Chemometric approach based characterization and selection of mid-early cauliflower for bioactive compounds and antioxidant activity

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Abstract The present study was aimed to analyse bioactive compounds (total phenolics, ascorbic acid and sinigrin) and antioxidant activity in 14 mid-early cauliflower genotypes. Significant differences (pb 0.05) were observed among the genotypes for all bioactive compounds and antioxidant activity. Total phenolics content of curd were ranged from 20.36 to 48.93 mg gallic acid equivalent (GAE) 100 g⁻¹ fresh weight (FW) which showed 2.5 times variation. The ascorbic acid content was maximum in DC522 (88.53 mg 100 g⁻¹ FW) followed by Pusa Sharad (65.64 mg 100 g⁻¹ FW) while minimum in DC310 (39.62 mg 100 g⁻¹ FW). Wide variation was observed for cupric reducing antioxidant capacity and ferric reducing antioxidant power ranging from 9.04 to 20.83 mg GAE 100 g⁻¹ FW and 13.11 to 26.31 mg GAE 100 g⁻¹ FW, respectively. Sinigrin was found to be highest in DC306 (39.50 µmol 100 g⁻¹ FW) for leaf and in DC326 (36.93 µmol 100 g⁻¹ FW) for curd sample. The cauliflower genotypes were classified based on chemometric

approaches namely principal component analysis (PCA) and agglomerative hierarchical clustering (AHC). The first two principal components (PC1 and PC2) explained 50.62% and 23.28% of total variance, respectively. The AHC as revealed by heat map classified cauliflower genotypes into four main groups based on measured traits. The information is useful for developing varieties and/or hybrids rich in bioactive compounds and antioxidant activity.

Keywords Cauliflower · Bioactive compounds · Antioxidant · PCA · AHC

Introduction

Brassica vegetables are important sources of dietary nutrients and good for health due to presence of phytochemical compounds namely vitamins, phenolics and glucosinolates (Gratacos-Cubarsi et al. 2010). These compounds have antioxidant and anti-carcinogenic activities and reduce ailments (Deng et al. 2013; Bhandari and Kwak 2015). Cauliflower (*Brassica olerace* var. *botrytis* L.) belongs to Brassicaceae family and rich source of natural antioxidants such as phenolics (Picchi et al. 2012), ascorbic acid (Ferrerres et al. 2007), carotenoids (Jahangir et al. 2009) and glucosinolates (Bhandari and Kwak 2015). The main edible parts of cauliflower is a ‘curd’ (a highly suppressed pre-floral apical meristem) and contains various bioactive compounds namely glucosinolates, ascorbic acid, polyphenols, and carotenoids. It is known to have anti-cancerous property due to presence of glucosinolates (Razis and Noor 2013). Among glucosinolates, sinigrin (2-propenyl glucosinolate) is the major one and is precursor of anti-cancerous compound allyl isothiocyanate. The crop is

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rich in most abundant antioxidant polyphenolics (Cartea et al. 2011). These compounds also involve in enzyme regulation and cell cycle control. The content of these compounds varies with varieties, plant tissue, soil nutrient, crop growing season and other external factors (Bhandari and Kwak 2014). Ascorbic acid is a water-soluble vitamin which act against cell death and serve as agent for lipid peroxidation chain-breakage (Gliszczynska-Swiglo et al. 2006; Kumar et al. 2011). Therefore, emphasis has been given to identify genotypes rich in such compounds in cauliflower.

In India, cauliflower is a widely grown winter vegetable crop which accounts for 5.3% share of country's total vegetable production (NHB 2016). A large number of varieties of cauliflower are grown by farmers but the information on the concentration of bioactive compounds and antioxidant activity was not available for those. However, few reports have been published regarding the content of glucosinolate, ascorbic acid, phenolics and flavonoid in other *Brassica* crops (Cartea et al. 2011; Lee et al. 2012). Generation of information on antioxidant properties of Indian varieties will be useful as a reference material and also helpful for breeder and consumer. In the present study, fourteen genotypes/breeding lines of cauliflower were investigated for bioactive compounds and antioxidant activities. Besides, principal component analysis (PCA) and agglomerative hierarchical clustering (AHC) were used to classify the genotypes and to find relation between bioactive compounds and antioxidant activity to enable selection of genotypes with higher bioactive compounds and antioxidant activity for use in breeding programme.

Materials and methods

Plant materials

The plant materials comprised of fourteen diverse genotypes of cauliflower including commercial varieties and advanced breeding lines of mid-early maturity group. The seeds were sown in mid September on raised nursery beds at research farm of Division of Vegetable Science, ICAR-Indian Agricultural Research Institute, New Delhi, India. 1 month old seedlings were transplanted on raised bed at spacing of 60 × 45 cm. Each genotype had 20 plants which were arranged in randomized block design (RBD) with three replications. The recommended standard cultivation practices were followed for raising the crop as per Singh and Sharma (2003).

Estimation of total phenolics

Fresh curd sample (1 g) was grounded in 5 mL 100% ethanol. Then, the homogenate was centrifuged at 5000 rpm for 20 min and supernatant was separated. The centrifuged sample was re-extracted 5 times using 5 mL 80% ethanol every time and finally all the supernatants were pooled. The supernatant was filtered with Whatman No. 42 filter paper. The supernatant was dried through evaporation and finally dissolved in 5 mL distilled water from which different aliquots of 0.2 to 2 mL were taken in test tube and their volume was made to 3 mL. Folin–Ciocalteu reagent (0.5 mL) was added to each test tube and after 3 min, 2 mL of 20% Na₂CO₃ solution was added. The solution was mixed thoroughly and left for 60 min. Observation was recorded against the reagent blank at 650 nm absorbance in spectrophotometer. A standard curve was drawn with various concentrations of gallic acid. The total phenolics content was estimated according to the standard curve and expressed as mg GAE 100 g⁻¹ fresh weight (FW) (Malick and Singh 1980).

Estimation of ascorbic acid

The ascorbic acid was estimated as per the protocol given by Jagota and Dani (1982) was followed. Fresh curd sample (10 g) was added with equal quantity of activated charcoal. The mixture was grounded with equal volume of 6% metaphosphoric acid-EDTA solution and volume was made up to 50 mL with 4.5% metaphosphoric acid. The mixture was centrifuged at 5000 rpm for 10 min and filtered through Whatman No. 42 filter paper and collected in volumetric flask. A series of 0.1–0.6 mL working standard solution (L-ascorbic acid) was taken into test tubes. Then, 1.1–0.60 mL of 3% metaphosphoric acid was added to the test tubes and volume was made up to 1.2 mL. Then, 2.8 mL distilled water was added to each test tube to made volume to 4 mL and mixed well. Finally, 0.4 mL of folin–ciocalteu reagent was added, mixed and incubated for 10 min at room temperature. The contents were then centrifuged at 3000 rpm for 10 min. The blank solution was prepared by adding all the reagents except the ascorbic acid solution. After centrifugation, supernatant solutions were read against the blank solution in a spectrophotometer at 760 nm. The concentration of ascorbic acid in the sample was calculated from the slope of the ascorbic acid standard curve and expressed as mg of ascorbic acid 100 g⁻¹ fresh weight (FW).

Estimation of sinigrin

Sinigrin content in curd and leaf tissues was analysed as per procedure described by Tsao et al. (2002) with slight

modification. In brief, freshly harvested curd and leaf samples (1 g each) were extracted separately thrice with 50% (v/v) warm acetonitrile (25 mL) for 10 min. During sonication, the extracts were cooled to room temperature, filtered and concentrated to a volume of 1.5 mL. All samples were filtered through 0.45 µm syringe filter (Gelman Sciences Inc., Ann Arbor, MI, USA) and analysed by RP-HPLC (Alliance, Waters Corp., Milford, USA). The stock solution (100 µg mL⁻¹) of monohydrate sinigrin (Sigma-Aldrich) was prepared in HPLC grade water and stored at 4 °C. This was diluted to various concentrations (0.1–100 g mL⁻¹) to prepare calibration curve. Each point of the calibration was measured thrice and mean along with standard deviation were calculated. The HPLC was fitted with controller Empower 2[®] software programme, equipped with e2695 quaternary pump, auto injector (20 µL loop), and a 2998 PDA detector. A RP-18 column (250 mm × 4.6 mm × 5 µm) Supelco Discovery[®] was used as the stationary phase. Standard reference sinigrin (Sigma Aldrich) was analysed in RP-HPLC with a gradient system at a flow rate of 0.5 mL min⁻¹ using ACN: H₂O. The system was run with the following gradient programme: 99% A and 1% B (v/v) for 1 min, then linear increases to 50% each A and B in 5 min, held for 5 min and then brought back to 99% A and 1% B at 20 min. The stocks solutions were prepared in HPLC grade ACN and 20 µL volume of each sample was injected through auto injector (every time). Sharp peak was detected at λ_{max} of 227.5 nm. The retention time (t_R) and area of the identified sinigrin was recorded to further calculate concentration.

Antioxidant activity

Extraction of antioxidant

Fresh curd tissue (1 g) was crushed using mortar pestle with 5 mL of 100% ethanol. The sample was centrifuged at 5000 rpm for 15 min and re-extracted with 80% ethanol and finally the supernatants were pooled. The volume was made to 10 mL in volumetric flask with 80% ethanol and filtered through Whatman No. 42 filter paper. The sample extract was used for CUPRAC and FRAP assay.

Cupric reducing antioxidant capacity (CUPRAC) assay

The CUPRAC assay was done as per protocol described by Apak et al. (2004). Briefly, CuCl₂ (1 mL) was taken into a test tube containing 0.5 mL sample extract. Neocuprione (1 mL) and aqueous ammonium acetate (1 mL) buffer (pH 7) were added into each test tube. After that standard solution (50 µL) and distilled water (1040 µL) were added. Each test tube was shaken properly and incubated for 30 min. Finally, absorbance was measured at 450 nm in spectrophotometer. Antioxidant activity was calculated from the standard curve and expressed as mg GAE 100 g⁻¹ FW.

Ferric reducing antioxidant power (FRAP) assay

The FRAP assay was performed as described by Benzie and Strain (1996). Sample extract (25 µL) was taken into

Table 1 Bioactive compounds and antioxidant activity of fourteen mid early cauliflower genotypes

Cauliflower genotypes	Total phenolics (mg GAE 100 g ⁻¹ FW)	CUPRAC (mg GAE 100 g ⁻¹ FW)	FRAP (mg GAE 100 g ⁻¹)	Ascorbic acid (mg 100 g ⁻¹ FW)	Leaf sinigrin (µmol 100 g ⁻¹ FW)	Curd sinigrin (µmol 100 g ⁻¹ FW)
DC306	23.21 ± 0.36 ^{g,f}	9.04 ± 0.04 ^g	13.11 ± 0.47 ^e	54.71 ± 0.71 ^{d,e}	39.50 ± 0.08 ^a	29.91 ± 0.04 ^c
DC308	21.43 ± 0.71 ^{g,h}	12.65 ± 0. ^d	12.68 ± 0.04 ^e	40.17 ± 0.24 ^h	14.61 ± 0.08 ^{e,f}	28.55 ± 0.05 ^d
Pusa-Sharad	20.36 ± 0.36 ^h	10.92 ± 0.12 ^{e,f}	12.16 ± 0.47 ^c	65.64 ± 0.83 ^b	11.84 ± 0.10 ^{f,g}	23.94 ± 0.13 ^f
DC310	27.86 ± 1.43 ^d	10.65 ± 0.19 ^{e,f}	12.16 ± 0.47 ^c	39.62 ± 0.48 ^h	11.01 ± 0.11 ^g	8.45 ± 0.37 ^j
DC310-22	26.79 ± 1.07 ^{d,e}	14.48 ± 0.08 ^c	16.41 ± 0.94 ^d	46.24 ± 1.02 ^{g,f}	15.87 ± 0.17 ^{e,d}	9.01 ± 0.13 ^j
DC312	25.71 ± 0.71 ^{d,e}	12.67 ± 0.20 ^d	18.11 ± 0.93 ^c	55.20 ± 0.30 ^{d,e}	13.51 ± 0.50 ^{e,f,g}	6.52 ± 0.38 ^k
DC321	27.50 ± 0.36 ^{d,e}	14.76 ± 0.22 ^c	17.67 ± 0.14 ^c	44.59 ± 1.30 ^g	14.91 ± 0.43 ^e	12.97 ± 0.16 ⁱ
DC325	48.93 ± 1.07 ^a	17.27 ± 0.91 ^b	17.05 ± 0.48 ^{d,c}	58.88 ± 1.54 ^c	21.23 ± 0.32 ^b	17.30 ± 0.12 ^g
DC326	22.50 ± 0.36 ^{g,h}	9.64 ± 0.81 ^{f,g}	17.05 ± 0.04 ^{d,c}	45.79 ± 0.83 ^{g,f}	19.50 ± 0.02 ^{b,c}	36.93 ± 0.09 ^a
DC340	25.36 ± 0.36 ^{e,f}	10.25 ± 0.38 ^{e,f,g}	13.11 ± 0.47 ^e	57.03 ± 3.75 ^{d,c}	13.53 ± 0.27 ^{e,f,g}	16.25 ± 0.32 ^h
DC371	36.45 ± 0.02 ^b	20.17 ± 0.37 ^a	16.88 ± 0.47 ^{d,c}	47.78 ± 0.42 ^f	16.17 ± 0.27 ^{e,d}	16.08 ± 0.15 ^h
DC383	34.64 ± 0.36 ^b	20.83 ± 1.03 ^a	26.31 ± 0.47 ^a	54.63 ± 1.35 ^{d,e}	38.67 ± 3.51 ^a	32.43 ± 0.09 ^b
DC385	31.79 ± 0.36 ^c	12.64 ± 0.03 ^d	21.12 ± 0.94 ^b	52.88 ± 1.32 ^e	17.81 ± 0.26 ^{c,d}	26.59 ± 0.51 ^e
DC522	30.71 ± 0.71 ^c	11.72 ± 0.91 ^{d,e}	16.46 ± 0.05 ^{d,c}	88.53 ± 1.19 ^a	36.79 ± 0.33 ^a	26.31 ± 0.20 ^e

Values are mean of two replicates ± standard error. Mean followed by the same superscripts are not significantly different (at $p < 0.05$)

test tube and added with 2200 μL freshly prepared FRAP reagent (0.1 M acetate buffer having pH 3.6, TPTZ 10 mM in 40 mM HCl, 20 mM $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ in ratio 10:1:1). Final volume was made to 2500 μL with water. It was then vortex and incubated in water bath at 37 °C for 15 min. The absorbance was recorded at 593 nm using a UV–VIS spectrophotometer. Data were calculated against the calibration curve for different concentration of gallic acid. The results are expressed as mg GAE 100 g^{-1} fresh weight (FW).

Statistical analysis

Chemometric component

For data analysis, a matrix of order 14×6 , representing fourteen cauliflower genotypes and six biochemical parameters (total phenolics, CUPRAC, FRAP, ascorbic acid, curd sinigrin and leaf sinigrin) was created. For each biochemical parameter, average of two replication was used for statistical analysis involving one way analysis of variance (ANOVA), Pearson correlation, PCA and AHC. We applied PCA which is a data reduction mathematical procedure that recognizes patterns in the correlated data, reduces the variable to achieve smaller number of artificial variables, called principal components which accounts for most of the variance in the observed variables (Granato et al. 2010). The AHC was performed to examine the possibility of classification of cauliflower genotypes into clusters based on the similarities observed among them for the biochemical parameters (Johnson and Wichern 2007). The criterion of average distance was used to perform agglomerative hierarchical clustering procedure. The analysis was done in SAS ver. 9.3 and R package. A dendrogram was made for genotypes using SAS ver. 9.3 to

obtain a two-dimensional projection of the similarity or dissimilarity of the entire genotypes.

Results and discussion

Total phenolics and ascorbic acid content

The natural phenolic compounds have an antimicrobial, anti-cancerous, neuro-protective activity and also help to manage obesity through insulin secretion (Grussu et al. 2011). Total phenolics in cauliflower curd were evaluated using the Folin's method and results are presented in Table 1. The total phenolics content was significantly different ($p < 0.05$) among the cauliflower genotypes which varied from 20.36 to 48.93 mg GAE 100 g^{-1} FW with 48.93, 36.45 and 34.64 mg GAE 100 g^{-1} FW in DC325, DC371 and DC383, respectively. Phenolics are the important bioactive compounds responsible for their antioxidant effects (Kwon et al. 2008). Volden et al. (2009) found total phenolics of 62.5 GAE 100 g^{-1} and 74.2 GAE 100 g^{-1} in white and green cauliflower cultivar, respectively which was higher than the content found in our study. The variations in total phenolics in curd tissues is due to factors like different genotypes grown, environmental condition and management practices of crop as reported by Chipurura et al. (2010). The content of total phenolics found in the present study is in agreement with previous studies of Lo Scalzo et al. (2007).

Ascorbic acid or vitamin C is an important phytochemical and most effective antioxidant in plants (Smirnoff 1996). Ascorbic acid content in cauliflower genotypes ranged from 39.62 to 88.53 mg 100 g^{-1} FW depicting twofold variation with maximum in DC522 (88.53 mg 100 g^{-1} FW) followed by Pusa Sharad (65.64 mg 100 g^{-1} FW) and DC325 (58.88 mg 100 g^{-1} FW). The range of

Table 2 Pearson correlation coefficient between the biochemical parameters across cauliflower genotypes

	Total phenolics	CUPRAC	FRAP	Ascorbic acid	Leaf sinigrin	Curd sinigrin
Total phenolics	1					
CUPRAC	.702** (.004)	1				
FRAP	.407	.577* (.024)	1			
Ascorbic acid	.163	– .092	.052	1		
Leaf sinigrin	.216	.168	.331	.488	1	
Curd sinigrin	– .138	– .094	.189	.204	.579* (.024)	1

$N = 14$, $\text{prob} > |r|$ under H_0 : $\rho = 0$

**Correlation is significant at the 0.01 level (2-tailed)

*Correlation is significant at the 0.05 level (2-tailed)

Fig. 1 Scree plot explaining proportion of variance accounted for by principal components

Fig. 2 Bi-plot presentation of genotypes and antioxidant activities, phenol: total phenolics; acid: ascorbic acid; sleaf: leaf sinigrin; scurd: curd sinigrin

ascorbic acid corresponded to previous report of Davey et al. (2000).

Antioxidant activity

Antioxidant activity studies are being given more importance in various vegetables which provides useful information on health promoting substances (Scalfi et al. 2000). The natural antioxidants in food work synergistically and/or antagonistically by multiple reaction mechanism. Therefore, a simple universal method needs to be applied to measure total antioxidant activity accurately and quantitatively. Estimation of minimum two antioxidant analysis is desirable to compare food samples under various reaction mechanisms (Sun et al. 2009). In this experiment, we

have used two in vitro assays, namely CUPRAC, FRAP and the results are presented in Table 1. Wide variation was observed among the cauliflower genotypes which ranged from 9.04 to 20.83 mg GAE 100 g⁻¹ FW for CUPRAC, 13.11 to 26.31 mg GAE 100 g⁻¹ FW for FRAP. The genotypes DC383, DC371 and DC325 had higher CUPRAC values of 20.83, 20.17 and 17.27 mg GAE 100 g⁻¹ FW, respectively. The corresponding sequence based on tests with the FRAP method was DC383 > DC385 > DC312 > DC321 > DC325 > DC326 > DC371 > DC-310-22 > DC522 > DC306 > DC340 > DC308 > DC310 > Pusa Sharad. The FRAP values recorded in our study were higher than earlier report (Volden et al. 2009). High antioxidant activity in CUPRAC may be attributed due to the presence of phenolics and ascorbic acid in cauliflower curd extract. Bhandari and Kwak (2014) also found significant variation in antioxidant (vitamin C, total phenolics) contents in different cultivars of cauliflower.

Sinigrin content

In cruciferous crops, sinigrin (2-propenyl glucosinolate) is a major glucosinolate which act as a precursor of the anticancer compound allyl-isothiocyanate (Girgin and El 2015). Among the fourteen cauliflower genotypes, leaf sinigrin was highest in DC306 (39.50 µmol 100 g⁻¹ FW) followed by DC383 (38.67 µmol 100 g⁻¹ FW) and DC522 (36.79 µmol 100 g⁻¹ FW). Curd sinigrin was highest in DC326 (36.93 µmol 100 g⁻¹ FW) followed by DC383 (32.43 µmol 100 g⁻¹ FW), DC306 (29.91 µmol 100 g⁻¹ FW). In nine genotypes, sinigrin content in leaves was higher than curd due to high translocation efficiency of glucosinolates from leaves to curd (Bhandari and Kwak 2014). During crossing programme, the levels of glucosinolate in various genotypes are required to develop

Fig. 3 Hierarchical cluster analysis and heatmap of biochemical compounds, in fourteen cauliflower genotypes

suitable varieties and/or hybrids. The sinigrin content found in the present study was higher than the previous reports which may be due to differences in genotypes, the plant matrix, growing conditions and analytical protocols (Volden et al. 2009).

Correlation coefficient

Correlation is a statistical technique used to test the relationship between variables. Table 2 showed the associations between the measured parameters of cauliflower genotypes based on Pearson correlation coefficient. A significant correlation of 0.702 was observed between CUPRAC and phenolics at 1% level of significance and 0.577 between FRAP and phenolics at 5% level of significance. Leaf sinigrin and curd sinigrin showed significant correlation of 0.579. The relationship between total phenolics and antioxidant activity in different vegetables showed that there is increase in antioxidant activity due to high concentration of total phenolics (Amenour et al. 2010; Saeed et al. 2012; Kaur et al. 2014). Similar observation was found in this study due to the fact that phenolic compounds are a major contributor to antioxidant capacity.

Chemometric techniques

Chemometrics is an interdisciplinary research field that involves multivariate statistics, mathematical modelling and computing, especially applied to chemical data. In various studies, these tools are widely used in quality control of dairy products, bioactive and antioxidant compound study in food sample (Cruz et al. 2013). The data obtained from fourteen cauliflower genotypes were subjected to PCA to visualize underlying structure in experimental data and relationship between cauliflower genotypes and various antioxidant parameters. Figure 1 showed the scree plot and the variance explained by the principal components. It was observed that maximum variance (91.87%) could be explained by four principal components. Based on the factor loadings of the PCA, these fourteen cauliflower genotypes were grouped. These factor loadings are the correlation coefficients between the fourteen genotypes and the six biochemical parameters. The first principal component (PC1) explained 50.62% of the variance and second principal component (PC2) could explain 23.28% of the variance as evident from bi-plot (Fig. 2). It was observed that genotypes DC385, Pusa sharad, DC340, DC371 and DC321 had abundance of

Fig. 4 Hierarchical cluster analysis of fourteen cauliflower genotypes

CUPRAC and FRAP and DC325 was rich in total phenolics. These biochemical antioxidants were more prominent in most of the cauliflower genotypes. Heat map in the Fig. 3 is the graphical representation of antioxidants in cauliflower genotypes under study where the individual values in a matrix are represented as colours. It was observed that these genotypes formed four major clusters. One cluster was formed by the genotypes DC321, DC310-22, DC310, DC340 and DC312 based on the biochemical parameters. The other cluster comprised of genotypes DC385, DC371 and DC325. The other two clusters had DC326, DC308, DC309 grouped together and DC383, DC306 and DC522 in one cluster. Hierarchical cluster analysis performed on fourteen cauliflower genotypes was illustrated as dendrogram in Fig. 4. Based on the similarities among the genotypes for the six biochemical parameters (total phenolics, CUPRAC, FRAP, ascorbic acid, leaf sinigrin, curd sinigrin), clusters were formed. The major cluster classified the genotypes DC310-22, DC321, DC310, DC371, DC312 and DC340 in one. DC308, DC326 and DC385 were grouped in one cluster while DC306 and DC383 genotypes were in single cluster. DC522 and Pusa Sharad were outgrouped.

Conclusion

The results obtained from the present study indicated considerable variation for all bioactive compounds and antioxidant activity among the genotypes which will have potential interest to plant breeders. The mid-early cauliflower are potential sources of anti-cancerous compounds and natural antioxidants and they were classified by chemometric tools like PCA and AHC. Analysis of total phenolics, antioxidant capacity and sinigrin will help to identify the important genotypes with higher antioxidant compound. The use of antioxidant rich cauliflower genotypes by consumer will increase the intake of health promoting compounds through diet and thereby prevent chronic human diseases. Besides, genotypes rich in bioactive compounds can be used in crop improvement programme to develop varieties and/or hybrids with high nutraceuticals value.

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