

PLAMED-2011-01-0064-OP.R2

Supporting Information

Metabolomic Differentiation of Maca (*Lepidium meyenii*) Accessions Cultivated under Different Conditions Using NMR and Chemometric Analysis

**Jianping Zhao¹, Bharathi Avula¹, Michael Chan^{2,3}, Céline Clément⁴, Michael
Kreuzer⁴, Ikhlas A. Khan^{1,2}**

Affiliation

¹ National Center for Natural Products Research, Research Institute of Pharmaceutical
Sciences, University of Mississippi, University, MS, USA

² Department of Pharmacognosy, School of Pharmacy, University of Mississippi,
University, MS, USA

³ British Columbia Institute of Technology, Burnaby, B.C., Canada

⁴ ETH Zurich, Institute of Agricultural Sciences, Zurich, Switzerland

Correspondence

Prof. Dr. Ikhlas A. Khan

National Center for Natural Products Research
Research Institute of Pharmaceutical Sciences
University of Mississippi

University, MS 38677

USA

Phone: + 662-915-7821

Fax: + 662-915-7989

ikh@olemiss.edu

Table 1S List of parameters for the ^{13}C and 2D NMR experiments.

A. ^{13}C NMR Experimental Parameters

```
##TITLE= Parameter file, TOPSPIN  Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##$ANAVPT= 1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_zg>
##$BF1= 100.612769
##$BF2= 400.13
##$BF3= 100.612769
##$BF4= 100.612769
##$BYTORDA= 0
##$CFDGTYP= 0
##$CFRGTYP= 5
##$CPDPRG= <waltz16>
##$CPDPRG2= <waltz16>
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 8
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 6
##$FTLPGN= 0
##$FW= 90000
##$FnMODE= 0
##$GP031= 0
##$GRPDLY= -1
##$HDDUTY= 20
##$HDRATE= 20
##$HL1= 3
##$HL2= 83
##$HL3= 83
##$HL4= 83
##$HOLDER= 0
##$LFILTER= 10
##$LGAIN= -10
##$MASR= 4200
##$MASRLST= <masrlst>
##$NBL= 1
##$NC= 0
##$NS= 10000
##$NUC1= <13C>
##$NUC2= <1H>
##$O1= 11067.40459
```

```
##$O2= 1600.51999995403
##$PAPS= 2
##$PHP= 2
##$PH_ref= 0
##$PRGAIN= 0
##$PROBHD= <33>
##$PROSOL= no
##$PULPROG= <zgpg30>
##$PW= 0
##$SFO1= 100.62383640459
##$SFO2= 400.13160052
##$SOLVENT= <MeOD>
##$SW= 238.894305736935
##$TD= 65536
##$TD0= 1
##$TE= 300
##$WBST= 1024
##$WBSW= 4
```

B.2D COSY NMR experimental parameters

```
##TITLE= Parameter file, TOPSPIN Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##$ANAVPT= 1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlcosy>
##$BF1= 400.13
##$BF2= 400.13
##$BF3= 400.13
##$BF4= 400.13
##$BYTORDA= 0
##$CFDGTYP= 0
##$CFRGTY= 5
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 48
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 6
##$DR= 18
##$DS= 4
##$GRPDLY= -1
##$HDDUTY= 20
##$HDRATE= 20
##$HL1= 1
```

```
##$HL2= 35
##$HL3= 8
##$HL4= 26
##$MASR= 4200
##$MASRLST= <masrlst>
##$NBL= 1
##$NC= 0
##$NS= 16
##$NUC1= <1H>
##$NUC2= <off>
##$NUC3= <off>
##$NUC4= <off>
##$NUCLEI= 0
##$NUCLEUS= <off>
##$O1= 2000.65
##$O2= 2000.65
##$O3= 1853.21993700427
##$O4= 1853.21993700427
##$PAPS= 2
##$PARMODE= 1
##$POWMOD= 0
##$PR= 1
##$PRGAIN= 0
##$PROBHD= <33>
##$PULPROG= <cosyqf45>
##$PW= 0
##$PYNM= <acqu.py>
##$PYNMP= <proc.py>
##$QNP= 1
##$RECPH= 0
##$RG= 64
##$RO= 0
##$SEOUT= 0
##$SFO1= 400.13200065
##$SFO2= 400.13200065
##$SFO3= 400.131853219937
##$SFO4= 400.131853219937
##$SOLVENT= <MeOD>
##$SW= 10.0127214266842
##$SW_h= 4006.41025641026
##$TD= 2048
##$TD0= 1
##$TE= 300
##$WBST= 1024
##$WBSW= 4
```

C.2D TOCSY NMR experimental parameters

```
##TITLE= Parameter file, TOPSPIN Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##$AQSEQ= 0
##$AQ_mod= 3
```

##\$AUNM= <au_getlcosy>
##\$BF1= 400.13
##\$BF2= 400.13
##\$BF3= 400.13
##\$BF4= 400.13
##\$BYTORDA= 0
##\$CFDGTYP= 2
##\$CFRGTYTYP= 5
##\$CPDPRG4= <mlev>
##\$CPDPRG5= <mlev>
##\$CPDPRG6= <mlev>
##\$CPDPRG7= <mlev>
##\$CPDPRG8= <mlev>
##\$DBP07= 0
##\$DE= 6
##\$DECBNUC= <off>
##\$DECIM= 48
##\$DECNUC= <off>
##\$DECSTAT= 4
##\$DIGMOD= 1
##\$DIGTYP= 6
##\$DR= 18
##\$DS= 16
##\$FL1= 90
##\$FL2= 90
##\$FL3= 90
##\$FL4= 90
##\$FOV= 20
##\$FTLPGN= 0
##\$FW= 90000
##\$FnMODE= 0
##\$GP031= 0
##\$HDDUTY= 20
##\$HDRATE= 20
##\$HL1= 256
##\$HL2= 90
##\$HL3= 14
##\$HL4= 90
##\$MASR= 4200
##\$MASRLST= <masrlst>
##\$NBL= 1
##\$NC= 0
##\$NS= 64
##\$NUC1= <1H>
##\$NUC2= <off>
##\$NUC3= <off>
##\$NUC4= <off>
##\$NUCLEI= 0
##\$NUCLEUS= <off>
##\$O1= 1841.85846700302
##\$O2= 1841.85846700302
##\$O3= 1841.85846700302
##\$O4= 1841.85846700302
##\$PAPS= 2

```
##$PARMODE= 1
##$PH_ref= 0
##$POWMOD= 0
##$PR= 1
##$PRGAIN= 0
##$PROSOL= no
##$PULPROG= <mlevph>
##$PW= 0
##$QNP= 1
##$RD= 0
##$RG= 64
##$RO= 0
##$SFO1= 400.131841858467
##$SFO2= 400.131841858467
##$SFO3= 400.131841858467
##$SFO4= 400.131841858467
##$SOLVENT= <MeOD>
##$SW= 10.2090533492367
##$SW_h= 4084.96732026144
##$TD= 2048
##$TD0= 1
##$TE= 300
##$V9= 5
##$WBST= 1024
##$WBSW= 4
```

D.2D J-resolved NMR experimental parameters

```
##TITLE= Parameter file, TOPSPIN Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##$ANAVPT= 1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlcosy>
##$BF1= 400.13
##$BF2= 400.13
##$BF3= 400.13
##$BF4= 400.13
##$BYTORDA= 0
##$CFDGTYP= 0
##$CPDPRG4= <mlev>
##$CPDPRG5= <mlev>
##$CPDPRG6= <mlev>
##$CPDPRG7= <mlev>
##$CPDPRG8= <mlev>
##$DE= 6
##$DECBNUC= <off>
##$DECIM= 24
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 1
##$DIGTYP= 6
##$DP07= 0
```

##\$DQDMODE= 0
##\$DR= 18
##\$DS= 4
##\$DSPFIRM= 0
##\$DSPFVS= 0
##\$DTYPA= 0
##\$FL1= 1
##\$FL2= 83
##\$FL3= 83
##\$FL4= 83
##\$FOV= 20
##\$FTLPGN= 0
##\$FW= 90000
##\$FnMODE= 0
##\$GRPDLY= -1
##\$HDDUTY= 20
##\$HDRATE= 20
##\$HL1= 1
##\$HL2= 35
##\$HL3= 8
##\$HL4= 26
##\$MASR= 4200
##\$MASRLST= <masrlst>
##\$NBL= 1
##\$NC= 0
##\$NS= 16
##\$NUC1= <1H>
##\$O1= 2400.78
##\$O2= 2000.65
##\$O3= 1853.21993700427
##\$O4= 1853.21993700427
##\$PAPS= 2
##\$PARMODE= 1
##\$PH_ref= 0
##\$POWMOD= 0
##\$PR= 1
##\$PRGAIN= 0
##\$PROBHD= <33>
##\$PROSOL= no
##\$PULPROG= <lcjresprqf>
##\$PW= 0
##\$PYNM= <acqu.py>
##\$PYNMP= <proc.py>
##\$QNP= 1
##\$RECPH= 0
##\$RG= 80.6
##\$SEOUT= 0
##\$SFO1= 400.13240078
##\$SFO2= 400.13200065
##\$SFO3= 400.131853219937
##\$SFO4= 400.131853219937
##\$SOLVENT= <MeOD>
##\$SW= 16.0203382624365
##\$SW_h= 6410.25641025641

##\$TD= 32768
##\$TD0= 1
##\$TE= 300
##\$V9= 5
##\$WBST= 1024
##\$WBSW= 4

E.2D HSQC NMR experimental parameters

##TITLE= Parameter file, TOPSPIN Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##\$ANAVPT= 1
##\$AQSEQ= 0
##\$AQ_mod= 3
##\$AUNM= <au_getlinv>
##\$BF1= 400.13
##\$BF2= 100.612769
##\$BF3= 400.13
##\$BF4= 400.13
##\$BYTORDA= 0
##\$CFDGTYP= 0
##\$CFRGTY= 5
##\$CPDPRG2= <garp>
##\$CPDPRG5= <mlev>
##\$CPDPRG6= <mlev>
##\$CPDPRG7= <mlev>
##\$CPDPRG8= <mlev>
##\$DE= 6
##\$DECBNUC= <off>
##\$DECIM= 32
##\$DECNUC= <off>
##\$DECSTAT= 4
##\$DIGMOD= 1
##\$DIGTYP= 6
##\$DQDMODE= 0
##\$DR= 18
##\$DR_end= 6
##\$DR_set= 12
##\$DR_strt= 12
##\$DS= 4
##\$FL1= 83
##\$FL2= 83
##\$FL3= 83
##\$FL4= 83
##\$FOV= 20
##\$FTLPGN= 0
##\$FW= 90000
##\$FnMODE= 0
##\$GP031= 0
##\$GRPDLY= -1
##\$HDDUTY= 20
##\$HDRATE= 20

```
##$HL1= 256
##$HL2= 55
##$HL3= 83
##$HL4= 83
##$MASR= 4200
##$NBL= 1
##$NC= 0
##$NS= 128
##$NUC1= <1H>
##$NUC2= <13C>
##$NUCLEI= 0
##$O1= 1885.01
##$O2= 9055.14921
##$O3= 1880.61099999004
##$O4= 1880.61099999004
##$PH_ref= 0
##$POWMOD= 0
##$PR= 1
##$PRGAIN= 0
##$PROBHD= <33>
##$PROSOL= no
##$PULPROG= <hmqcphpr>
##$PW= 0
##$PYNM= <acqu.py>
##$PYNMP= <proc.py>
##$QNP= 1
##$RG= 287.4
##$SFO1= 400.13188501
##$SFO2= 100.62182414921
##$SFO3= 400.131880611
##$SFO4= 400.131880611
##$SOLVENT= <MeOD>
##$SW_h= 4807.69230769231
##$TD= 2048
##$TD0= 1
##$TE= 300
##$V9= 5
##$WBST= 1024
##$WBSW= 4
```

F.2D HMBC NMR experimental parameters

```
##TITLE= Parameter file, TOPSPIN Version 1.3
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##$ANAVPT= 1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlinv>
##$BF1= 400.13
##$BF2= 100.612769
##$BF3= 400.13
##$BF4= 400.13
##$BYTORDA= 0
```

##\$CFDGTYP= 0
##\$CFRGTYP= 5
##\$CPDPRG= <garp>
##\$CPDPRG2= <garp>
##\$CPDPRG4= <mlev>
##\$CPDPRG5= <mlev>
##\$CPDPRG6= <mlev>
##\$CPDPRG7= <mlev>
##\$CPDPRG8= <mlev>
##\$DBP07= 0
##\$DE= 6
##\$DECBNUC= <off>
##\$DECIM= 48
##\$DECNUC= <off>
##\$DECSTAT= 4
##\$DIGMOD= 1
##\$DIGTYP= 6
##\$DQDMODE= 0
##\$DR= 18
##\$DR_end= 6
##\$DR_set= 12
##\$DR_strt= 12
##\$DS= 16
##\$FL1= 83
##\$FL2= 83
##\$FL3= 83
##\$FL4= 83
##\$FOV= 20
##\$FRQLO3= 0
##\$FRQLO3N= 0
##\$FTLPGN= 0
##\$FW= 90000
##\$FnMODE= 0
##\$GRPDLY= -1
##\$HDDUTY= 20
##\$HDRATE= 20
##\$HL1= 90
##\$HL2= 83
##\$HL3= 83
##\$HL4= 83
##\$HOLDER= 0
##\$MASR= 4200
##\$MASRLST= <masrlst>
##\$NBL= 1
##\$NC= 0
##\$NS= 256
##\$NUCLEI= 0
##\$O1= 2000.65
##\$O2= 11067.40459
##\$O3= 1853.22796386345
##\$O4= 1853.22796386345
##\$PH_ref= 0
##\$POWMOD= 0
##\$PR= 3

```

##$PROBHD= <33>
##$PROSOL= no
##$PULPROG= <hmbclpndqf>
##$PW= 0
##$PYNM= <acqu.py>
##$PYNMP= <proc.py>
##$QNP= 1
##$RECPH= 0
##$RG= 287.4
##$RO= 0
##$SFO1= 400.13200065
##$SFO2= 100.62383640459
##$SFO3= 400.131853227964
##$SFO4= 400.131853227964
##$SOLVENT= <MeOD>
##$SW= 10.0127214266842
##$SW_h= 4006.41025641026
##$TD= 4096
##$TD0= 1
##$TE= 300
##$V9= 5
##$VD= 0
##$WBST= 1024
##$WBSW= 4

```

Table 2S Model overview list of the PCA for all the accessions of maca from the two growing sites.

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.494558	0.494558	0.472475	0.00869703	0.472475
Comp 2	0.150104	0.644662	0.265114	0.0087409	0.612329
Comp 3	0.108435	0.753096	0.270525	0.00878525	0.717204
Comp 4	0.0944576	0.847554	0.354961	0.00883013	0.817585
Comp 5	0.0349006	0.882455	0.191421	0.00887549	0.852503
Comp 6	0.0199711	0.902426	0.124034	0.00892138	0.870798
Comp 7	0.0156486	0.918074	0.118154	0.00896776	0.886064
Comp 8	0.0136307	0.931705	0.132443	0.00901473	0.901154
Comp 9	0.0106949	0.9424	0.110984	0.00906217	0.912124
Comp 10	0.00830168	0.950702	0.101786	0.00911021	0.921069
Comp 11	0.00633773	0.957039	0.0872161	0.00915885	0.927953
Comp 12	0.00513522	0.962175	0.0603683	0.00920802	0.932302
Comp 13	0.00468482	0.96686	0.0807057	0.00925779	0.937766
Comp 14	0.00375908	0.970619	0.0477842	0.0093081	0.94074
Comp 15	0.00363308	0.974252	0.087177	0.00935912	0.945906
Comp 16	0.00298704	0.977239	0.0747434	0.00941068	0.949949
Comp 17	0.00251898	0.979758	0.0567324	0.00946289	0.952788
Comp 18	0.00226886	0.982027	0.0628603	0.00951576	0.955756
Comp 19	0.00215512	0.984182	0.0644852	0.00956929	0.958609
Comp 20	0.0018626	0.986044	0.071836	0.00962347	0.961583
Comp 21	0.0015293	0.987574	0.0567319	0.00967836	0.963762

Comp 22	0.00142879	0.989002	0.0840939	0.00973392	0.96681
Comp 23	0.00101824	0.990021	0.0320896	0.00979018	0.967875
Comp 24	0.000912454	0.990933	0.042743	0.00984722	0.969248
Comp 25	0.000813249	0.991746	0.0509671	0.00990498	0.970815
Comp 26	0.000719288	0.992466	0.0521543	0.00996345	0.972337
Comp 27	0.00062012	0.993086	0.0312697	0.0100228	0.973202
Comp 28	0.000589083	0.993675	0.032492	0.0100828	0.974073
Comp 29	0.000502222	0.994177	0.0212389	0.0101437	0.974624
Comp 30	0.000458324	0.994635	0.0267514	0.0102054	0.975302
Comp 31	0.000424198	0.99506	0.0218136	0.0102679	0.975841
Comp 32	0.000387135	0.995447	0.0161891	0.0103313	0.976232
Comp 33	0.000377296	0.995824	0.0205367	0.0103955	0.97672
Comp 34	0.000363514	0.996188	0.0426767	0.0104607	0.977714
Comp 35	0.000342529	0.99653	0.0521971	0.0105268	0.978877
Comp 36	0.000304112	0.996834	0.0436306	0.0105938	0.979799
Comp 37	0.00027443	0.997109	0.0358335	0.0106618	0.980523
Comp 38	0.000245735	0.997354	0.0291927	0.0107307	0.981091
Comp 39	0.000215092	0.997569	0.0318754	0.0108007	0.981694
Comp 40	0.000204699	0.997774	0.0417587	0.0108716	0.982458
Comp 41	0.000201006	0.997975	0.0399729	0.0109436	0.98316
Comp 42	0.000176325	0.998151	0.022933	0.0110167	0.983546
Comp 43	0.000172041	0.998324	0.0513576	0.0110909	0.984391
Comp 44	0.000150135	0.998474	0.0456377	0.0111662	0.985103
Comp 45	0.000128299	0.998602	0.0163463	0.0112426	0.985347
Comp 46	0.000124869	0.998727	0.0322487	0.0113203	0.985819

Table 3S Model overview list of the PCA for the maca accessions from the Patalá site (**A**) and the Alpacayán site (**B**).

A

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.480782	0.480782	0.441784	0.0145257	0.441784
Comp 2	0.231835	0.712618	0.416575	0.0146757	0.674323
Comp 3	0.0762296	0.788847	0.190481	0.0148293	0.736358
Comp 4	0.0579642	0.846812	0.202229	0.0149865	0.789674
Comp 5	0.0399504	0.886762	0.22391	0.0151474	0.836768
Comp 6	0.0279505	0.914712	0.192109	0.0153124	0.868127
Comp 7	0.0229182	0.937631	0.237992	0.0154814	0.899511
Comp 8	0.00945064	0.947081	0.0487306	0.0156546	0.904408
Comp 9	0.00814368	0.955225	0.101914	0.0158322	0.91415
Comp 10	0.00680158	0.962027	0.0697591	0.0160145	0.920139
Comp 11	0.00621553	0.968242	0.0943041	0.0162015	0.92767
Comp 12	0.0056828	0.973925	0.109622	0.0163934	0.935599
Comp 13	0.00448923	0.978414	0.101983	0.0165905	0.942167
Comp 14	0.00364296	0.982057	0.118593	0.0167931	0.949026
Comp 15	0.00308335	0.985141	0.108274	0.0170012	0.954545
Comp 16	0.00220243	0.987343	0.0743603	0.0172151	0.957925
Comp 17	0.00198669	0.98933	0.0808976	0.0174353	0.961329
Comp 18	0.00155042	0.99088	0.0587233	0.0176617	0.9636
Comp 19	0.00152521	0.992405	0.0952409	0.0178948	0.967066

Comp 20	0.00119798	0.993603	0.0822024	0.018135	0.969774
Comp 21	0.00109478	0.994698	0.0850624	0.0183824	0.972345
Comp 22	0.000860868	0.995559	0.0674584	0.0186374	0.97421
Comp 23	0.000840156	0.996399	0.145034	0.0189005	0.977951
Comp 24	0.000684717	0.997084	0.132774	0.019172	0.980878
Comp 25	0.000543633	0.997627	0.136632	0.0194523	0.983491
Comp 26	0.000454343	0.998082	0.132909	0.0197419	0.985685
Comp 27	0.000330998	0.998413	0.0818467	0.0200413	0.986857
Comp 28	0.000301416	0.998714	0.122611	0.0203509	0.988468
Comp 29	0.000221013	0.998935	0.122472	0.0206713	0.989881
Comp 30	0.000167786	0.999103	0.0393558	0.0210031	0.990279
Comp 31	0.000149263	0.999252	0.128249	0.021347	0.991526
Comp 32	7.77415e-005	0.99933	0.0493333	0.0217035	0.991944

B

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.601189	0.601189	0.578912	0.0149655	0.578912
Comp 2	0.15364	0.754829	0.339663	0.0151263	0.72194
Comp 3	0.0778239	0.832653	0.28414	0.0152912	0.800948
Comp 4	0.0371255	0.869779	0.171571	0.01546	0.835099
Comp 5	0.0322342	0.902013	0.191239	0.0156332	0.866635
Comp 6	0.0245717	0.926584	0.203972	0.0158107	0.893838
Comp 7	0.015237	0.941821	0.147601	0.0159928	0.909507
Comp 8	0.0135458	0.955367	0.18028	0.0161797	0.925821
Comp 9	0.0117514	0.967119	0.233832	0.0163715	0.943167
Comp 10	0.00566498	0.972784	0.122083	0.0165685	0.950105
Comp 11	0.00458232	0.977366	0.114194	0.0167709	0.955803
Comp 12	0.00409527	0.981461	0.112464	0.0169789	0.960773
Comp 13	0.00321875	0.98468	0.117147	0.0171928	0.965369
Comp 14	0.00275539	0.987435	0.120447	0.0174127	0.96954
Comp 15	0.00188966	0.989325	0.0922357	0.0176391	0.972349
Comp 16	0.00182611	0.991151	0.12058	0.0178721	0.975684
Comp 17	0.0014048	0.992556	0.0856291	0.0181121	0.977766
Comp 18	0.00118052	0.993736	0.0875972	0.0183594	0.979713
Comp 19	0.000949203	0.994686	0.0752941	0.0186143	0.981241
Comp 20	0.000889652	0.995575	0.115802	0.0188773	0.983413
Comp 21	0.000589922	0.996165	0.0302988	0.0191486	0.983916
Comp 22	0.00056928	0.996734	0.0559244	0.0194288	0.984815
Comp 23	0.000531	0.997266	0.123408	0.0197183	0.986689
Comp 24	0.000445633	0.997711	0.0918836	0.0200175	0.987912
Comp 25	0.000359595	0.998071	0.0735575	0.020327	0.988801
Comp 26	0.000330222	0.998401	0.0786223	0.0206473	0.989682
Comp 27	0.000293488	0.998694	0.097097	0.020979	0.990684
Comp 28	0.000244983	0.998939	0.125331	0.0213227	0.991851
Comp 29	0.000222776	0.999162	0.133021	0.0216792	0.992935
Comp 30	0.000146143	0.999308	0.130063	0.0220491	0.993854
Comp 31	0.000103895	0.999412	0.0844248	0.0224332	0.994373
Comp 32	6.16661e-005	0.999474	0.0549135	0.0228324	0.994682

Table 4S Model overview list of the PCA for the maca accessions from the four growing areas: **A.** never cultivated area at the Patalá site; **B.** previously cultivated area at the Patalá site; **C.** never cultivated area at the Alpacayán site; **D.** previously cultivated area at the Alpacayán site.

A

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.457822	0.457822	0.400538	0.0234306	0.400538
Comp 2	0.252336	0.710158	0.433935	0.0238796	0.660666
Comp 3	0.103918	0.814076	0.316326	0.0243478	0.768006
Comp 4	0.05991	0.873986	0.250534	0.0248366	0.826128
Comp 5	0.0450643	0.91905	0.309722	0.0253473	0.87998
Comp 6	0.0255922	0.944642	0.275762	0.0258815	0.913077
Comp 7	0.0141559	0.958798	0.20642	0.0264407	0.93102
Comp 8	0.00867843	0.967477	0.112573	0.027027	0.938785
Comp 9	0.00834507	0.975822	0.192811	0.0276423	0.950588
Comp 10	0.00519674	0.981019	0.0882712	0.0282887	0.95495
Comp 11	0.00472078	0.985739	0.130099	0.0289689	0.960811
Comp 12	0.00437146	0.990111	0.241461	0.0296854	0.970273
Comp 13	0.00300904	0.99312	0.207514	0.0304414	0.976442
Comp 14	0.00182481	0.994945	0.173192	0.0312402	0.980522
Comp 15	0.00158843	0.996533	0.235242	0.0320855	0.985104
Comp 16	0.00128112	0.997814	0.332461	0.0329818	0.990056
Comp 17	0.000478497	0.998293	0.142182	0.0339335	0.99147
Comp 18	0.000363003	0.998656	0.101891	0.0349463	0.992339
Comp 19	0.000246075	0.998902	0.0958131	0.036026	0.993073
Comp 20	0.000208895	0.999111	0.15014	0.0371797	0.994113

B

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.560617	0.560617	0.529733	0.0303566	0.529733
Comp 2	0.18826	0.748877	0.396335	0.031155	0.716116
Comp 3	0.0762903	0.825167	0.269316	0.032	0.792571
Comp 4	0.0592382	0.884405	0.277805	0.0328958	0.850196
Comp 5	0.0358289	0.920234	0.213903	0.0338472	0.882239
Comp 6	0.0260704	0.946305	0.169542	0.0348595	0.902205
Comp 7	0.0201622	0.966467	0.293279	0.0359389	0.930886
Comp 8	0.0129051	0.979372	0.317075	0.0370923	0.9528
Comp 9	0.00838749	0.987759	0.337058	0.0383275	0.968709
Comp 10	0.00449644	0.992256	0.298067	0.0396538	0.978036
Comp 11	0.0031062	0.995362	0.334388	0.0410815	0.985381
Comp 12	0.00182808	0.99719	0.330721	0.0426229	0.990215
Comp 13	0.000870423	0.998061	0.213626	0.0442922	0.992306
Comp 14	0.000529771	0.99859	0.17947	0.046106	0.993687
Comp 15	0.000329929	0.99892	0.122803	0.0480841	0.994462

C

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
-----------	------	-----------	------	----------	-----------

Comp 1	0.632427	0.632427	0.605001	0.0263989	0.605001
Comp 2	0.128246	0.760673	0.306805	0.0269849	0.726189
Comp 3	0.0791112	0.839784	0.1542	0.0276	0.76841
Comp 4	0.066088	0.905872	0.384736	0.0282463	0.857511
Comp 5	0.0301258	0.935998	0.23797	0.0289262	0.891419
Comp 6	0.0166453	0.952644	0.182632	0.0296425	0.91125
Comp 7	0.0133376	0.965981	0.140116	0.0303983	0.923685
Comp 8	0.0107842	0.976765	0.262518	0.0311969	0.943719
Comp 9	0.00650951	0.983275	0.144805	0.0320421	0.951869
Comp 10	0.00532329	0.988598	0.239714	0.0329381	0.963407
Comp 11	0.00396482	0.992563	0.303905	0.0338897	0.974527
Comp 12	0.00184722	0.99441	0.157562	0.0349022	0.978541
Comp 13	0.00146167	0.995872	0.0886939	0.0359817	0.980444
Comp 14	0.00137203	0.997244	0.288653	0.0371353	0.986089
Comp 15	0.000826249	0.99807	0.223793	0.0383707	0.989202
Comp 16	0.000548134	0.998618	0.165823	0.0396972	0.990993
Comp 17	0.000291318	0.99891	0.113185	0.0411251	0.992012
Comp 18	0.000215792	0.999125	0.145651	0.0426667	0.993176

D

Component	R2VX	R2VX(cum)	Q2VX	Q2 limit	Q2VX(cum)
Comp 1	0.47263	0.47263	0.429054	0.0282255	0.429054
Comp 2	0.257086	0.729716	0.451561	0.0289054	0.686871
Comp 3	0.119895	0.849611	0.383981	0.0296216	0.807106
Comp 4	0.045027	0.894638	0.247138	0.0303773	0.854778
Comp 5	0.0322044	0.926843	0.154878	0.0311758	0.87727
Comp 6	0.0273559	0.954198	0.336471	0.0320209	0.918565
Comp 7	0.0145888	0.968787	0.260613	0.0329168	0.939788
Comp 8	0.00876903	0.977556	0.191655	0.0338683	0.951328
Comp 9	0.005991	0.983547	0.142389	0.0348807	0.958258
Comp 10	0.00479019	0.988337	0.133235	0.0359601	0.96382
Comp 11	0.00351233	0.99185	0.166032	0.0371136	0.969827
Comp 12	0.00348092	0.995331	0.363624	0.038349	0.980798
Comp 13	0.00215734	0.997488	0.419276	0.0396753	0.988849
Comp 14	0.000670958	0.998159	0.207294	0.0411031	0.991161
Comp 15	0.000477029	0.998636	0.14888	0.0426446	0.992477
Comp 16	0.000344769	0.998981	0.186804	0.044314	0.993882
Comp 17	0.000199378	0.99918	0.129235	0.0461279	0.994673