

Table S1. *Trigonella foenum* L. population sites include name, longitude, and latitude for 50 regions

Region	Longitude	Latitude	Region	Longitude	Latitude
Mahnian	49.085535	35.52108	Azna	48.680525	33.488492
Kakareza	48.261338	33.720642	saveh	50.331931	35.037995
Kuhdasht	47.681523	33.563479	sabzevar	57.65865	36.224587
Khomein	50.317967	33.663119	parand	50.987826	35.478324
mardabad	50.537596	35.693079	chitgar	51.212207	35.729605
bandarabbas	56.285105	27.214064	Geshlagh	36.01861	50.419564
Hamadan	48.527574	34.835419	Boyinzahra	35.753171	50.058024
SagzAbad	49.934878	35.766543	birjand	59.254591	32.862695
Bishe	48.687335	33.444838	ghadim abad	49.968588	36.218293
Alashtar	48.268144	33.916449	mahalat	50.461191	33.91693
Borujerd	48.813873	33.805145	Gayene	59.169619	33.565837
Shiraz	52.233507	29.62115	shushtar	48.832836	32.121287
Khorramabad	47.996006	33.510018	Eslamshahr	51.246368	35.535401
Kazerun	51.944223	29.568908	aligudarz	49.699415	33.387433
haji-abad	56.363404	27.25745	BajiAbad	48.630759	31.476271
Minab	56.542827	27.323446	Hamidieh	48.516364	31.435083
Fasa	53.450804	29.137368	MazarSaghi	59.321318	33.145016
Gazvin	49.759621	36.340488	masjed soleiman	49.188288	32.053383
Joghtay	57.058914	36.618904	Takestan	36.078885	49.714336
salafchegan	50.472353	34.493022	Mirash	50.731482	36.182436
Kalateh	47.047711	33.760414	Darvan	51.036232	36.006212
Vardij	51.173727	35.810671	malayer	48.789939	34.294051
Ferdows	58.254167	34.311944	shazand	49.400067	33.949173
Kashmar	58.485833	35.464167	Nazarabad	35.970873	50.621609
Varish	51.173651	35.829366	dizan	50.955418	36.224762

Table S2. Equation of calibration curve and R² value of measured primary and secondary metabolites by HPLC and spectrophotometer except for antioxidant activity

metabolites	equation	R ² value
aspartic acid	y = 4717.4X - 119157	R ² = 0.99
glutamic	y = 1581X - 124	R ² = 0.99
isoleucine	y = 2744x - 2727.9	R ² = 0.99
leucin	y = 1087.3X - 1851.2	R ² = 0.99
phenylalanine	y = 1777.1X + 9045	R ² = 0.99
valine	y = 4998.2X + 2344	R ² = 0.99
lysin	y = 12375X - 1057	R ² = 0.99
4-hydroxy isoleucine	y = 4108X - 291.2	R ² = 0.99
Trigonelline	y = 455.25X - 200.81	R ² = 0.99
Phenol	y = 0.009X - 0.029	R ² = 0.99
Flavonoid	y = 0.008X - 0.002	R ² = 0.99

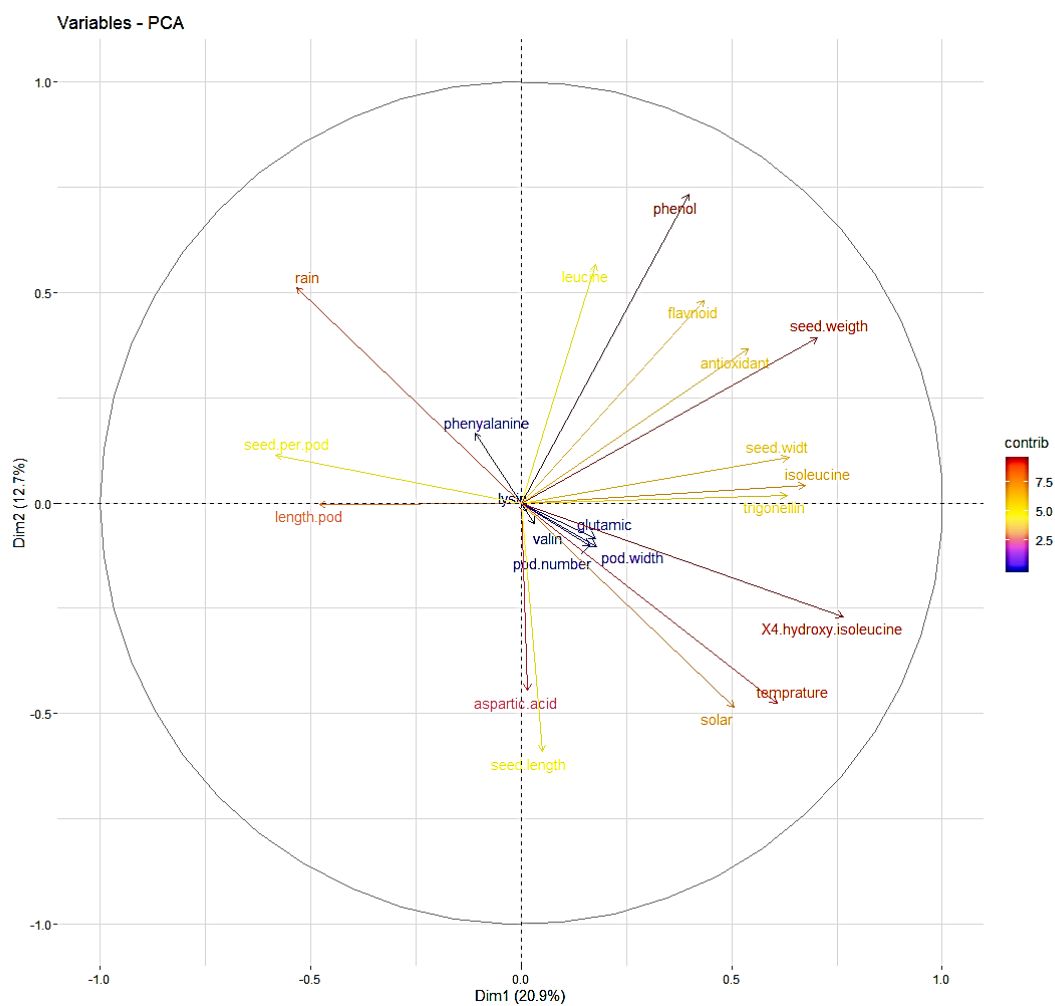


Figure S1. The association amongst measured variables and two first axis of PCA result. First and second dims explained 20.9% and 12.7% of the total variance, respectively. The color of vectors shows the rate of contribution of each variable to each dim.

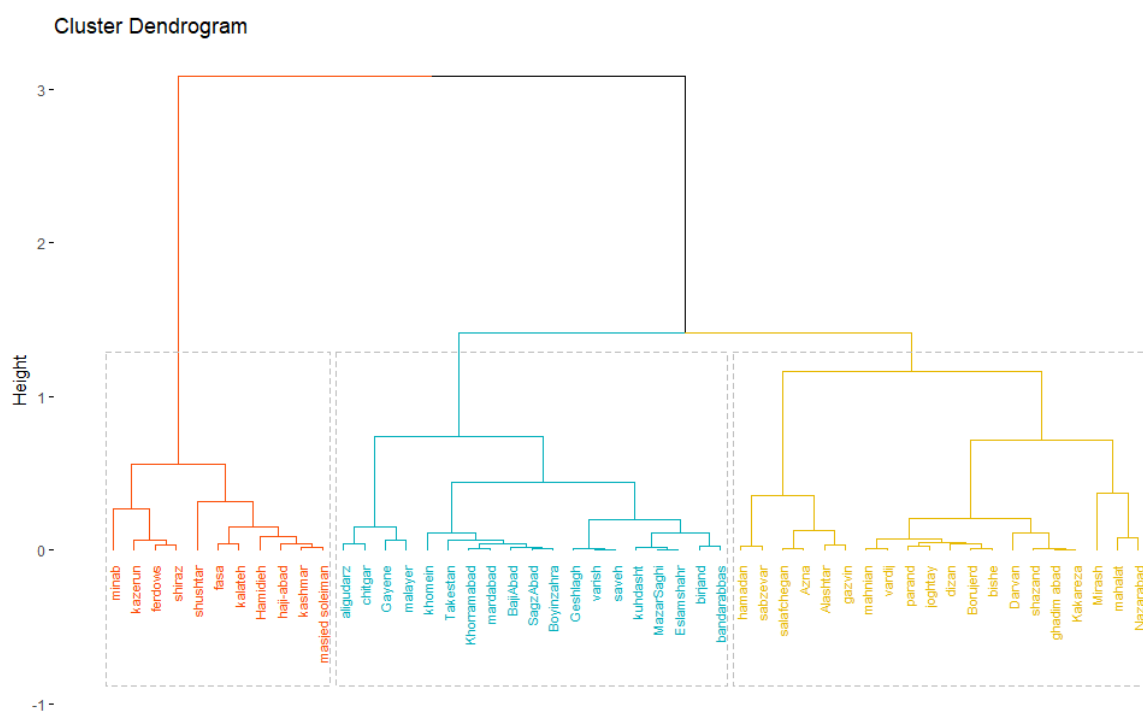


Figure S2. Dendrogram created by the hierarchical clustering based on HCPC result for studied regions.

Table S3. The eigenvalue, constrained inertia and cumulative percent of first two CCA

	Two first important axes	
	CCA1	CCA2
Eigenvalue	0.023	0.001
Constrained inertia (%)	0.87	0.07
Cumulative %	0.87	0.94

Table S4. The principal coordination of canonical variables with two first axis of CCA analysis.

Highest value and the lowest value displayed in green and red colors respectively in CCA1 and CCA2

	CCA1	CCA2
trigonelline	-0.110	0.083
4-hydroxy isoleucine	-0.335	0.024
Aspartic acid	-0.130	-0.051
Glutamic	-0.046	-0.110
valine	-0.035	-0.070
phenylalanine	0.138	-0.100
isoleucine	-0.225	0.116
leucine	0.392	0.349
antioxidant	-0.149	-0.135
flavonoid	0.012	-0.002
phenol	0.096	-0.014
Lysin	0.067	0.067
Pod number	0.061	-0.042
Seed per pod	0.319	0.020
Pod length	0.195	-0.014
Seed weight	0.047	0.070
Pod width	0.073	-0.019
Seed length	0.079	0.008
Seed width	0.025	0.017
Solar irradiation	-0.817	0.267
Temperature	-0.751	0.451
Rain	0.981	0.170

Table S5. Principal coordinates of regions to each axis by all vegetal traits with CCA1 and CCA2.
Highest value and the lowest value displayed in green and red colors respectively CCA1 and CCA2

	CCA1	CCA2
Shushtar	-1.332	-0.191
Hamidieh	-0.731	-1.429
Kazerun	-0.423	3.102

haji-abad	-0.715	0.157
Minab	-0.520	3.178
Fasa	-0.504	-1.013
Kalateh	-0.968	1.313
shiraz	-0.656	-1.014
Mirash	2.906	3.833
Hamadan	-0.053	-3.040
Khomein	1.778	-1.449
Khorramabad	2.061	-2.721
Mardabad	0.636	-2.062
Ferdows	-0.775	0.850
Sagz Abad	0.942	-1.465
Boyinzahra	1.760	-2.616
Masjed soleiman	-1.177	0.369

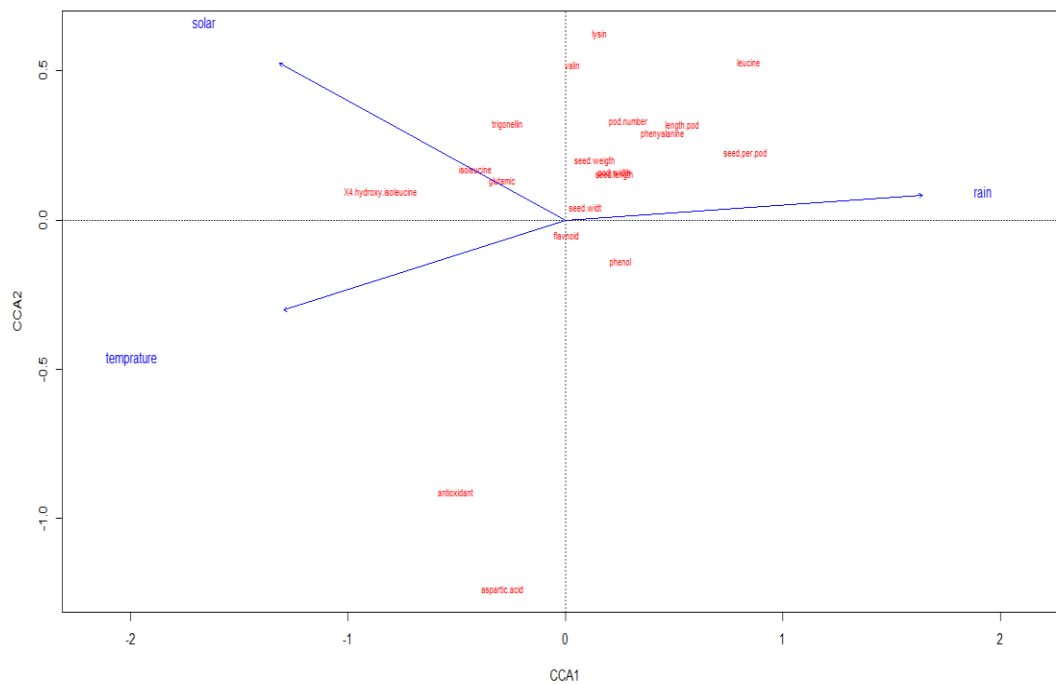


Figure S3. CCA plot of the relationship between environmental and vegetal variables. Blue arrows showed environmental variables and green text displayed vegetal traits

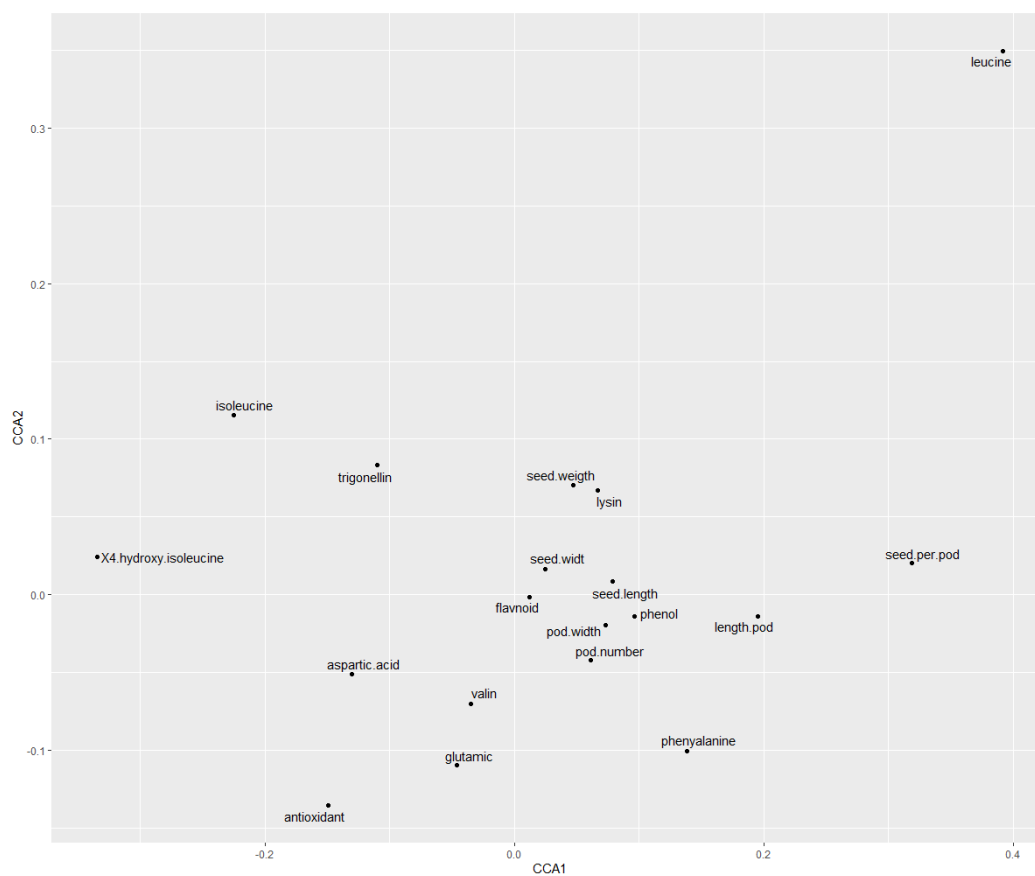


Figure S4. Scatter plot of CCA that shows the coordinates of variables to each dimension

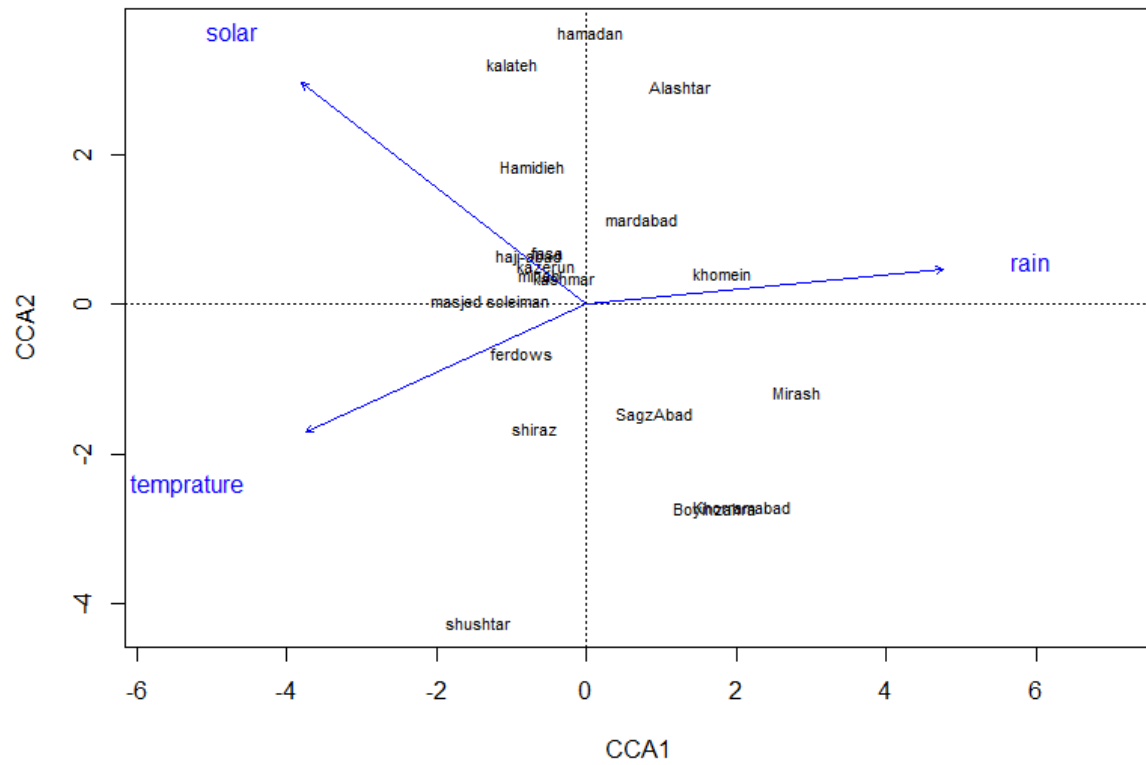


Figure S5. CCA ordination biplot of selected regions based on HCPC analysis, displaying environmental variables in blue arrows and each region in the black text.

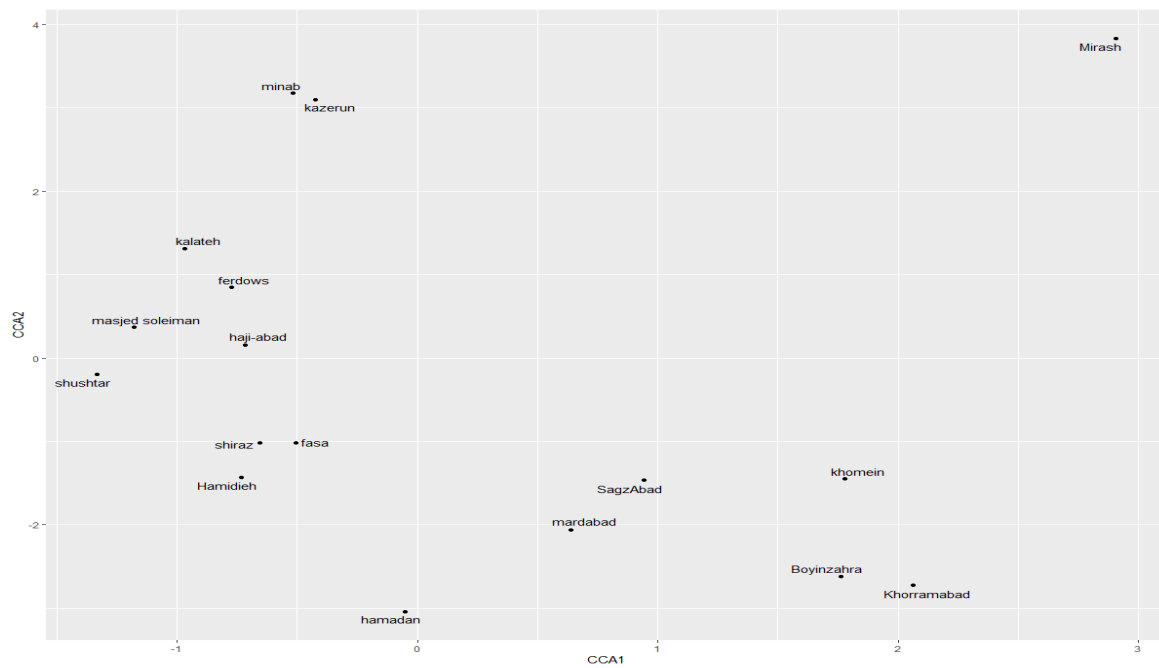


Figure S6. Scatter plot of CCA that shows the contribution of regions to each dim of CCA analysis.

