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Three-dimensional principal component analysis employed for the study of the β-glucosidase production of *Lentinus edodes* strains

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Abstract

The effect of cation type and concentration and fermentation time on the β-glucosidase production of four strains of *Lentinus edodes* was determined. Three-dimensional principal component analysis (3D-PCA) followed by nonlinear mapping technique (NLMAP) was employed for the assessment of similarities and dissimilarities between the enzymatic activities. No linear relationship was found between the effect of cations on the enzyme production and their ion radii, concentration and charge. Enzyme production was similar between 20 and 40 days of fermentation then changed considerably. The enzyme activities of strains also showed marked differences. The results proved that 3D-PCA followed by NLMAP is a valuable tool for the evaluation of three-dimensional data matrices in biology and microbiology too.

Keywords: β-Glucosidase production; *Lentinus edodes* strains; Three-dimensional principal component analysis

1. Introduction

Principal component analysis (PCA) a versatile and easy-to-use multivariate mathematical–statistical method has been developed for the extraction of maximal information from large data matrices containing numerous columns and rows [1]. PCA makes possible the elucidation of the relationship between the columns and rows of any data matrix without being one of the dependent variable. PCA has been frequently used in many fields of up-to-date research [2–4]. As the resulting matrices of PC loadings and variables are generally multidimensional, they cannot be evaluated by visual methods. Nonlinear mapping technique (NLMAP) has been developed for the reduction of the dimensionality of such matrices [5].

However, traditional PCA is a typical multivariate two-way statistical method unsuitable for the evaluation of three or more dimensional data matrices. A three-way PCA model (3D-PCA) has been developed independently and simultaneously and has been called parallel factor analysis (PARAFAC) [6], and canonical decomposition (CANDECOMP) [7]. A tutorial for PARAFAC model [8], the development of a

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direct fitting algorithm [9] and its application in chromatography [10] have been recently reported. The Tucker model of 3D-PCA has also been developed for the assessment of the similarities and dissimilarities between the members of three-dimensional data matrices [11,12]. The improvement of the method has also been published [13]. These techniques have been successfully used in many fields of up-to-date data evaluation such as the analysis of retention data in normal phase high-performance liquid chromatography [14], environmental analysis [15], person perception analysis in psychology [16], and medium-rank second-order calibration [17].

The concept of utilising excess biomass or wastes from agricultural and agro-industrial residues to produce energy, feeds or foods and other useful products is not necessarily new. For centuries, agricultural residues and wood have been used as sources of fuel, food, construction materials and papermaking, as well as for other purposes. Because of their capacity to degrade wood, white rot fungi are of increasing biotechnological interest [18]. They produce a wide range of extracellular enzymes that enable them to degrade insoluble lignocellulosic substrates into soluble substances, which can be uptaken by the mushroom as nutrition [19,20]. When degrading cellulose ultimately to glucose, the fungi utilise an assortment of extracellular hydrolytic enzymes, including endoglucanases (EC 3.2.1.94), exoglucanases (EC 3.2.1. 91) and β-glucoside-glucohydrolases (β-glucosidases, EC 3.2.1.21) acting sequentially and cooperatively. The different abilities of mushroom species to grow and fruit on a particular lignocellulosic substrate are determined by both fungus- and substrate-associated factors [21]. β-Glucosidases catalyse the hydrolysis of alkyl- and aryl-β-glucosides, diglucosides and oligosaccharides. The main role of β-glucosidase in the saccharification of cellulose is the degradation of cellobiose, an inhibitor of the depolymerizing enzymes, and cello-oligosaccharides to glucose.

The objectives of the study were the determination of the production of β-glucosidase during the complete life cycle of *Lentinus edodes* strains cultivated in liquid media composed of agro-industrial residues; the application of 3D-PCA for the separation of the effect of the composition of culture media, fermentation time and mushroom species on the production of β-glucosidase. The results may contribute to the better understanding of the underlying biochemical and biophysical processes and can find potential applications in the biotransformation of lignocellulose biomass. To the best of our knowledge, 3D-PCA has never been employed for the evaluation of the results of such type of mycological studies.

2. Experimental

2.1. Materials

$MgSO_4 \cdot 7H_2O$, $CaCl_2$, NaCl, $ZnSO_2 \cdot 7H_2$, $FeCl_3 \cdot 6H_2O$, $MnSO_4 \cdot H_2O$, CH_3COOH, CH_3COONa, NaOH and glycine (each of pro analysis quality) were purchased from Merck (Darmstadt, Germany); *o*-nitrophenyl-β-D-glucopiranoside (99 + %) and *o*-nitrophenol (98%) were purchased from Sigma-Aldrich (Steinheim, Germany). Each chemical has been employed as received.

2.2. Organisms and culture conditions

Strains of *L. edodes* (Berk.) Sing. (*L.e.1-3*, *L.e.16-3*, *L.e.6-6* and *L.e.am*) were taken from the culture collection of the National Agronomical Station (Oeiras, Portugal). They were maintained on potato dextrose agar (PDA) (Merck) at 4°C. They were cultivated in a liquid medium [22,23] in Erlenmeyer flasks of 1 l. Culture media was composed of 200 ml of distilled water, 200 ml of liquid medium, and 2.5 ml sawdust extract/l medium. Sawdust extract was prepared by boiling 200 g of chestnut sawdust in 1 l of distilled water for 1 h, then it was filtered and centrifuged. Cations in various concentrations were added to the media (see Tables 1–4). The medium was sterilised at 121°C for 20 min, cooled to 26°C and inoculated by adding a piece of agar (about 10 mm of diameter) with mycelium. Cultures were incubated at 24 ± 2°C in the dark for 30 days, then they were transferred to the fructification room (18 ± 2°C) with 12-h light/day for 30 days.

2.3. Determination of the activity of β-glucosidase

Each 10th day samples were taken from the culture medium under sterile conditions; they were cen-

Table 1
Effect of cations on the β-glucosidase activities of the strain (*L.e.1-3*)
No activities was observed at 10 days.

No.	Cation	Concentration (ppm)	Days of sampling				
			20	30	40	50	60
1	Mg(II)	0	0	0.66	0.66	1.09	0.71
2		84.1	0.12	0.37	1.31	1.60	1.68
3		168.2	0.09	0.36	1.09	1.43	1.41
4		252.3	0	0.36	1.33	3.67	2.77
5	Mn(II)	0	0	0.87	1.15	3.49	4.43
6		0.0233	0.14	0.59	1.60	2.17	2.74
7		0.0466	0.19	0.58	2.59	4.51	6.16
8		0.07	0	0.36	1.33	3.67	2.77
9	Ca(II)	0	0	0.65	0.96	1.53	2.19
10		0.3	0.20	0.42	2.30	2.76	2.62
11		0.6	0.09	0.35	0.98	1.35	1.48
12		0.9	0	0.36	1.33	3.67	2.77
13	Cu(II)	0	0	0.56	1.25	1.15	0.77
14		0.01	0.13	0.56	1.23	1.86	1.59
15		0.02	0.20	0.58	1.70	2.19	3.29
16		0.03	0	0.36	1.33	3.67	2.77
17	Na(I)	0	0	0.72	0.99	1.77	2.20
18		0.04	0.15	0.63	1.39	2.68	2.55
19		0.08	0.21	0.74	1.38	1.55	1.47
20		0.12	0	0.36	1.33	3.67	2.77
21	Fe(III)	0	0	0.58	0.66	0.83	1.40
22		0.0233	0.09	0.37	1.00	1.89	1.14
23		0.0466	0.15	0.57	1.13	2.54	2.65
24		0.07	0	0.36	1.33	3.67	2.77
25	Zn(II)	0	0	0.50	0.37	0.90	0.83
26		0.0383	0.10	0.20	1.04	1.46	1.20
27		0.0766	0.07	0.26	0.95	1.15	1.15
28		0.115	0	0.36	1.33	3.67	2.77

trifuged at 20,000 × *g* for 20 min, and the activity of β-glucosidase was determined by visible spectrophotometry (UNICAM 8700 Spectrophotometer, Cambridge, England) at 400 nm in a cuvette of 10 mm length [24]. Reaction mixture contained 250 μl of *o*-nitrophenyl-β-D-glucopiranoside (1.5 mg/ml), 250 μl of acetate buffer (0.2 M, pH 4.0) and 500 μl of culture medium appropriately diluted. After 60 min of incubation at 37°C, the reaction was stopped by adding 1 ml of 0.4 M glycine–NaOH buffer (pH 10.8), and the absorption was measured.

2.4. Data evaluation by multivariate methods

The Tucker model of 3D-PCA has been employed for the calculations. The data matrix consisted of the β-glucosidase activities determined at 28 ion concentrations (factor A), by four strains of *L. edodes* (factor B), and at five fermentation times (factor C) compiled in Tables 1–4. The dimensions of component matrices have been arbitrarily defined as 8, 3, 3. The dimensionality of the calculated component matrices has been reduced to two by NLMAP. The iteration has been carried out to the point where the difference between the last two iterations was lower than 10^{-8}. In order to elucidate the effect of the reduction of component matrices, the same calculations have been carried out with the component matrix of 3, 3, 2. The results obtained by the application of 8, 3, 3 and 3, 3, 2 component matrices were compared by calculating linear regressions between the first and second coordinates of the nonlinear maps (component matrix 8, 3, 3) and the first and second coordinates of the corresponding component matrices 3, 3, 2.

Table 2
Effect of cations on the β-glucosidase activities of the strain (*L.e.am*)
No activities was observed for 10 days.

No.	Cation	Concentration (ppm)	Days of sampling				
			20	30	40	50	60
1	Mg(II)	0	0	0.79	0.97	1.10	1.12
2		84.1	0.24	0.71	1.71	2.55	2.73
3		168.2	0.26	0.38	1.92	2.52	2.61
4		252.3	0	0.77	0.88	1.69	1.88
5	Mn(II)	0	0	0.85	2.48	5.30	7.75
6		0.0233	0.43	1.27	2.93	9.37	10.26
7		0.0466	0.48	0.77	2.99	5.09	6.35
8		0.07	0	0.77	0.88	1.69	1.88
9	Ca(II)	0	0	0.42	1.47	1.52	2.34
10		0.3	0.49	0.70	3.56	5.63	6.33
11		0.6	0.20	0.36	1.36	1.80	1.90
12		0.9	0	0.77	0.88	1.69	1.88
13	Cu(II)	0	0	0.81	2.09	2.55	5.24
14		0.01	0.41	0.47	1.55	3.17	3.40
15		0.02	0.31	0.50	1.90	3.65	4.27
16		0.03	0	0.77	0.88	1.69	1.88
17	Na(I)	0	0	0.56	2.73	5.44	7.36
18		0.04	0.24	0.53	1.75	2.61	2.15
19		0.08	0.31	0.58	1.47	2.15	2.01
20		0.12	0	0.77	0.88	1.69	1.88
21	Fe(III)	0	0	0.41	0.76	1.10	1.71
22		0.0233	0.38	0.53	2.08	7.50	7.89
23		0.0466	0.30	0.82	1.87	5.20	6.20
24		0.07	0	0.77	0.88	1.69	1.88
25	Zn(II)	0	0	1.04	1.14	1.47	1.80
26		0.0383	0.38	2.01	3.32	4.63	5.31
27		0.0766	0.30	0.68	1.50	4.50	6.08
28		0.115	0	0.77	0.88	1.69	1.88

The relationship between the effect of ions and their physicochemical parameters was assessed by stepwise regression analysis [25]. In the traditional multivariate regression analysis, the presence of independent variables exerting no significant influence on the dependent variable lessens the significance level of the independent variables that significantly influence the dependent variable. Stepwise regression analysis overcomes this difficulty by eliminating automatically from the selected equation the insignificant independent variables increasing in this manner the reliability of the calculation. The first and second coordinates of the two-dimensional nonlinear map of the component matrix **A** were separately the dependent variables. The concentration (ppm), charge, ion radii and their combinations (ppm × charge, ppm × ion radii, charge × ion radii, ppm × charge × ion radii) were the dependent variables. The number of accepted variables was not limited; the significance level was set to 95% in both instances.

Table 3
Effect of cations on the β-glucosidase activities of the strain (*L.e.16-3*)
No activities was observed at 10 days.

No.	Cation	Concentration (ppm)	Days of sampling				
			20	30	40	50	60
1	Mg(II)	0	0	0.94	1.07	1.25	0.80
2		84.1	0.32	0.36	1.57	2.35	2.83
3		168.2	0.46	0.36	1.20	1.32	1.29
4		252.3	0	0.45	0.74	0.99	1.02
5	Mn(II)	0	0	0.89	0.99	1.19	0.93
6		0.0233	0.56	0.90	1.91	3.21	3.00
7		0.0466	0.50	0.76	1.52	2.44	2.83
8		0.07	0	0.45	0.74	0.99	1.02
9	Ca(II)	0	0	1.23	0.83	1.15	0.68
10		0.3	0.37	0.44	1.10	1.49	1.06
11		0.6	0.39	0.68	1.52	2.18	1.98
12		0.9	0	0.45	0.74	0.99	1.02
13	Cu(II)	0	0	0.45	1.53	2.90	3.68
14		0.01	0.48	0.53	1.75	2.9	1.94
15		0.02	0.33	0.36	1.14	1.51	1.29
16		0.03	0	0.45	0.74	0.99	1.02
17	Na(I)	0	0	0.84	0.44	1.42	0.97
18		0.04	1.04	0.81	1.72	2.06	2.32
19		0.08	0.56	1.07	2.42	4.14	4.48
20		0.12	0	0.45	0.74	0.99	1.02
21	Fe(III)	0	0	0.84	1.12	4.07	3.49
22		0.0233	0.52	0.92	3.21	5.30	5.97
23		0.0466	0.67	1.29	3.39	4.55	4.30
24		0.07	0	0.45	0.74	0.99	1.02
25	Zn(II)	0	0	1.04	1.65	2.85	3.73
26		0.0383	0.47	0.79	1.25	2.22	2.14
27		0.0766	0.64	1.32	3.09	6.62	6.88
28		0.115	0	0.45	0.74	0.99	1.02

Table 4
Effect of cations on the β-glucosidase activities of the strain (*L.e.6-6*)
No activities was observed at 10 days.

No.	Cation	Concentration (ppm)	Days of sampling				
			20	30	40	50	60
1	Mg(II)	0	0	0.50	0.52	0.98	0.66
2		84.1	0.11	0.37	0.60	1.09	1.18
3		168.2	0.28	0.61	1.18	1.78	1.93
4		252.3	0	0.45	0.83	0.86	0.69
5	Mn(II)	0	0	0.75	0.67	1.42	0.77
6		0.0233	0.25	0.59	0.81	0.89	0.54
7		0.0466	0.26	0.78	1.30	2.55	2.01
8		0.07	0	0.45	0.83	0.86	0.69
9	Ca(II)	0	0	0.75	0.73	1.31	0.67
10		0.3	0.51	0.51	1.30	1.49	1.98
11		0.6	0.23	0.49	0.68	0.85	0.78
12		0.9	0	0.45	0.83	0.86	0.69
13	Cu(II)	0	0	0.79	0.69	1.00	1.29
14		0.01	0.24	0.76	0.86	0.74	0.97
15		0.02	0.27	0.65	0.71	0.79	0.69
16		0.03	0	0.45	0.83	0.86	0.69
17	Na(I)	0	0	0.45	0.53	2.53	1.86
18		0.04	0.13	0.65	1.24	1.73	1.41
19		0.08	0.38	1.01	1.79	5.24	4.12
20		0.12	0	0.45	0.83	0.86	0.69
21	Fe(III)	0	0	0.45	0.36	2.43	1.57
22		0.0233	0.35	0.68	1.43	5.03	4.55
23		0.0466	0.33	0.77	0.92	1.85	1.44
24		0.07	0	0.45	0.83	0.86	0.69
25	Zn(II)	0	0	0.94	0.84	2.57	2.27
26		0.0383	0.07	0.45	4.74	5.47	6.61
27		0.0766	0.26	0.88	0.85	1.19	0.84
28		0.115	0	0.45	0.83	0.86	0.69

Software for 3D-PCA was taken from N-WAY TOOLBOX, http:\\newton.mli.kvl.dk\foodtech.html prepared by Dr. C.A. Andersson and Dr. R. Bro. Softwares for NLMAP has been prepared by Dr. Barna Bordás, Plant Protection Institute, Hungarian Academy of Sciences (Budapest, Hungary), and software for stepwise regression analysis has been purchased from Compudrug (Budapest, Hungary).

3. Results and discussion

The enzymatic activities are compiled in Tables 1–4. The enzymatic activities show considerable dif-

ferences indicating that the type and concentration of cations, the nature of strains and the fermentation time equally influence the activity of β-glucosidase.

The main parameters of the 3D-PCA are compiled in Table 5. 3D-PCA using the model 8, 3, 3 reached the convergence criteria after the third iteration step; the total variance explained being 96.06%. This finding indicates that the reduction of the dimensionality of the original data matrix 24, 4, 5 to 8, 3, 3 can be performed with only 3.94% loss of information. Unfortunately, the 3D-PCA does not define these theoretical factors as concrete physicochemical entities only indicates their mathematical possibility. The first three factors explain the overwhelming majority of variance (86.68%) suggesting the basic similarities between the effect of the various cations, strains and fermentation times. The data further show that the impact of the second and third factors of component matrices **A** and **B** is also important.

The main results of 3D-PCA using a component matrix of 3, 3, 2 are compiled in Table 6. The considerable reduction in the dimensions of component matrix resulted only a 1.16% loss of variance explained indicating that the reduced component matrix is also suitable for the evaluation of the same data matrix.

The two-dimensional nonlinear map of component matrix **A** is shown in Fig. 1. Only cations added at the highest concentration to the fermentation broth form a clear-cut cluster; the other points representing various cations at different concentrations are widely distributed on the map. This distribution can be explained by the supposition that both the character and concentration of cations exert a similar impact on the β-glucosidase production, and the effect observed is the results of the interplay of various parameters. The results of stepwise regression analysis entirely supports our previous qualitative conclusions. It did not find significant relationships between the effect of cations on the production of β-glucosidase and their physicochemical parameters included in the calculation. It can be assumed that other parameters not included in the calculation may have a significant impact on the effect of cations.

Table 5
Main parameters of the three-dimensional PCA using component matrix of 8, 3, 3
No. of iterations: 3; total variance explained: 96.06%.

No.	No. of factors of component matrices			Variance explained of the total variance explained (%)
	A	**B**	**C**	
1	1	1	1	86.68
2	2	2	1	6.91
3	3	3	1	4.24
4	3	1	2	0.24
5	1	3	2	0.24
6	4	1	2	0.23
7	1	2	2	0.20

Table 6
Main parameters of the three-dimensional PCA using component matrix of 3, 3, 2
No. of iterations: 8; total variance explained: 94.90%.

No.	No. of factors of component matrices			Variance explained of the total variance explained (%)
	A	**B**	**C**	
1	1	1	1	87.74
2	2	2	1	6.99
3	3	3	1	4.29
4	3	1	2	0.26
5	1	3	2	0.23
6	4	2	2	0.22
7	2	2	2	0.10

Strains of *L.e.16-3* and *L.e.6-6* are very near to each other on the two-dimensional nonlinear map of component matrix **B**, while strains *L.e.1-3* and *L.e.am* are far away from each other and from the cluster of *L.e.16-3* and *L.e.6-6* (Fig. 2). This result emphasizes the basic similarity of strains *L.e.16-3* and *L.e.6-6* and the differences among the other strains.

The activity of β-glucosidase is similar between 20 and 40 days of fermentation as indicated on the two-dimensional nonlinear map of component matrix **C** (Fig. 3). However, the distribution of points on the map indicates that the enzyme production becomes markedly different at 50 and 60 days of fermentation.

Significant linear relationships have been found between the first and second coordinates of the two-dimensional nonlinear maps of matrix **A** and the first two members of the component matrix **A** 3, 3, 2 ($r_{calc.}$ were 0.4919 and 0.6301, respectively). No significant correlation was found for matrices **B**, and only the first coordinates of matrices **C** were significantly

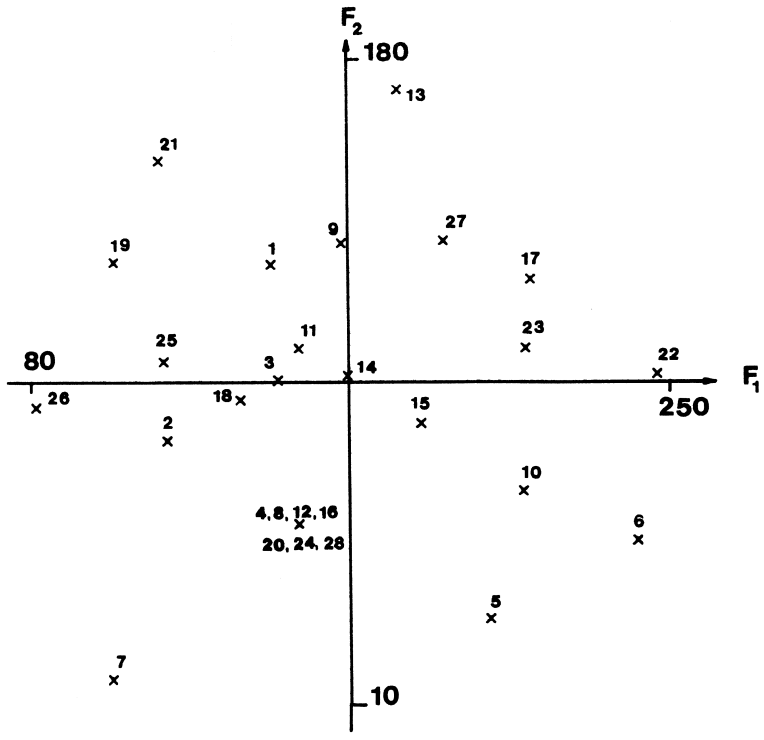

Fig. 1. Similarities and dissimilarities between the effect of cations on the β-glucosidase production simultaneously taking into consideration each strains of *L. edodes* and each fermentation time. Two-dimensional nonlinear map of component matrix **A**. No. of iterations: 738; maximum error: 7.61×10^{-2}. Numbers refer to cation type and concentration in Tables 1–4.

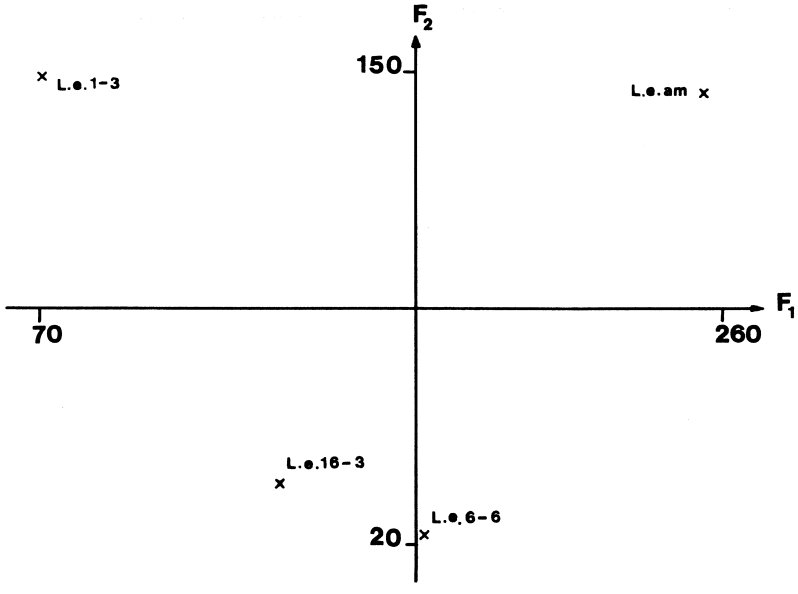

Fig. 2. Similarities and dissimilarities between the effect of *L. edodes* strains on the β-glucosidase production simultaneously taking into consideration each cation type and concentration and each fermentation time. Two-dimensional nonlinear map of component matrix **B**. No. of iterations: 19; maximum error: 3.48×10^{-6}.

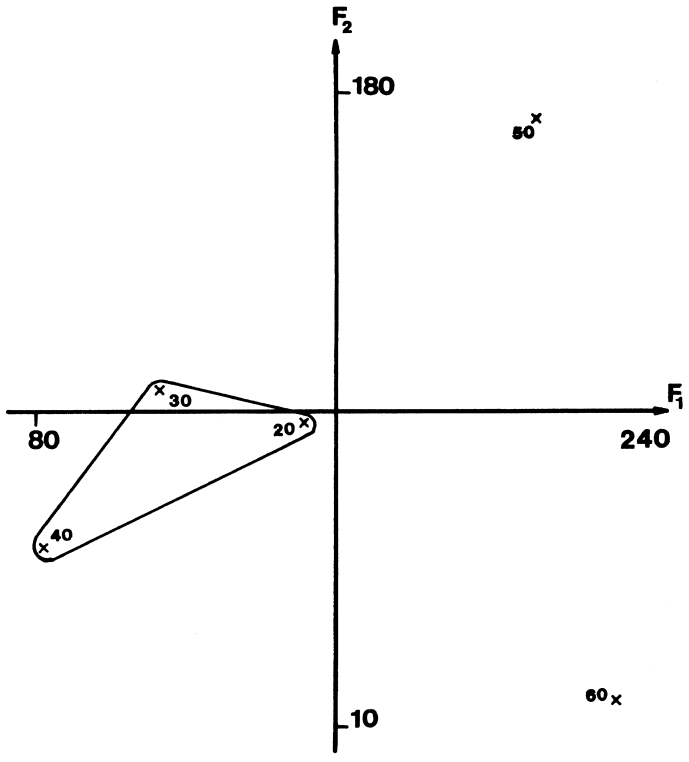

Fig. 3. Similarities and dissimilarities between the effect of fermentation time on the β-glucosidase production simultaneously taking into consideration each strains of *L. edodes* and each type and concentration of cations. Two-dimensional nonlinear map of component matrix **C**. No. of iterations: 121; maximum error: 4.17×10^{-3}. Numbers refer to fermentation time in days.

correlated ($r_{\text{calc.}} = 0.9206$). This finding suggests that the reduction of the dimensionality of component matrices exert a negligible effect on the variance explained but slightly modify the similarities and dissimilarities among the elements of the original matrix.

It can be concluded from the results that 3D-PCA can be successfully used for the separation of the effect of various fermentation parameters (composition of culture media, fungal strains, fermentation time) on the production of β-glucosidase. Nonlinear mapping technique applied to the component matrices facilitates the evaluation of such multidimensional data structures.

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