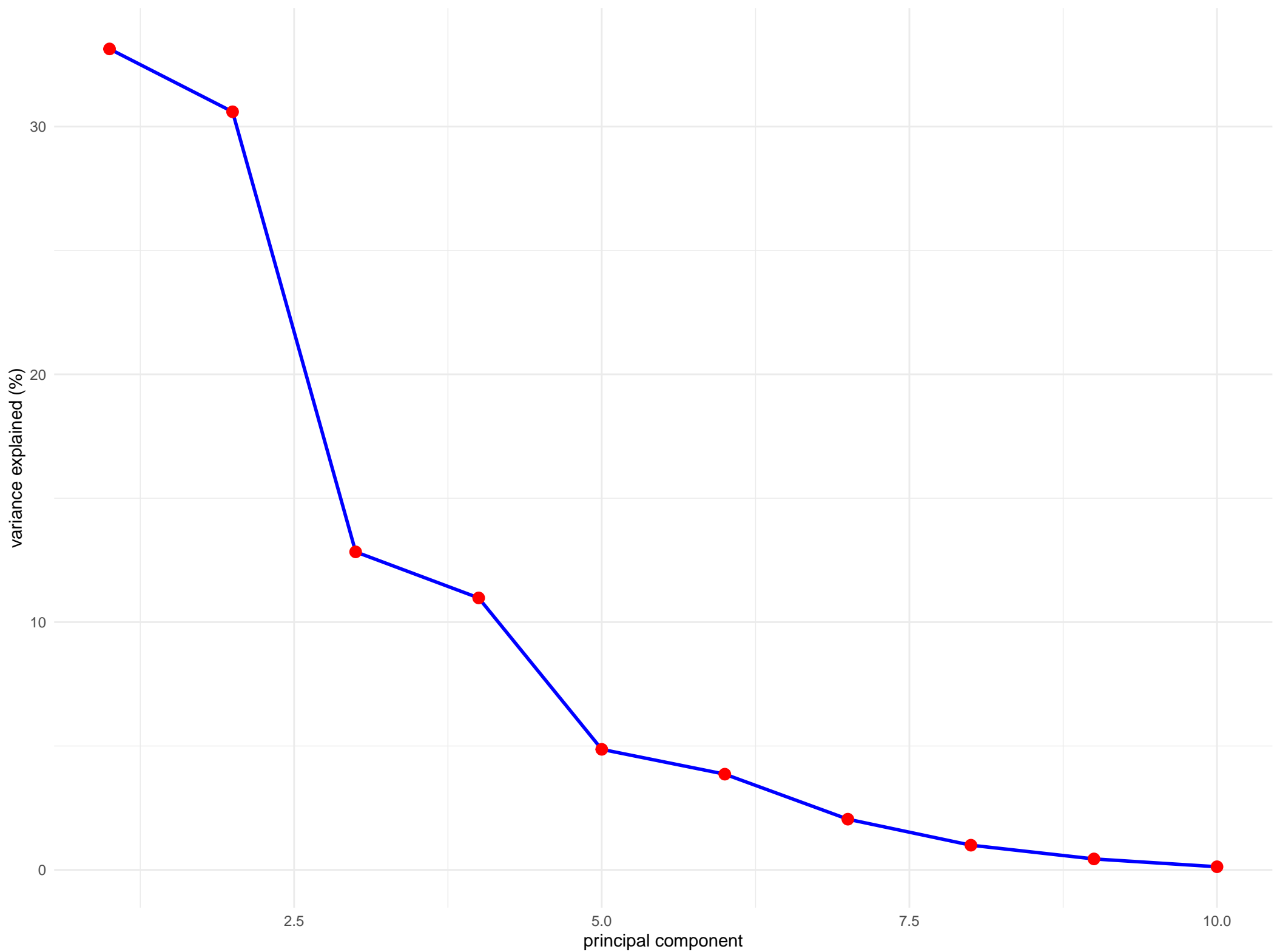


## pca sample identification – summary results

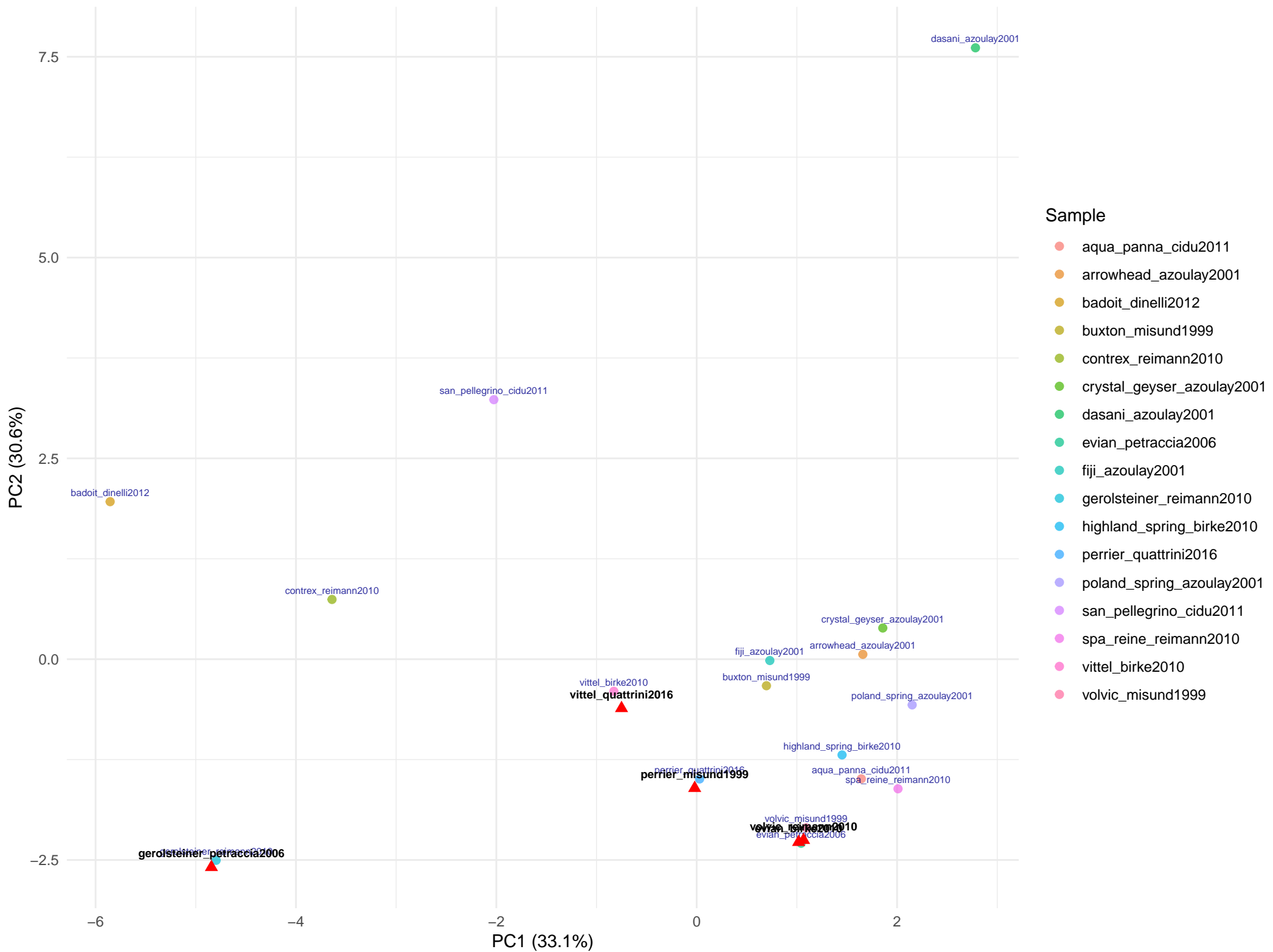
### Dataset Information:

- o Total samples: 22 (5 unknowns + 17 references)
- o Elements analyzed: 20 (0 excluded for zero variance)
- o PC1 variance: 33.13%
- o PC2 variance: 30.6%
- o Cumulative PC1+PC2: 63.73%

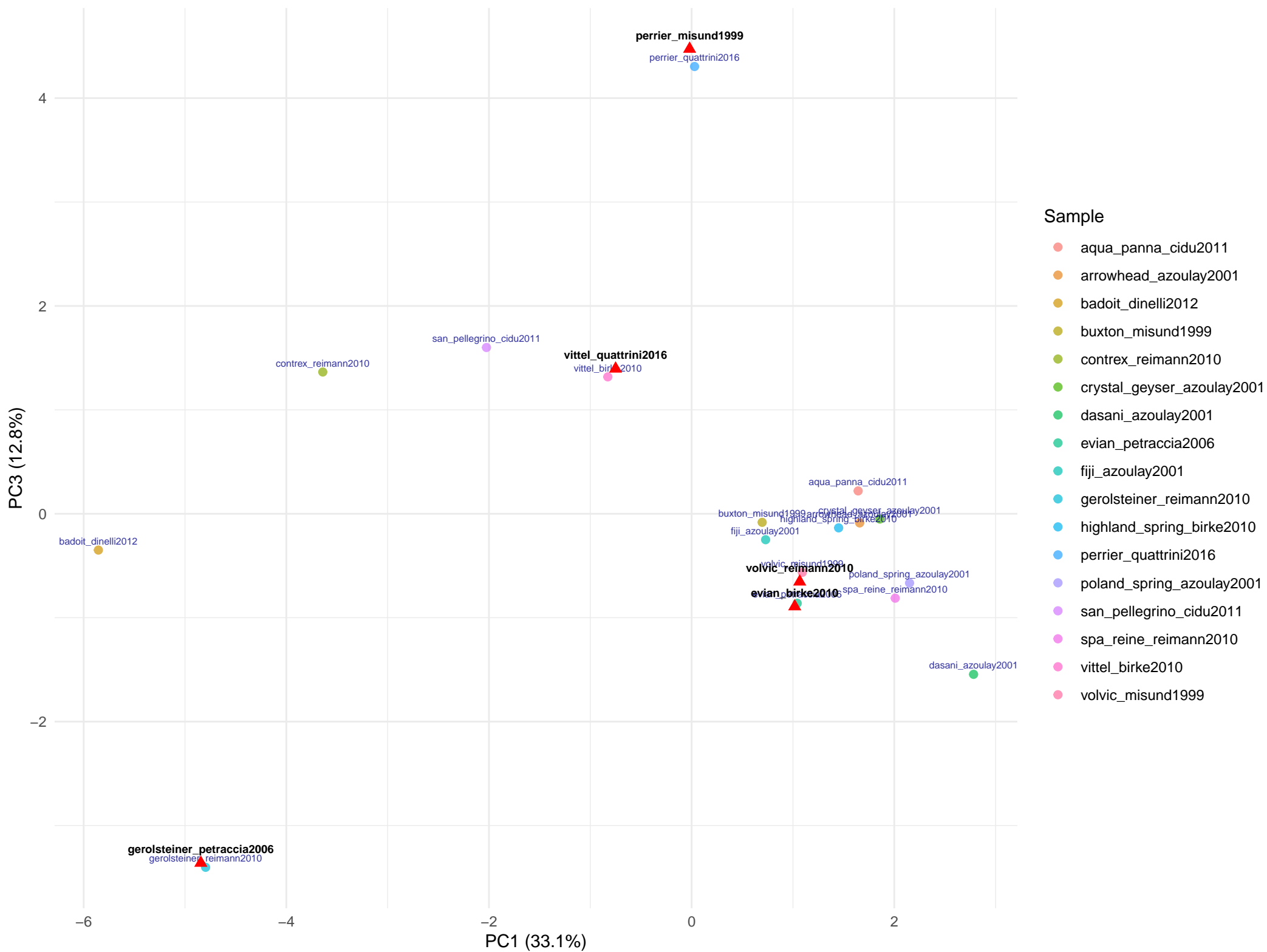
scree plot – variance explained by principal components



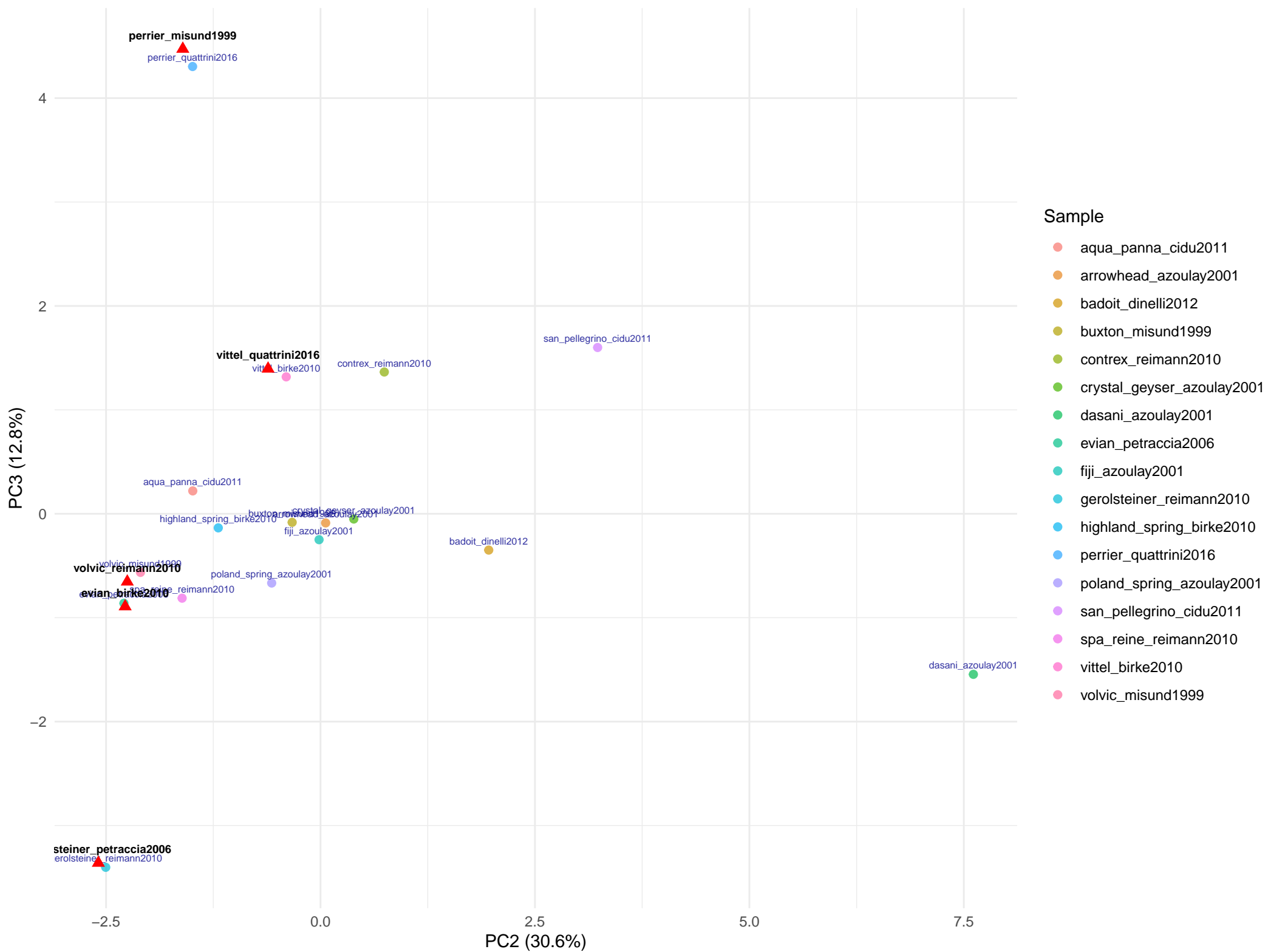
pca scores plot with unknown sample projections



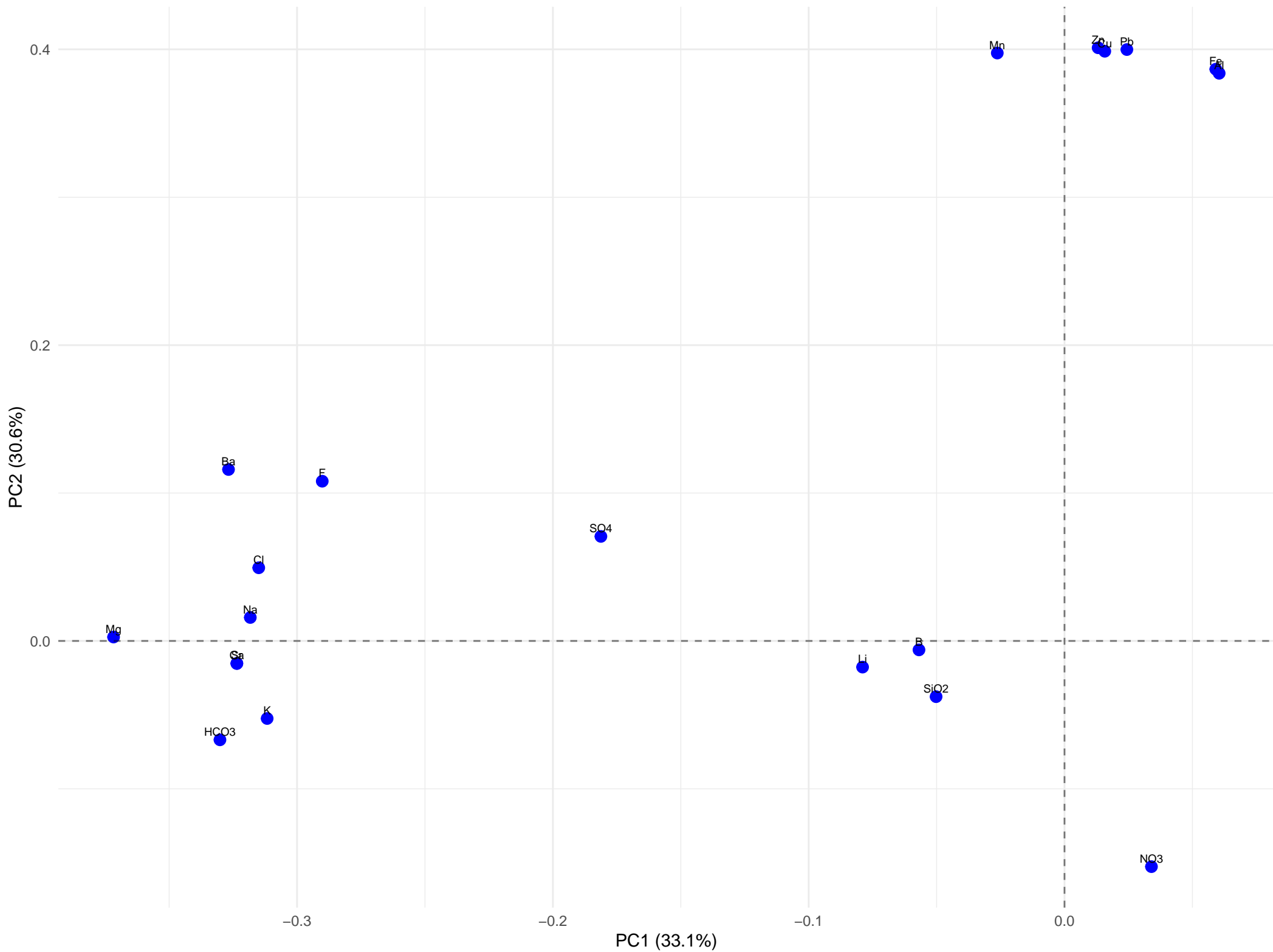
pca scores plot: PC1 vs PC3 with unknown sample projections



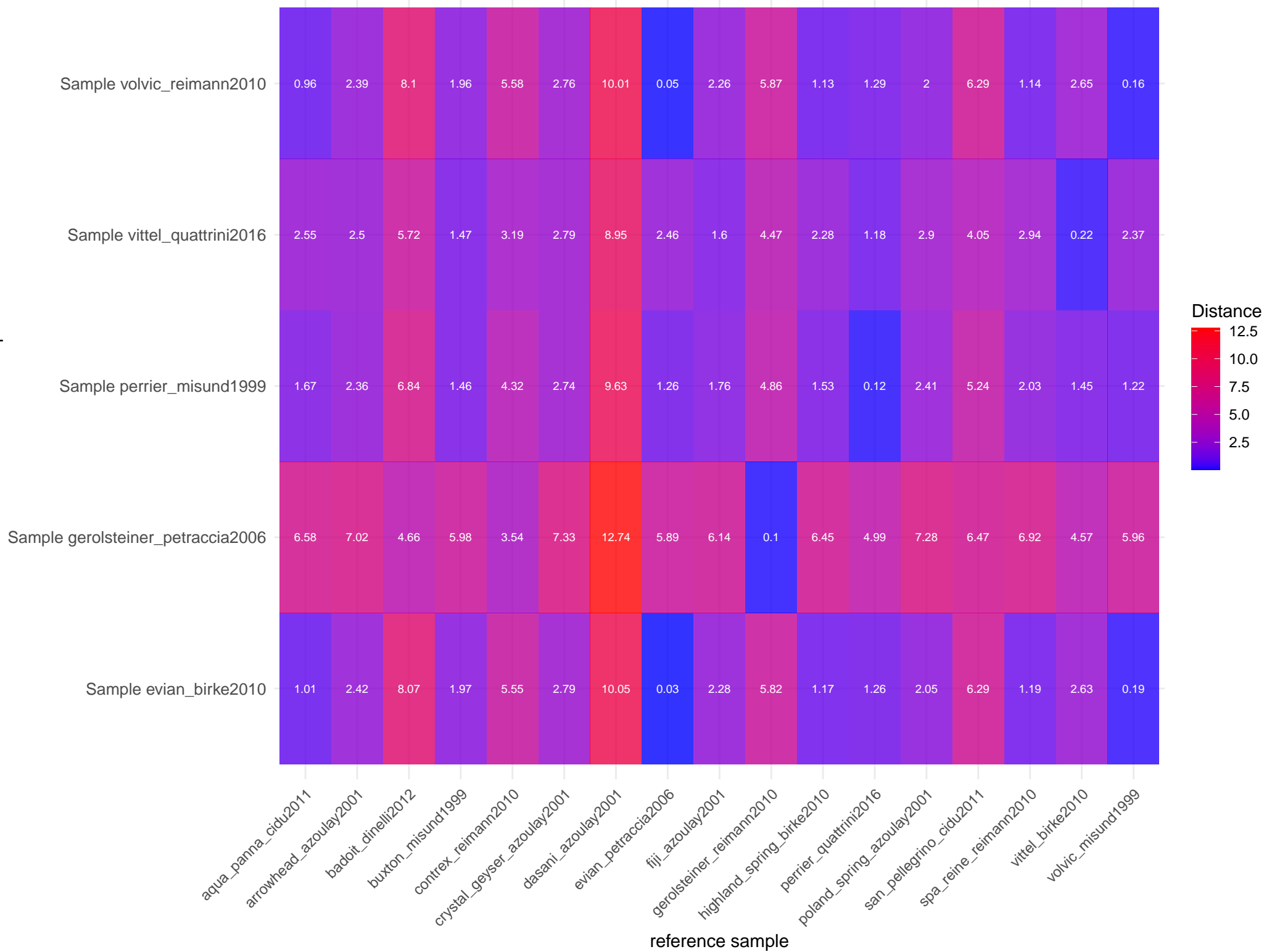
pca scores plot: PC2 vs PC3 with unknown sample projections



pca loadings plot – top 20 contributing elements

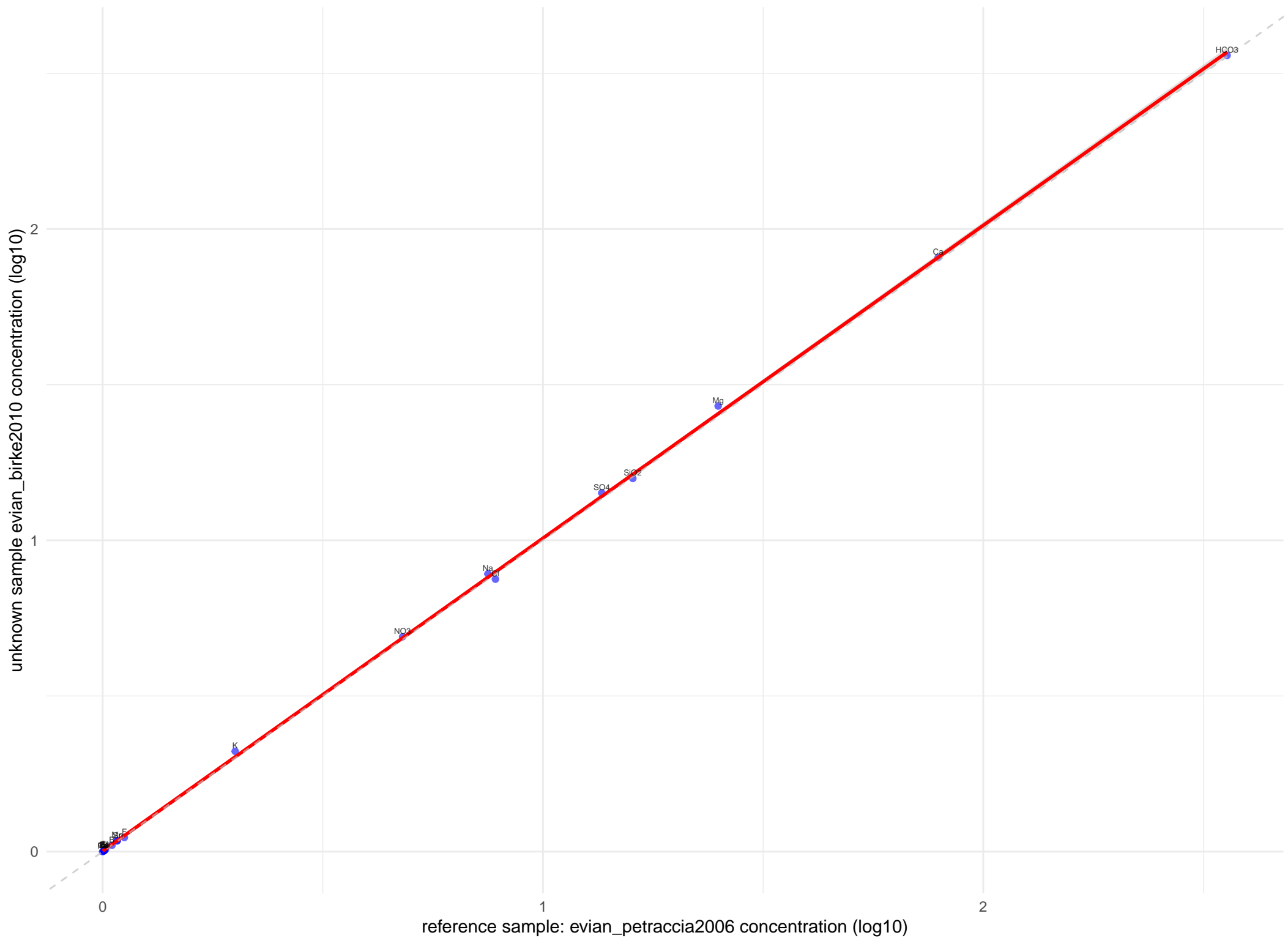


distance matrix – all unknown samples to all reference samples



# element correlation – sample evian\_birke2010 vs evian\_petraccia2006

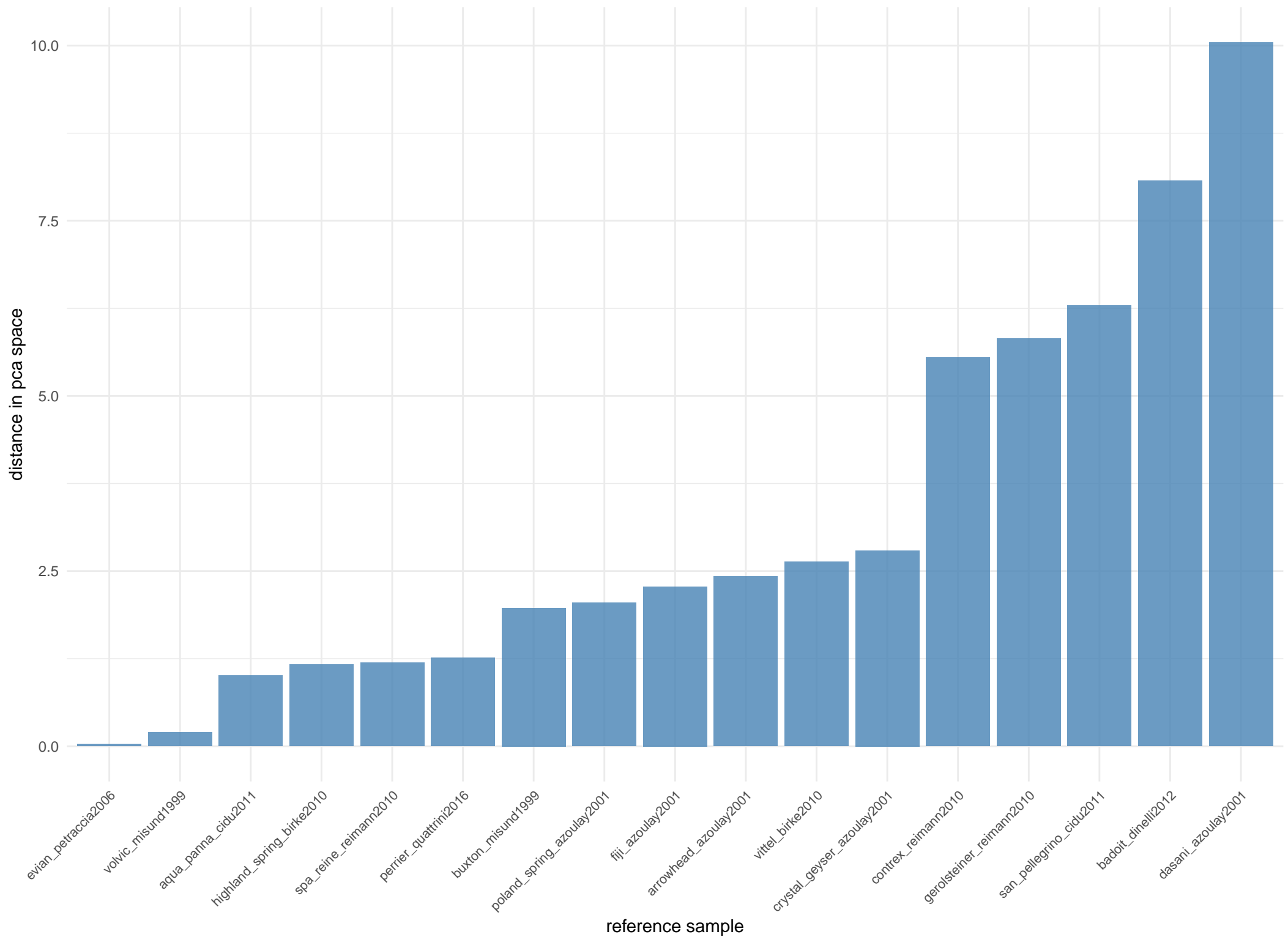
all 20 elements labeled (log scale) | correlation:  $r = 1$





# distance ranking – sample evian\_birke2010 to all reference samples

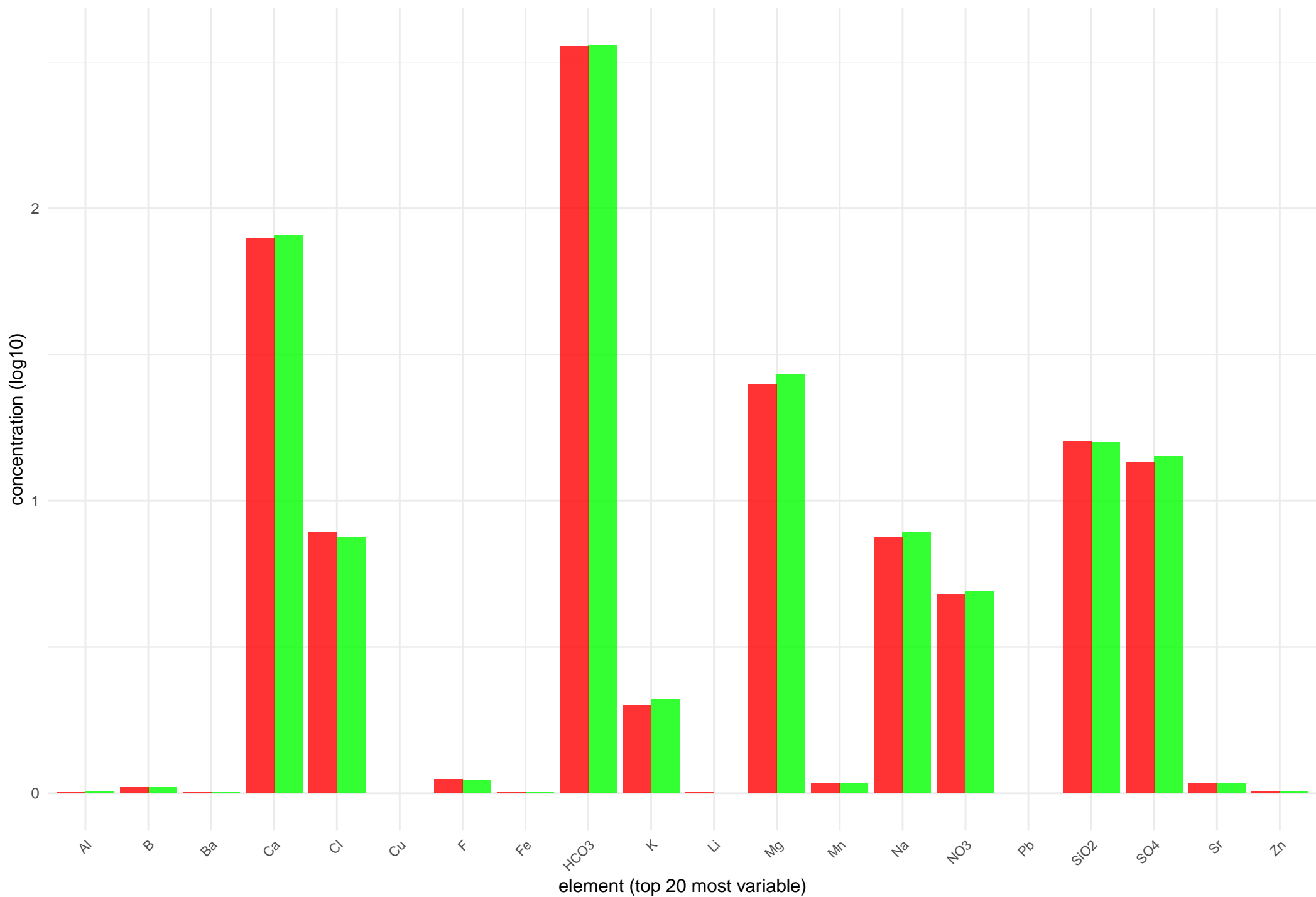
closest match: evian\_petraccia2006 | distance: 0.028



# element profile comparison – sample evian\_birke2010 vs evian\_petraccia2006

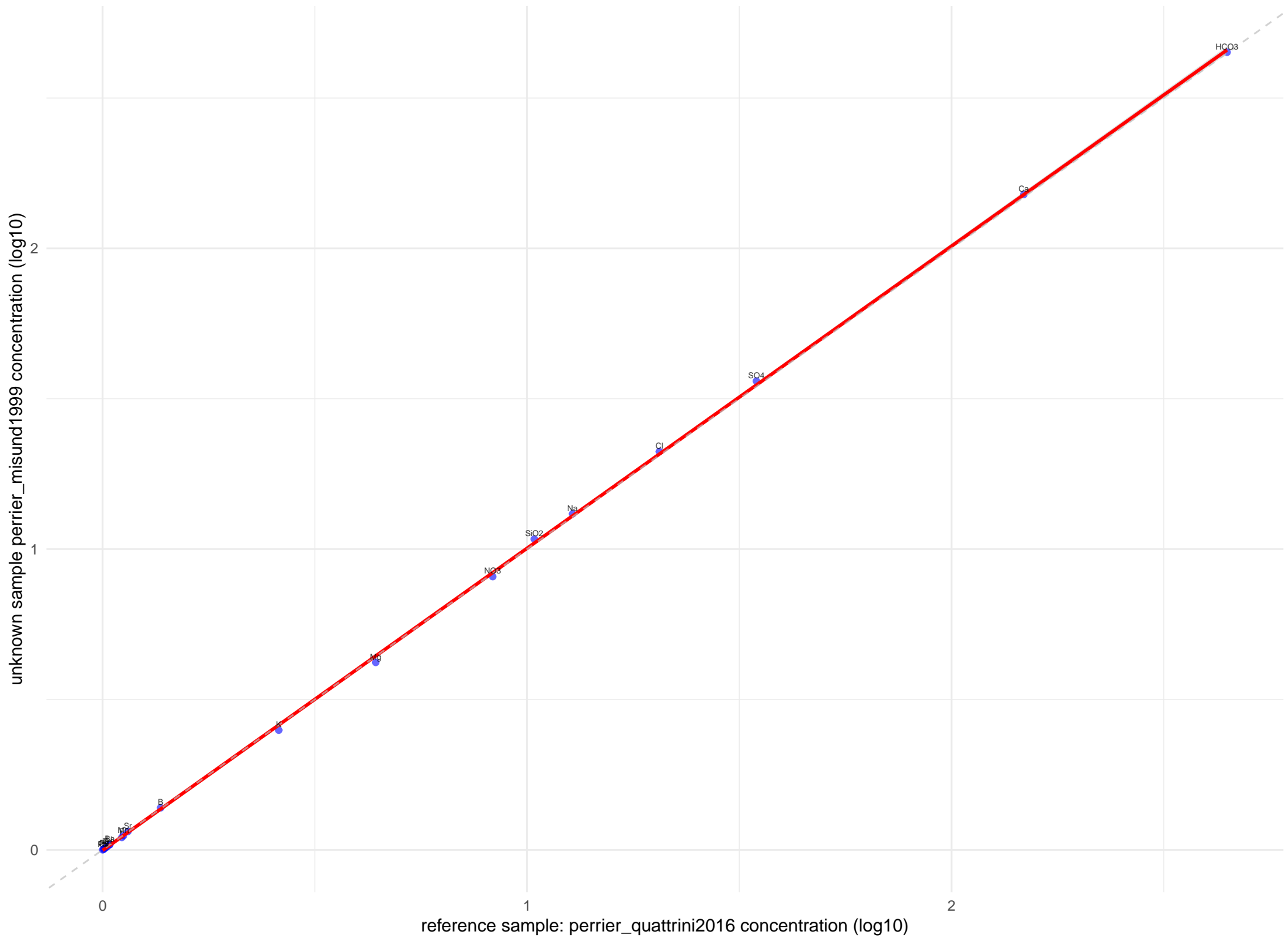
top 20 most variable elements (log scale) | distance: 0.028 | correlation: 1

sample ■ evian\_petraccia2006 ■ Sample evian\_birke2010



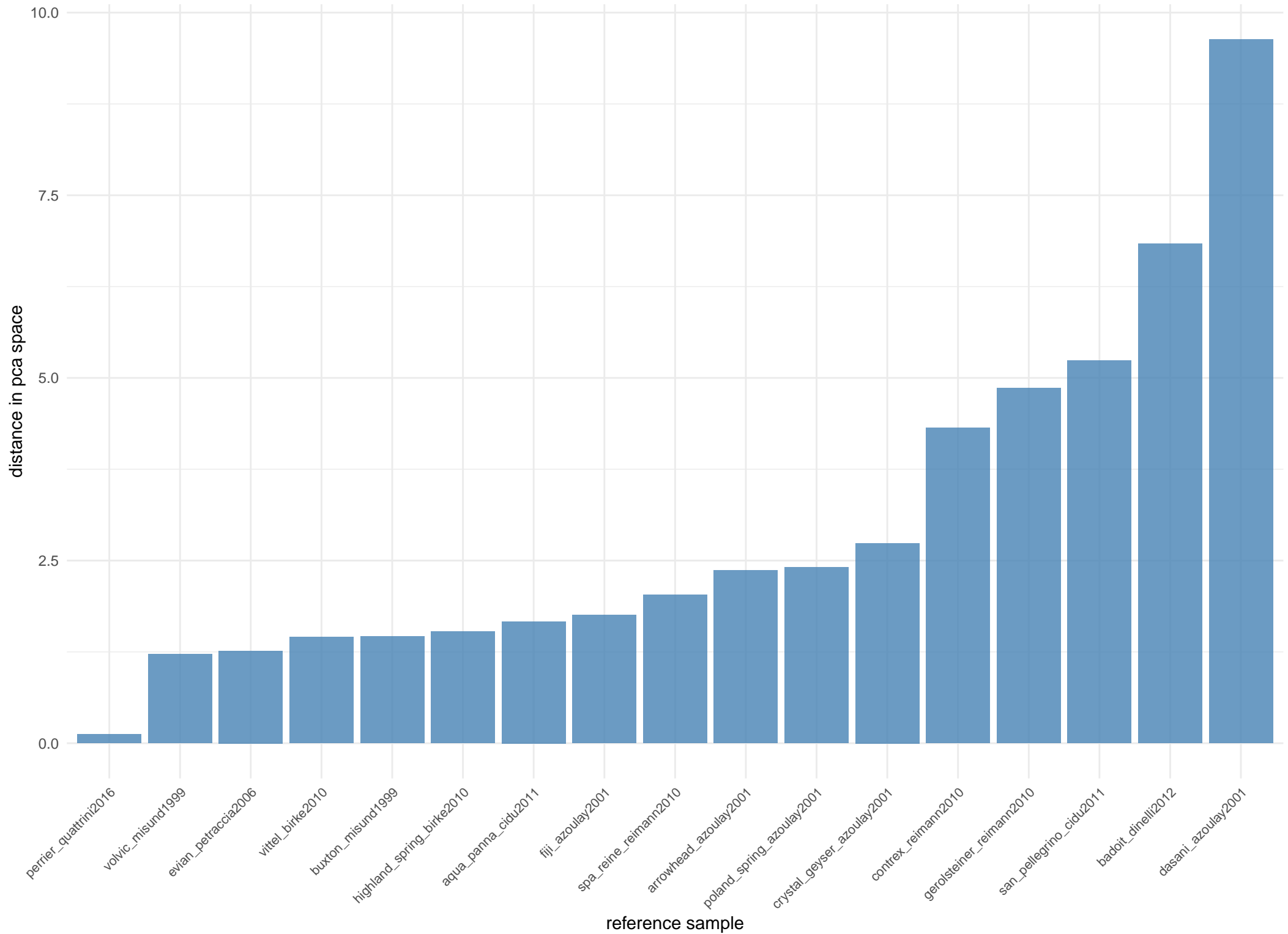
# element correlation – sample perrier\_misund1999 vs perrier\_quattrini2016

all 20 elements labeled (log scale) | correlation:  $r = 1$



# distance ranking – sample perrier\_misund1999 to all reference samples

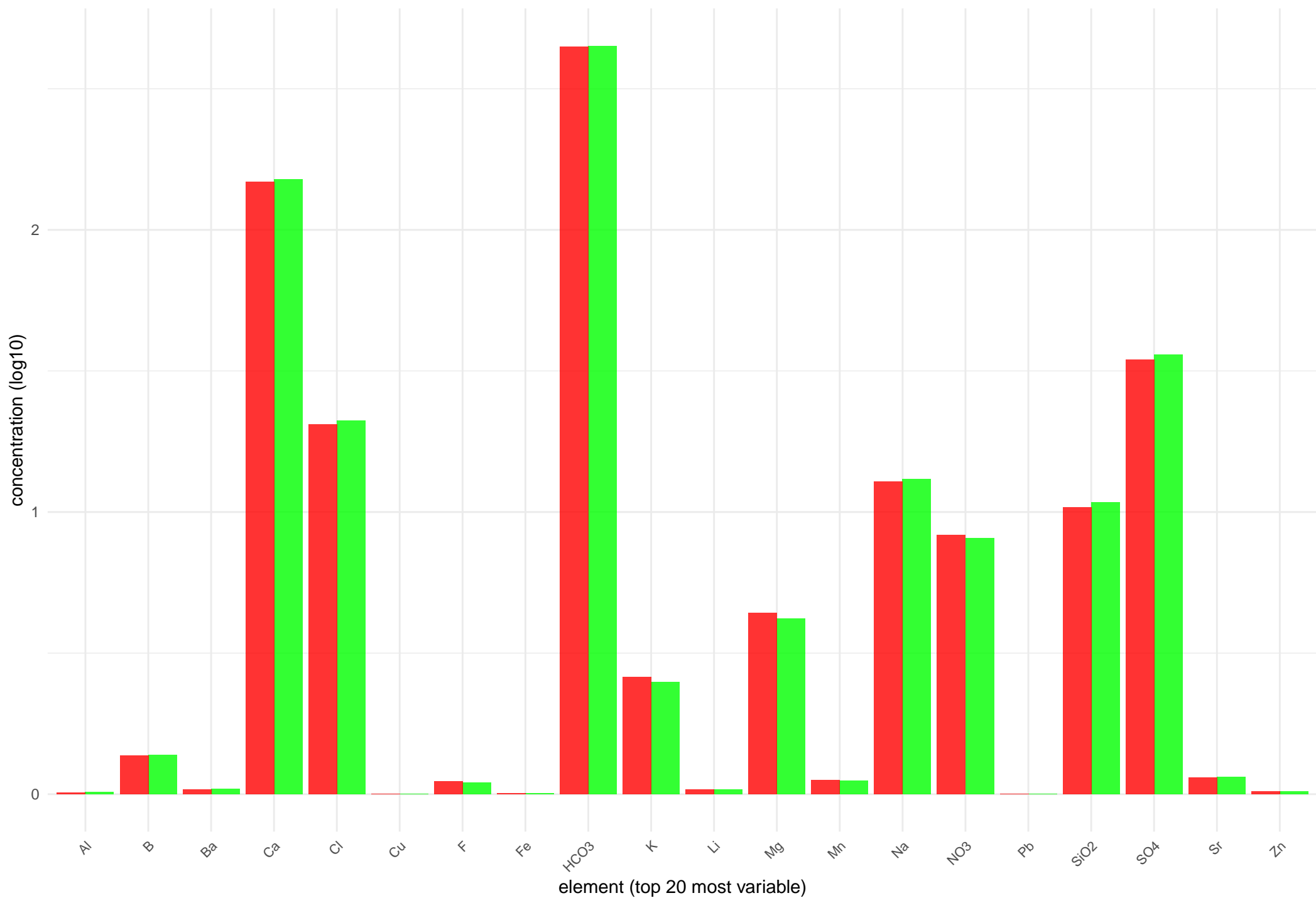
closest match: perrier\_quattrini2016 | distance: 0.124



# element profile comparison – sample perrier\_misund1999 vs perrier\_quattrini2016

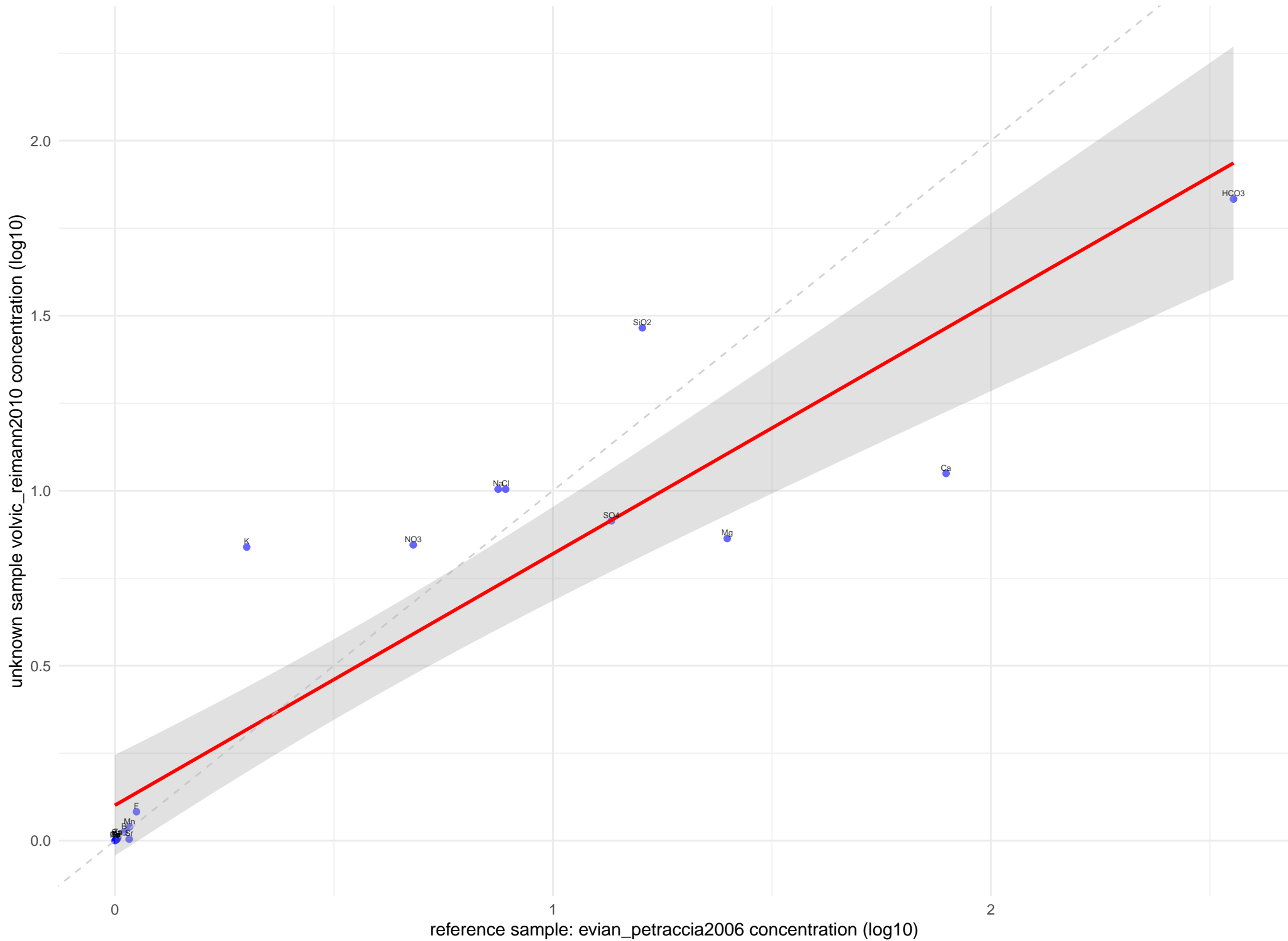
top 20 most variable elements (log scale) | distance: 0.124 | correlation: 1

sample ■ perrier\_quattrini2016 ■ Sample perrier\_misund1999



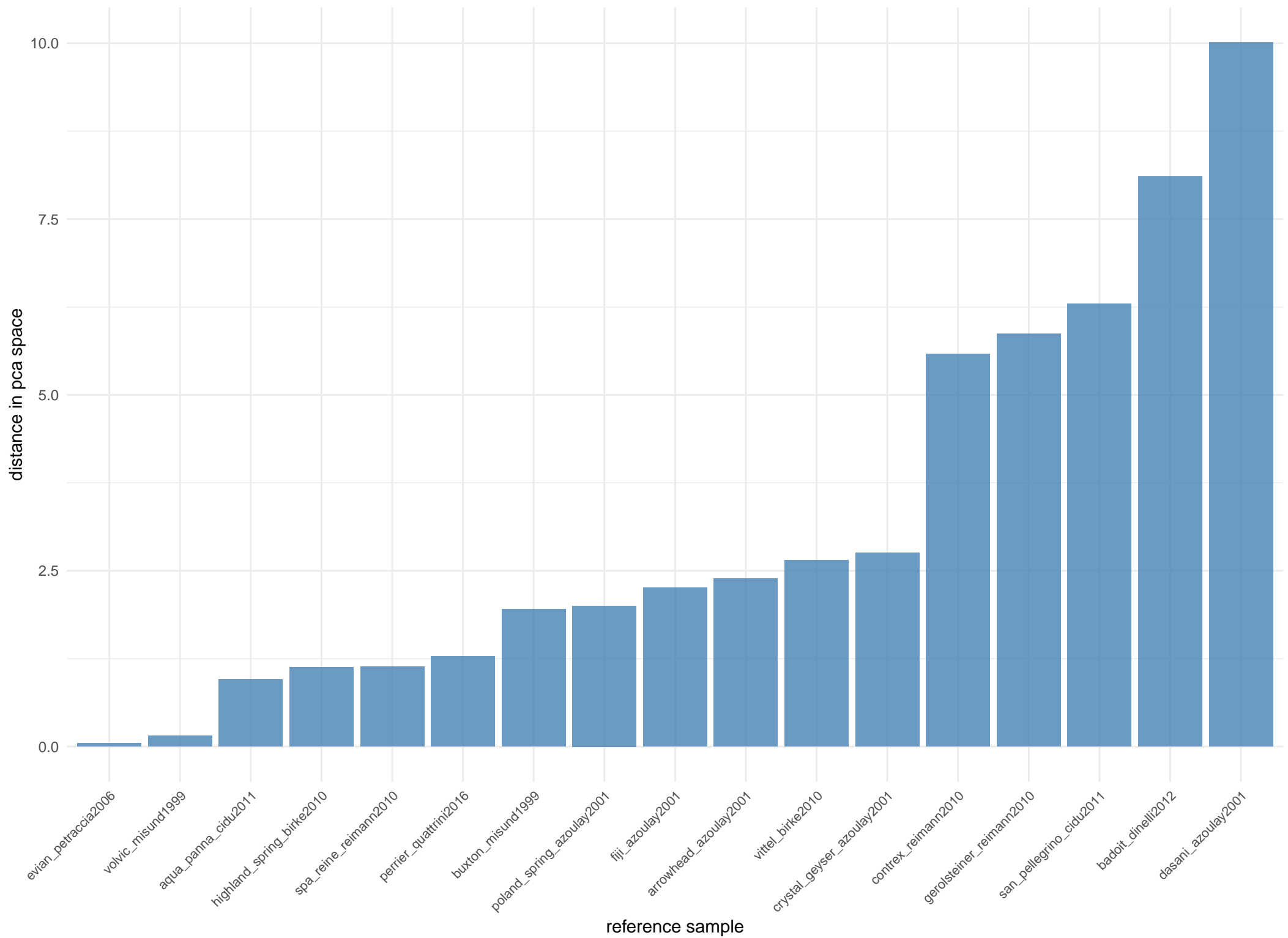
# element correlation – sample volvic\_reimann2010 vs evian\_petraccia2006

all 20 elements labeled (log scale) | correlation:  $r = 0.9192$



# distance ranking – sample volvic\_reimann2010 to all reference samples

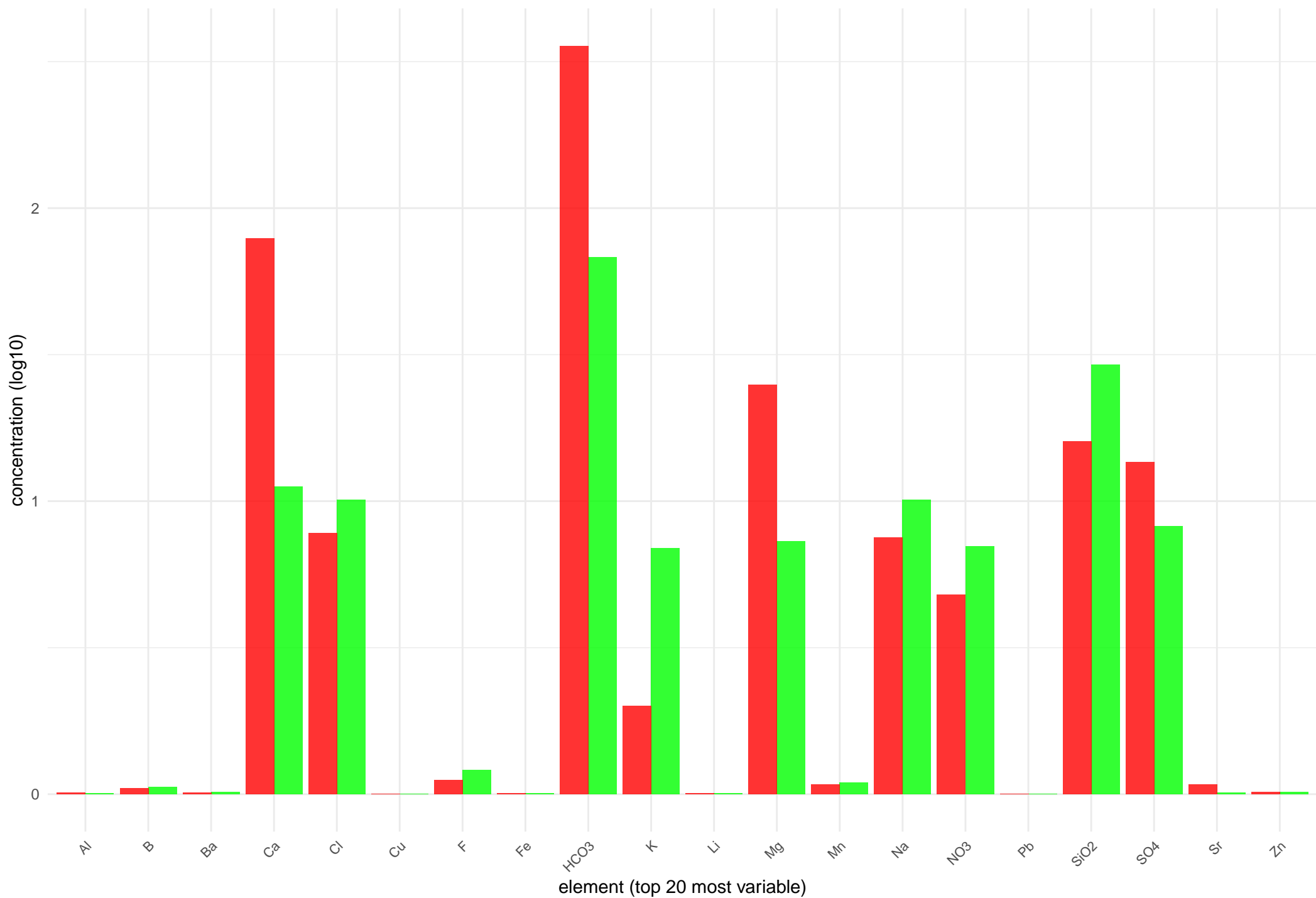
closest match: evian\_petraccia2006 | distance: 0.046



# element profile comparison – sample volvic\_reimann2010 vs evian\_petraccia2006

top 20 most variable elements (log scale) | distance: 0.046 | correlation: 0.9192

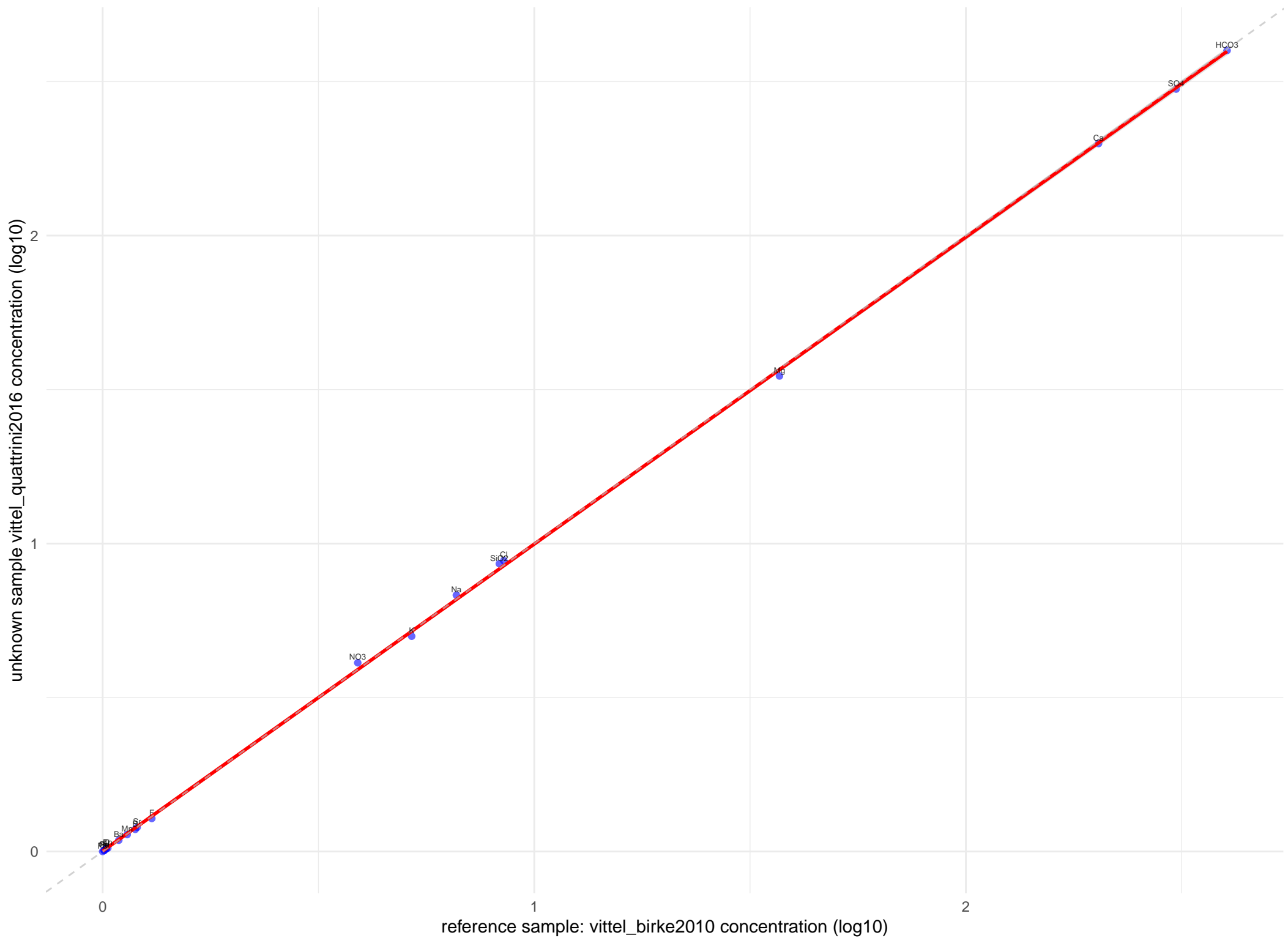
sample ■ evian\_petraccia2006 ■ Sample volvic\_reimann2010





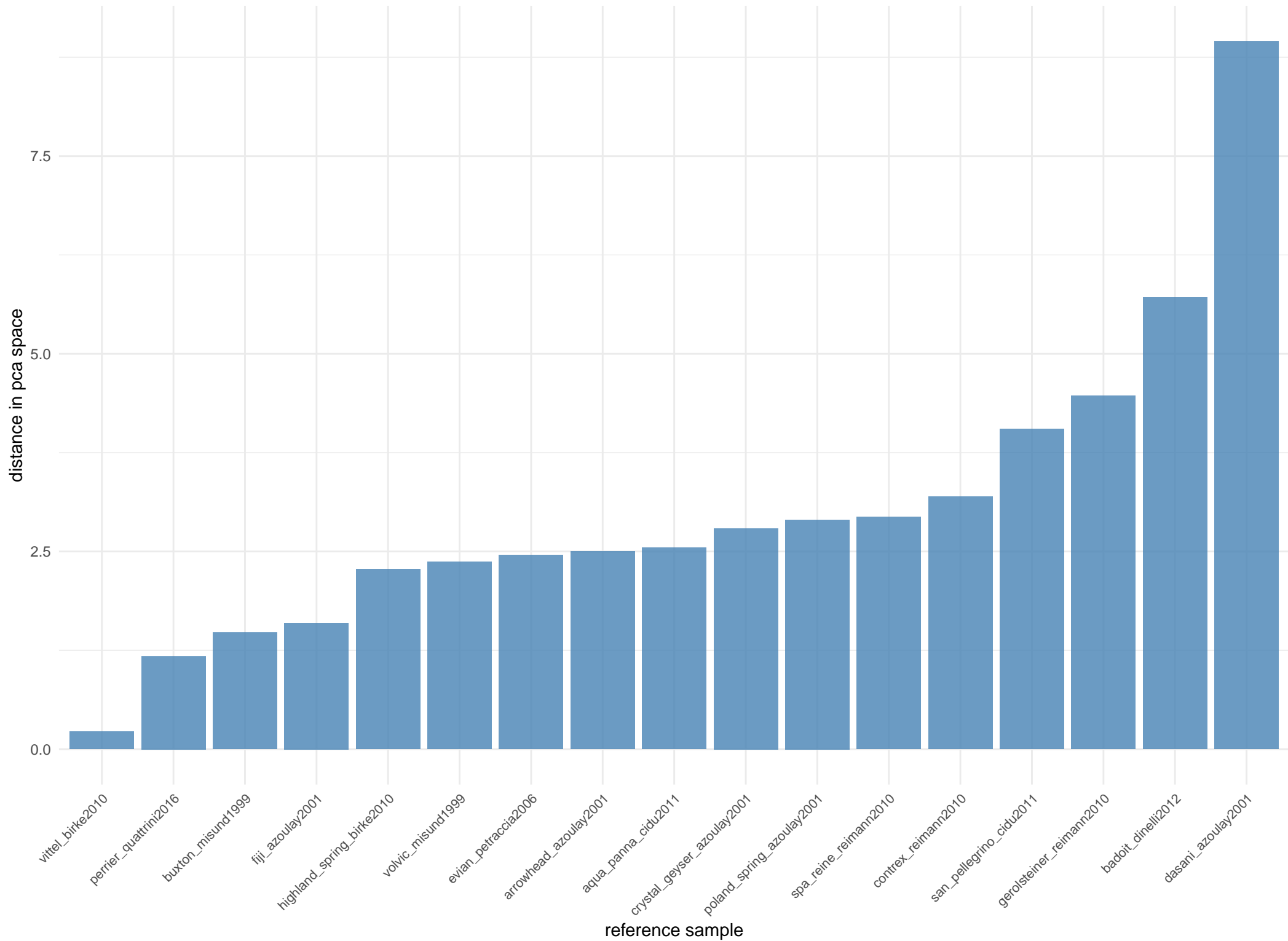
# element correlation – sample vittel\_quattrini2016 vs vittel\_birke2010

all 20 elements labeled (log scale) | correlation:  $r = 1$



# distance ranking – sample vittel\_quattrini2016 to all reference samples

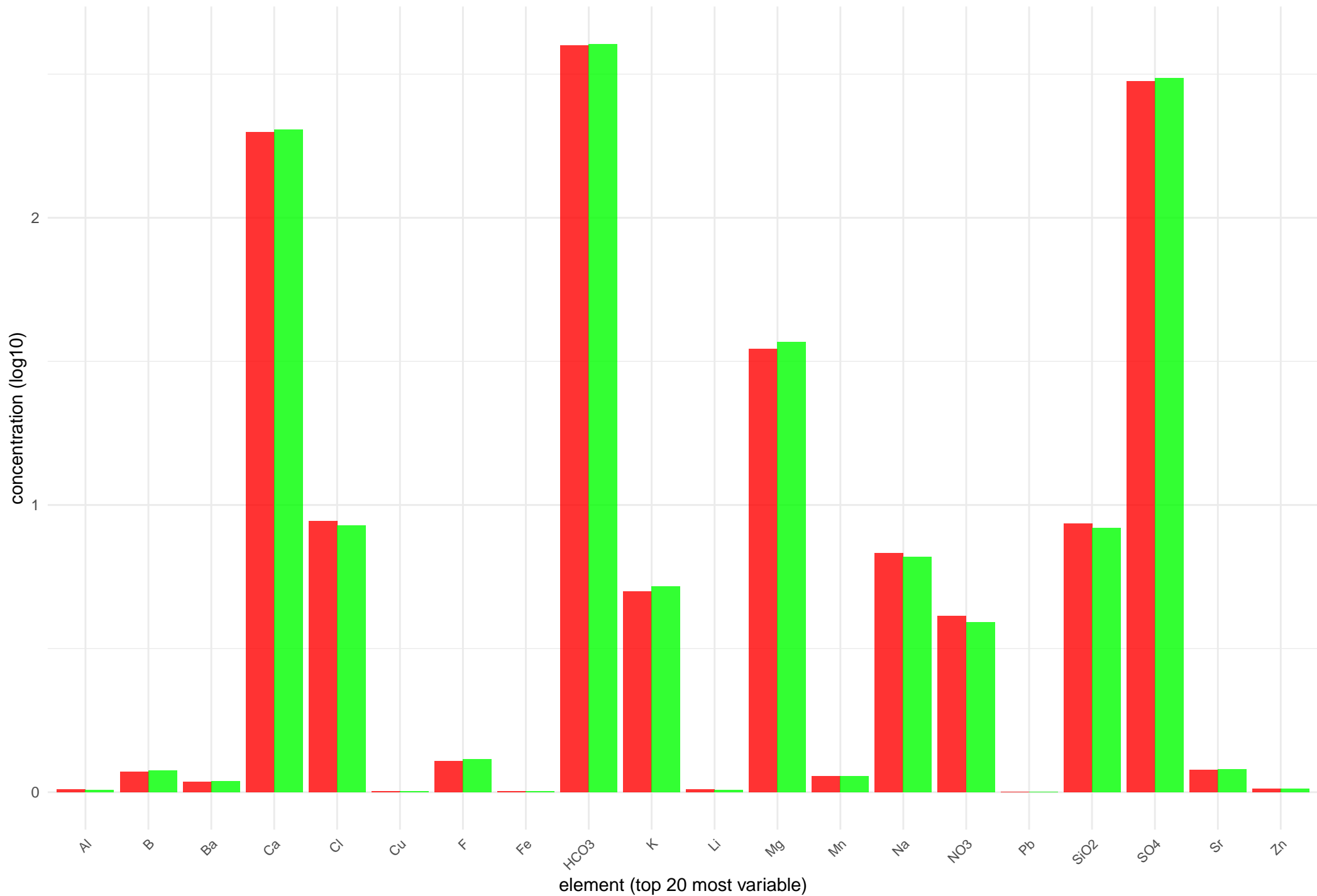
closest match: vittel\_birke2010 | distance: 0.225



# element profile comparison – sample vittell\_quattrini2016 vs vittell\_birke2010

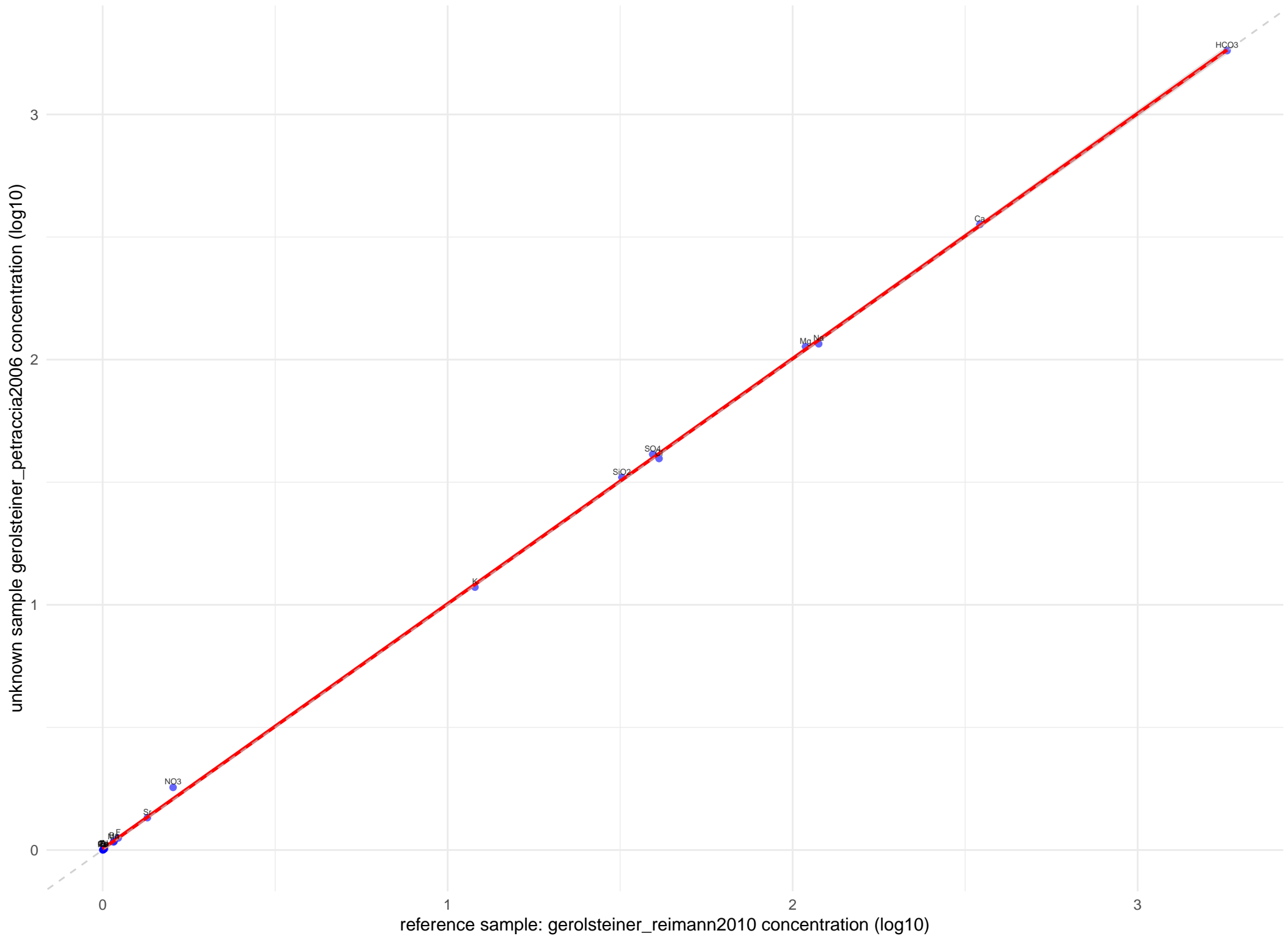
top 20 most variable elements (log scale) | distance: 0.225 | correlation: 1

sample ■ Sample vittell\_quattrini2016 ■ vittell\_birke2010



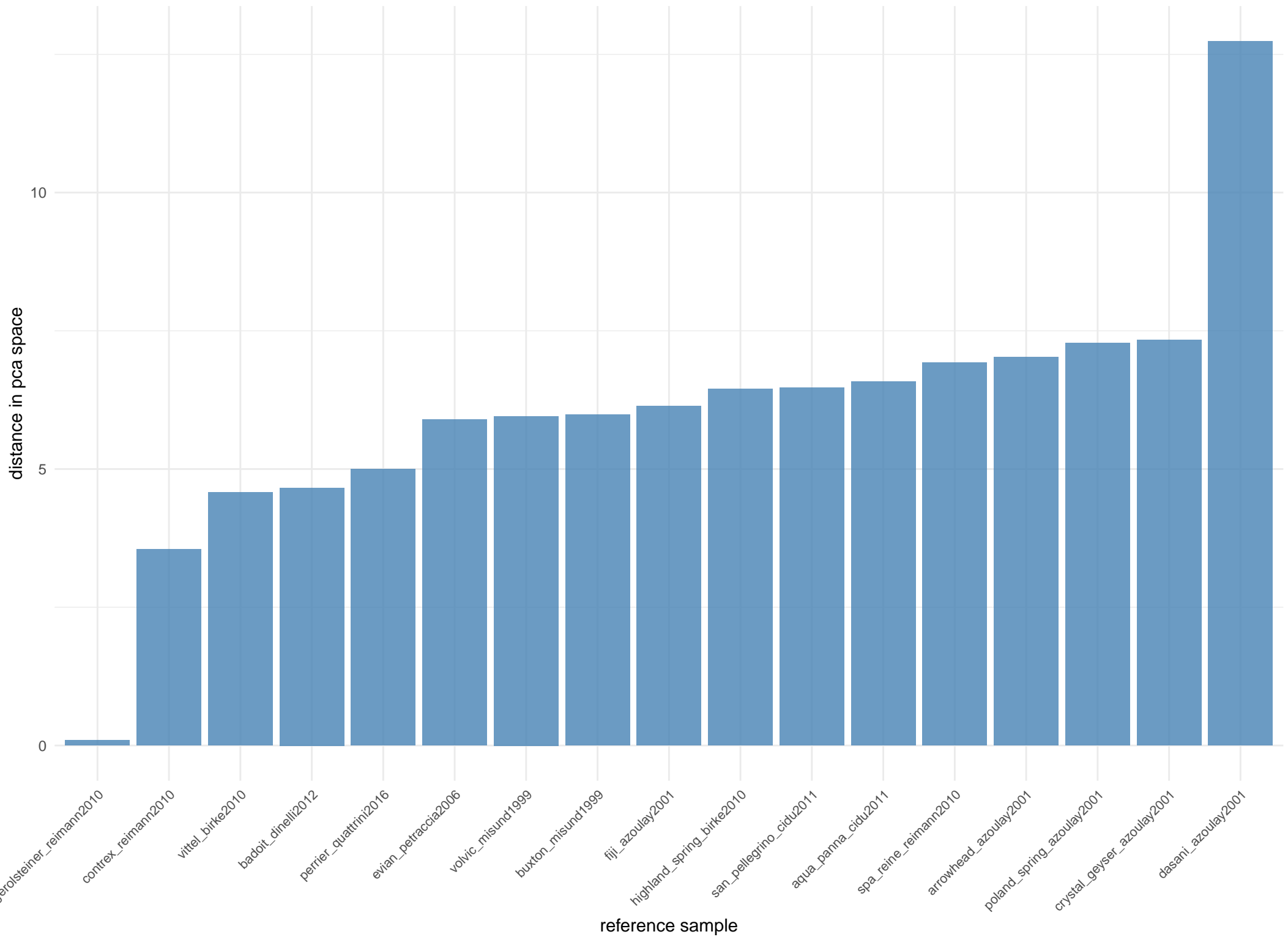
# element correlation – sample gerolsteiner\_petraccia2006 vs gerolsteiner\_reimann2010

all 20 elements labeled (log scale) | correlation:  $r = 1$



# distance ranking – sample gerolsteiner\_petraccia2006 to all reference samples

closest match: gerolsteiner\_reimann2010 | distance: 0.098



# element profile comparison – sample gerolsteiner\_petraccia2006 vs gerolsteiner\_reimann2010

top 20 most variable elements (log scale) | distance: 0.098 | correlation: 1

sample ■ gerolsteiner\_reimann2010 ■ Sample gerolsteiner\_petraccia2006

