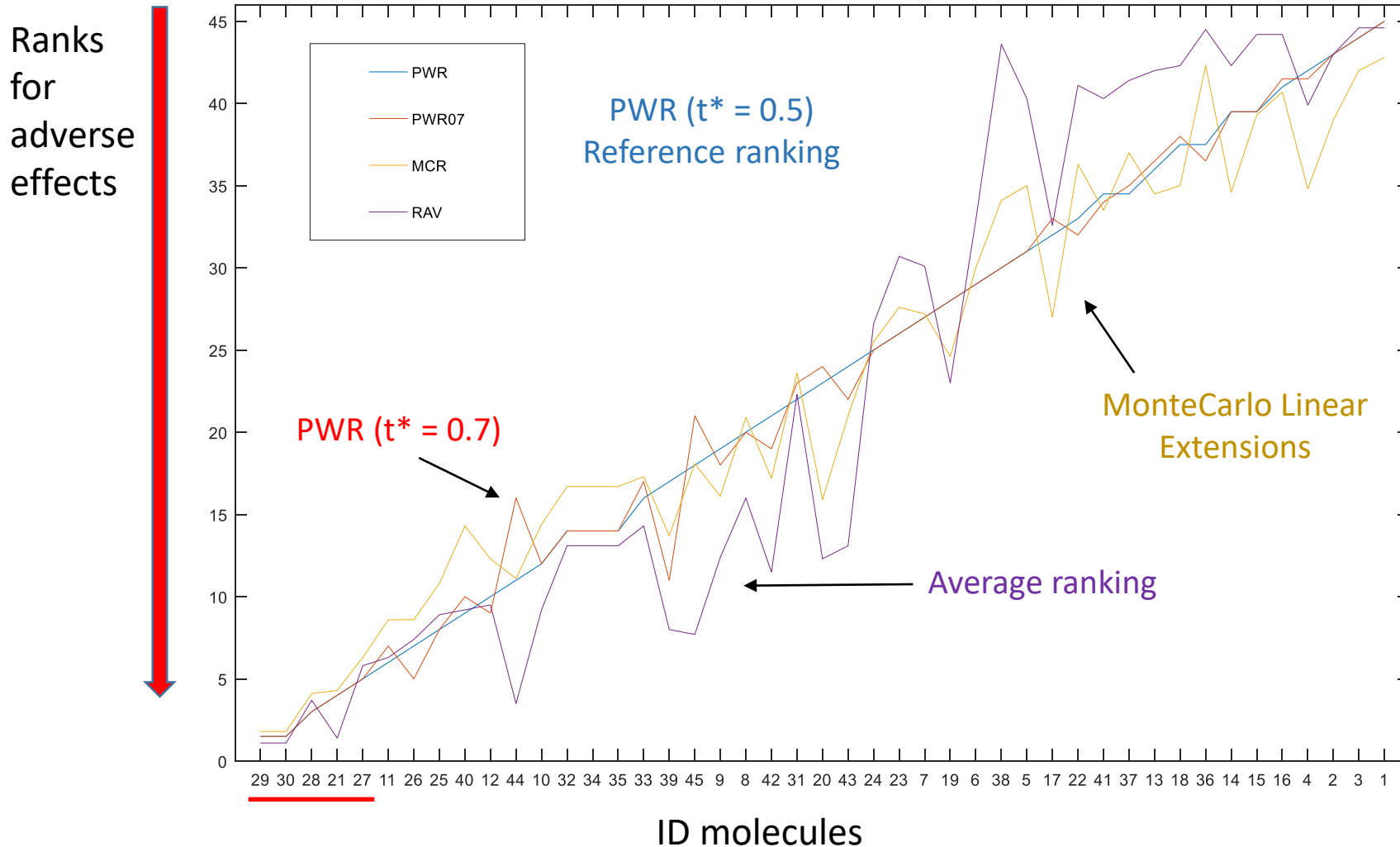
# Anilines: PWR diagram ( $t^* = 0.88$ )



Equal weights



# Anilines: ranks comparison



# Conclusions

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- **Possibility to weight the criteria**
- **Threshold selection offers different opportunities to rank the objects**
- **The Hasse transform from tournament table produces a family of regularized Hasse diagrams, thus also allowing a reduction of incomparabilities**
- **PWR is able to rank objects by a well founded theory**
- **PWR can remove inconsistencies from the tournament table**
- **PWR diagrams introduce a quantitative axis**
- **PWR diagrams can recover several incomparabilities present in the Hasse diagrams**
- **Statistical analysis can be performed on both the family of regularized-Hasse diagrams and the set of PWR rankings**