Supplementary Material (ESI) for Chemical Communications

Support Information

The Power of the Weak: Recognition of Ion Pairs in Water Using a Simple Array Sensor

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Contents:

Preparation of sub-microliter sensor arrays for anions,cations and Ion-pairs sensing.

The multi-well 10x8 (sub-microliter) chips were fabricated by ultrasonic drilling of microscope slides (a well diameter: 500 ±10 μm, depth: 500 ±10 μm). The sensor solutions (500 uM/L) were prepared by dissolving dyes S1-S6 in a PU-20 solution (4%, w/w), which was made by dissolving PU-20 in a mixture of solvents containing methanol and THF (v/v: 0.5/9.5). In a typical sensor array, the sensor solution was spotted onto the multi-well chip, the anions were then added as aqueous solutions (200nL, 500μM) of their corresponding salts, to each well containing a sensor. pH controlled experiments were carried out by adjusted with NaOH (0.01 M) and HCl (0.01 M) aqueous solutions. pH values of the anions solutions were measured by Titrator T50 (Mettler Toledo Co.).

Image Acquisition and Data Processing of a Sensor Array

Images from the sensor arrays were recorded using a Kodak Image Station 440CF. The scanned images (12 bit) are acquired with a resolution of 433x 441 pixels per inch and with grey levels over 1000 (12 second exposures). The sensor arrays are excited with a broadband UV lamp (300-400 nm, λ_{max}=365 nm) and up to four channels were used for emission detection: (1) Blue: band-pass filter 380-500 nm λ_{max}=435 nm, (2) Green: band pass filter 480-600 nm λ_{max}=525 nm, (3) Yellow: low pass filter 523 nm, (4) Red: low pass filter 590 nm. After acquiring the images, the integrated (non zero) grey pixel (*n*) value is calculated for each well of each channel. Images of the sensor chip were recorded before (*b*) and after (*a*) the addition of an analyte and their final responses (*R*) were evaluated as follows:

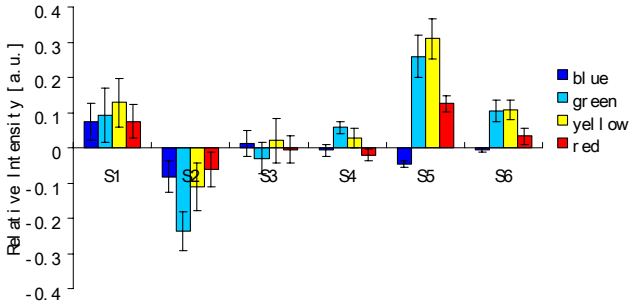
$$R = \sum_n \frac{a_n}{b_n} - 1$$

Sensors array responds for different analytes at different pH values

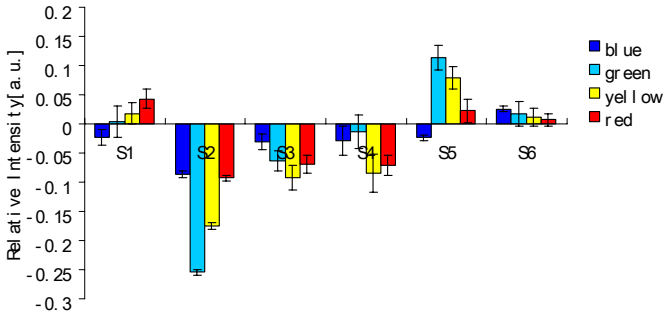
Lithium series anions analysis in the pH range of 5-9

Anions analysis at pH 5

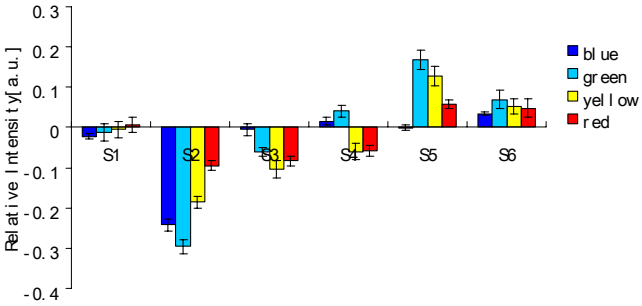
Fluoride



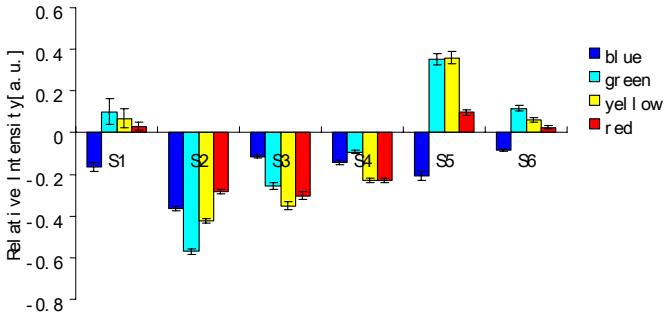
Chloride



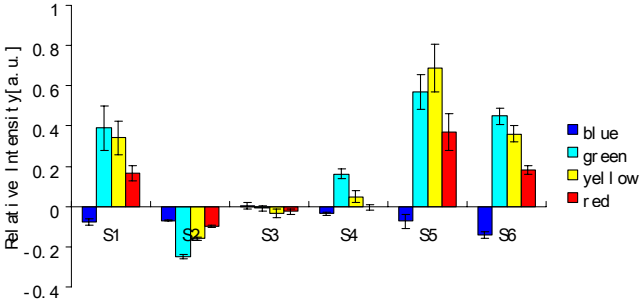
Bromide



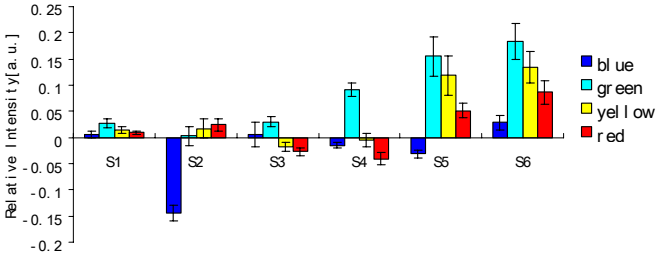
Iodine



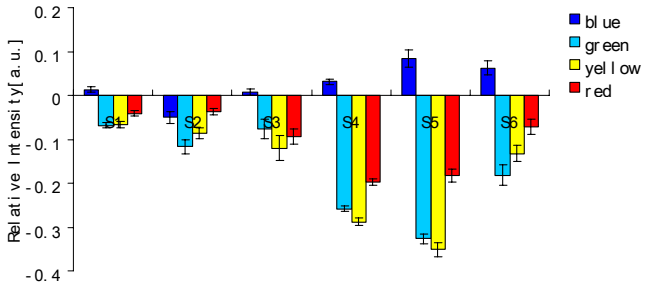
Acetate



Nitrate

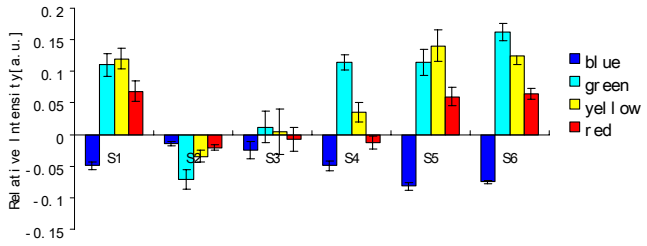


Dihydrogen phosphate



Anions analysis at pH 6

Fluoride



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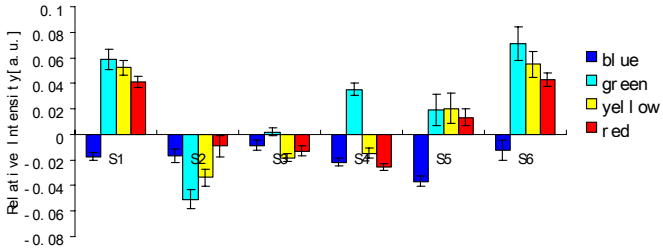

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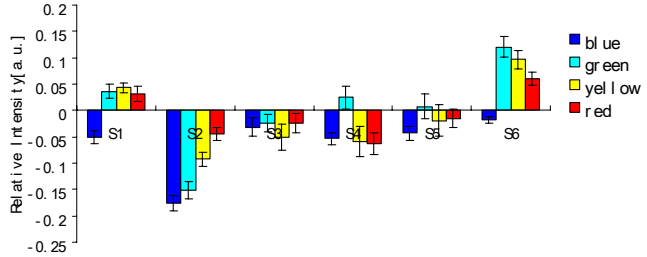

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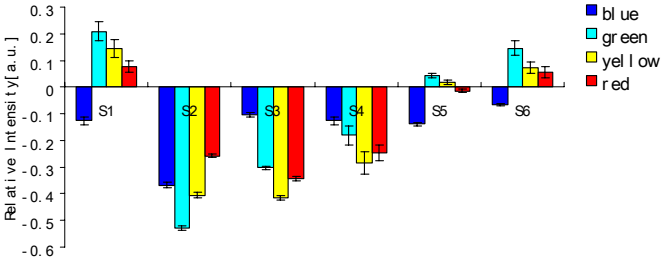

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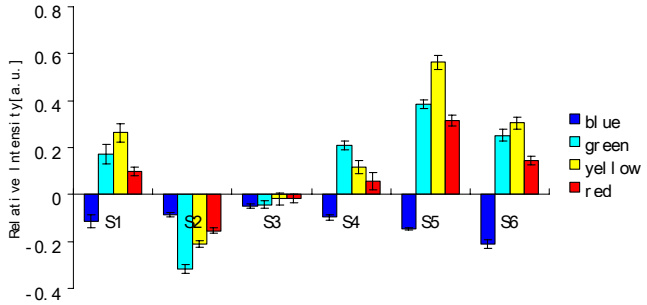

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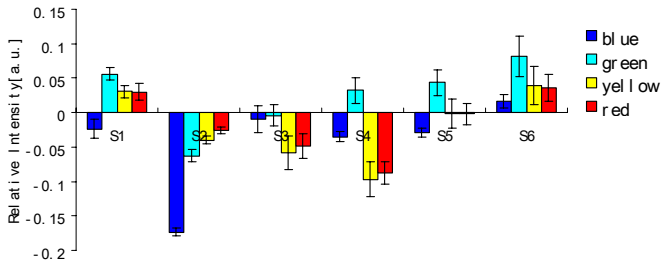
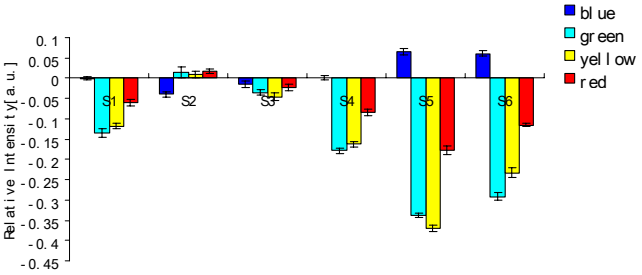
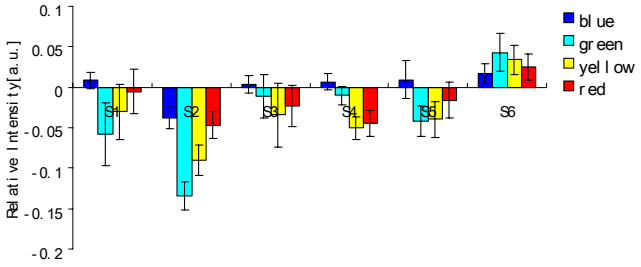


Dihydrogen phosphate



Anions analysis at pH 7

Fluoride



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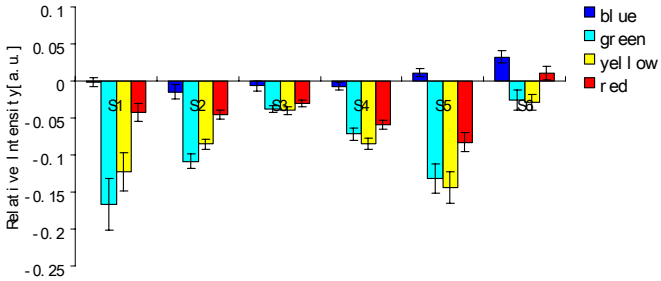

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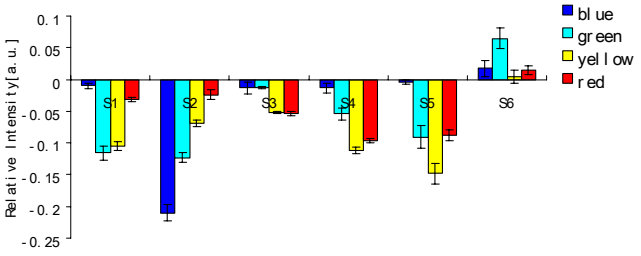

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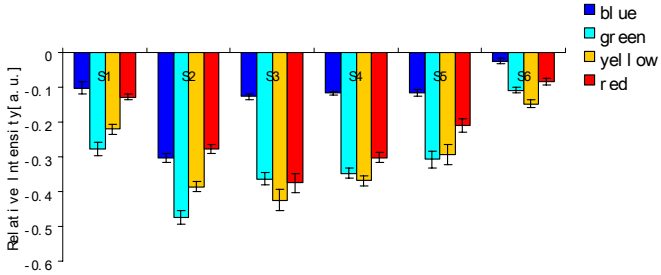

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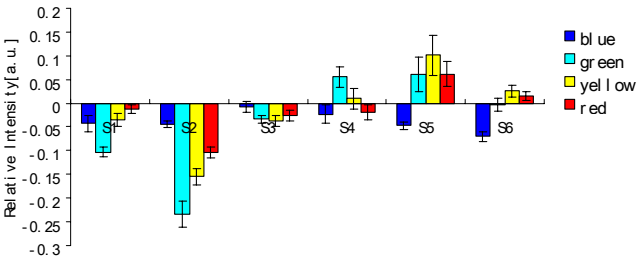

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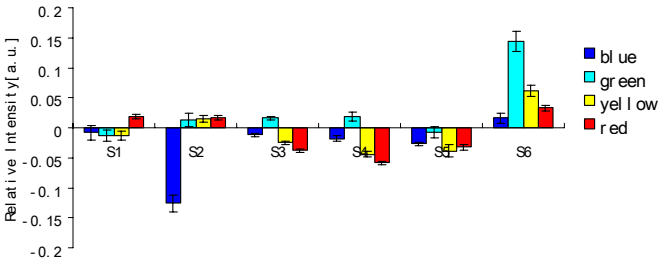
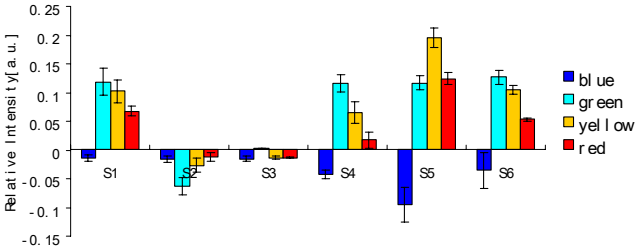
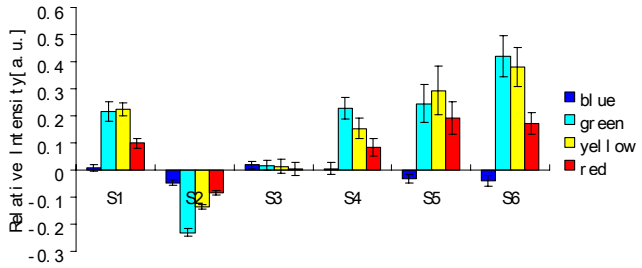


Dihydrogen phosphate



Anions analysis at pH 8

Fluoride



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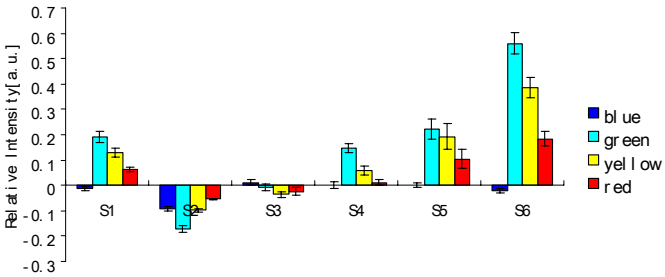

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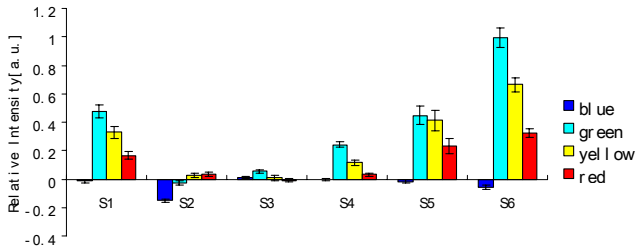

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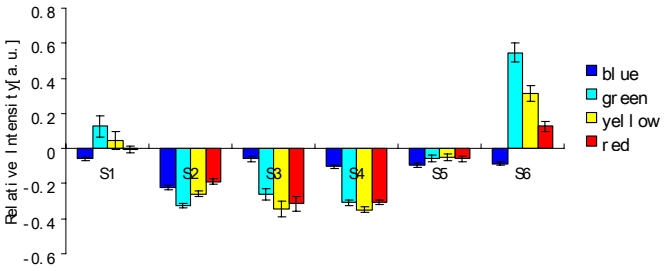

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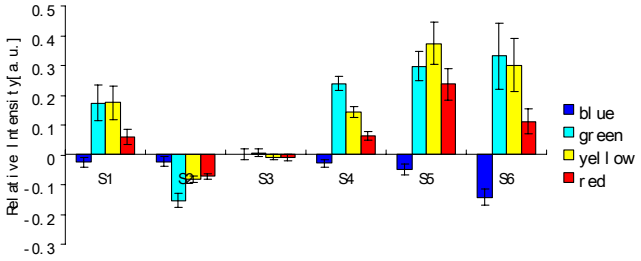

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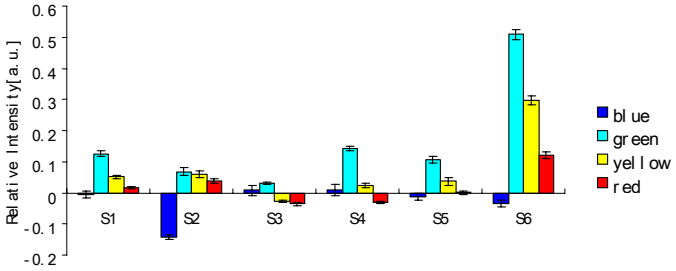
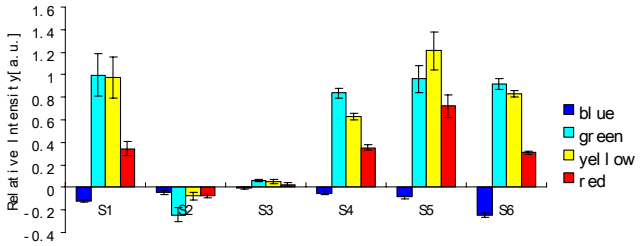
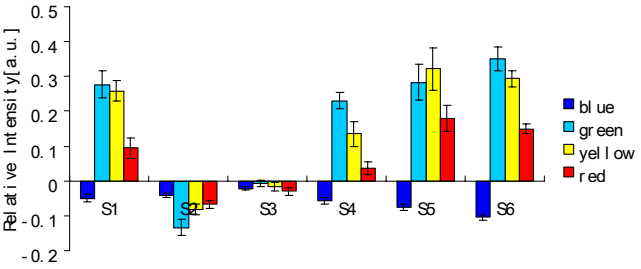


Dihydrogen phosphate



Anions analysis at pH 9

Fluoride



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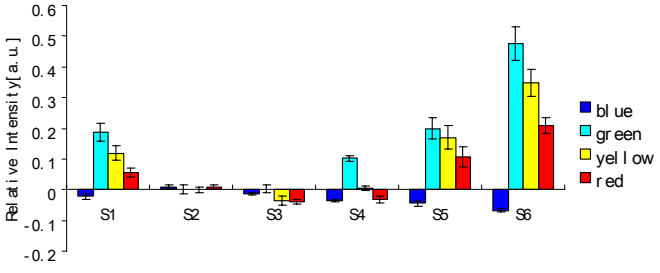

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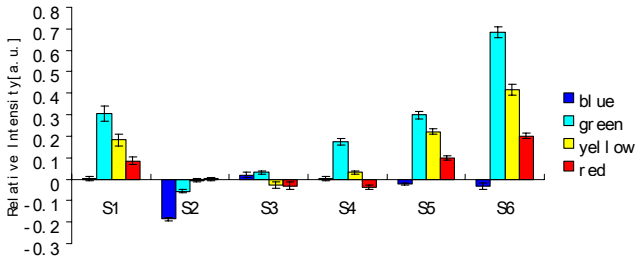

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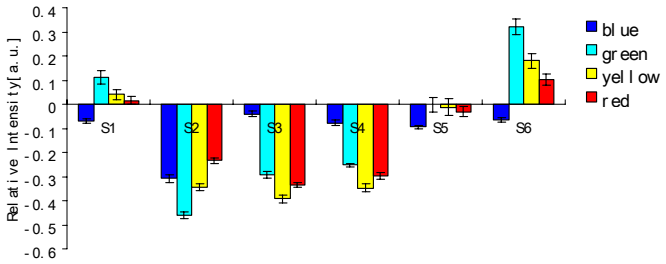

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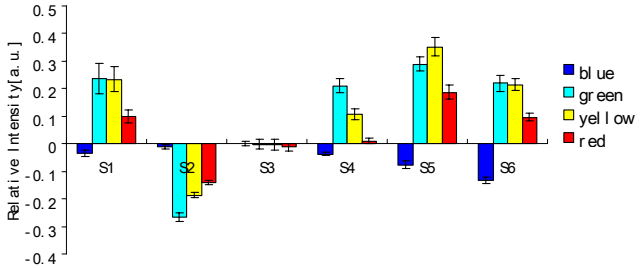

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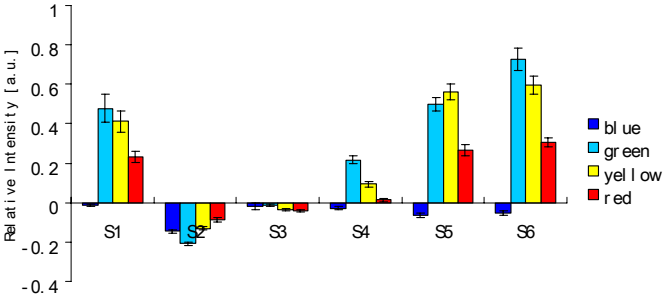
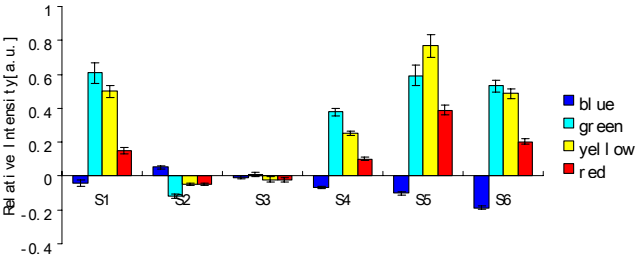


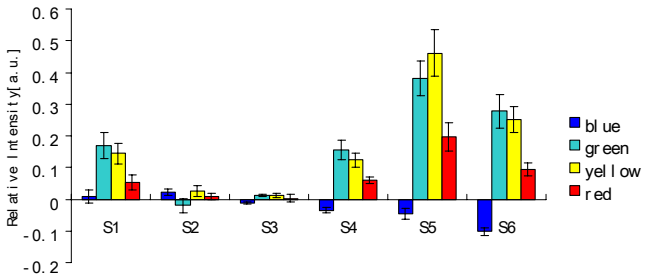
Dihydrogen phosphate



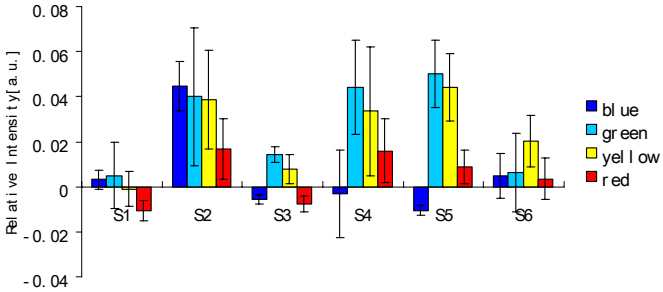
Sodium series anions analysis in the pH range of 5-9

Anions analysis at pH 5

Fluoride



Chloride



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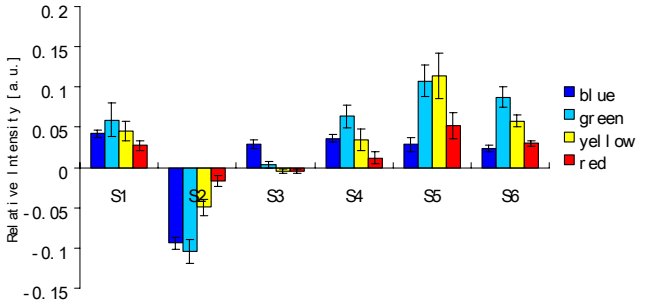
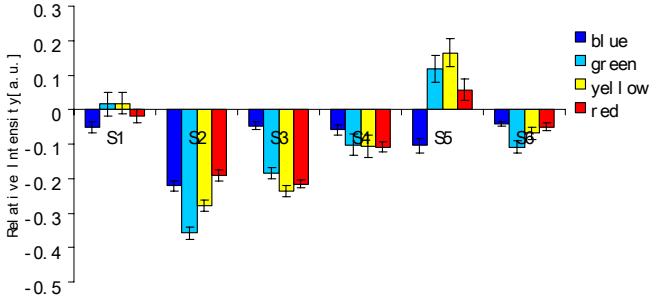
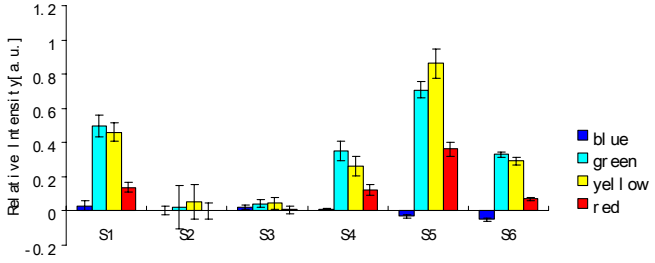


Iodine



Acetate



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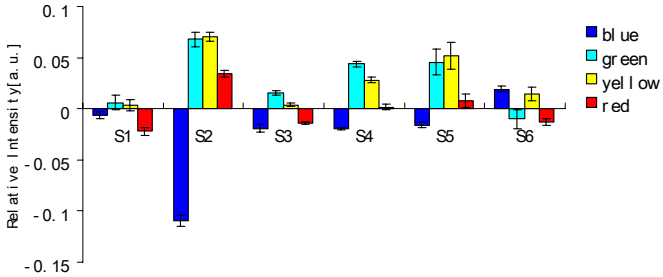
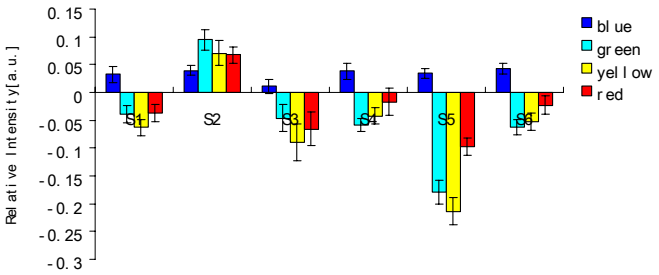
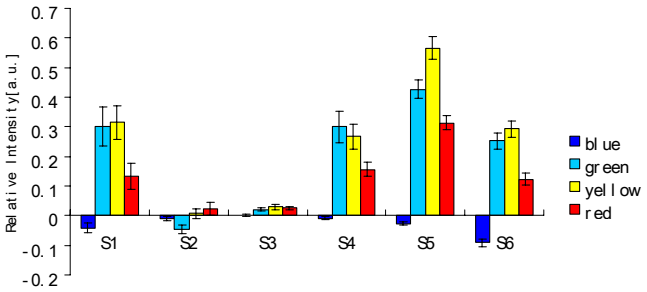


Dihydrogen phosphate

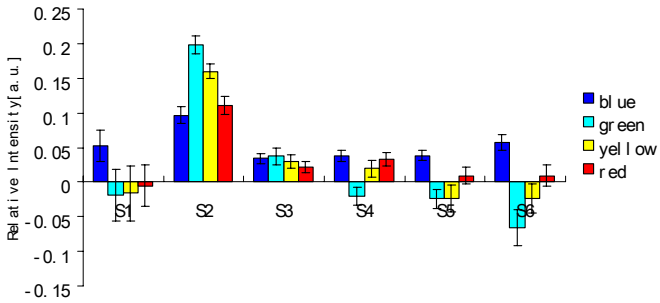


Anions analysis at pH 6

Fluoride



Chloride



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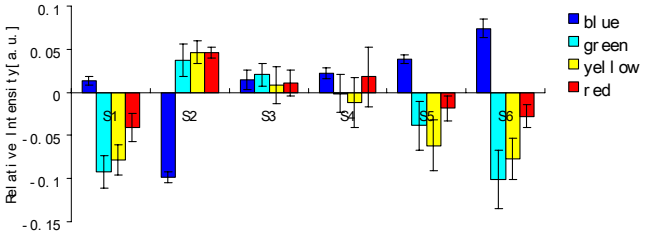

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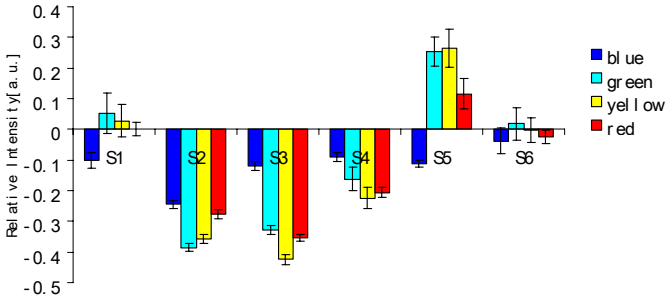

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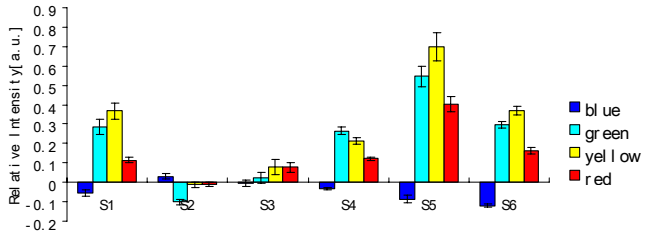

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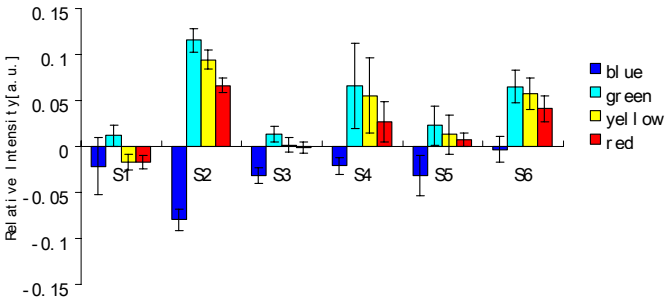
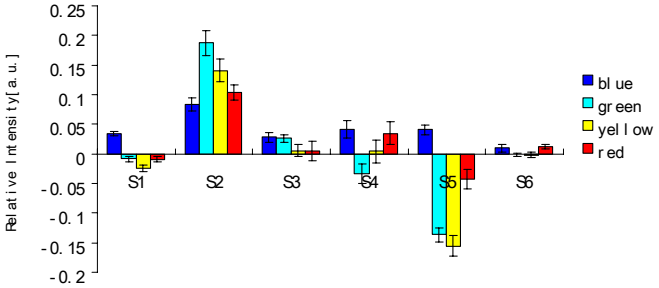
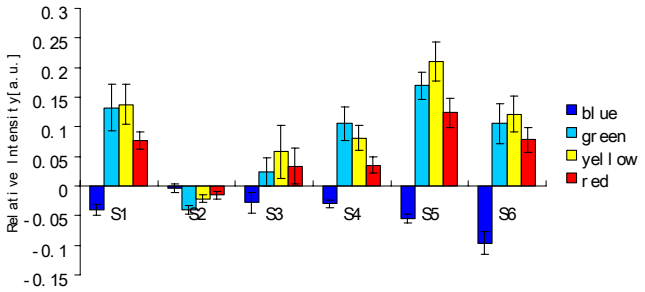


Dihydrogen phosphate



Anions analysis at pH 7

Fluoride



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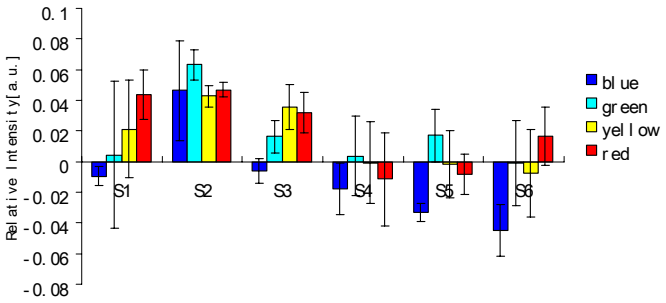

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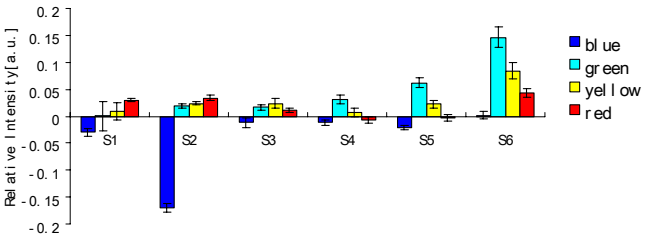
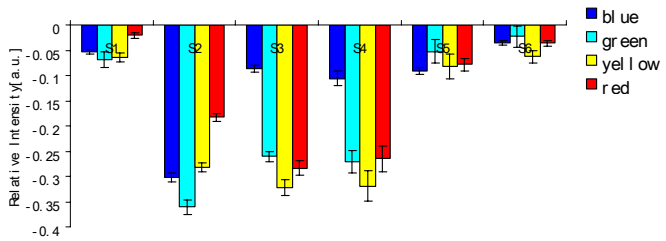


Iodine



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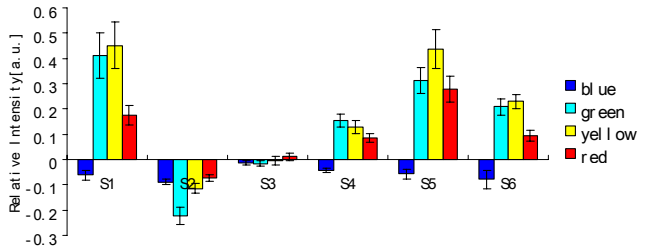
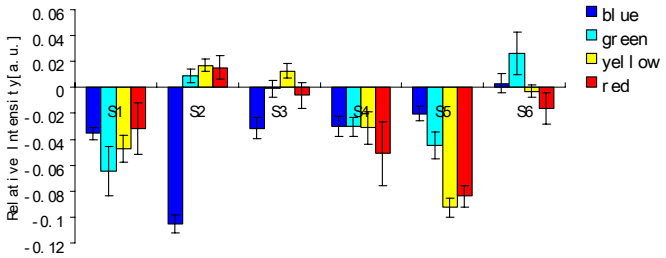
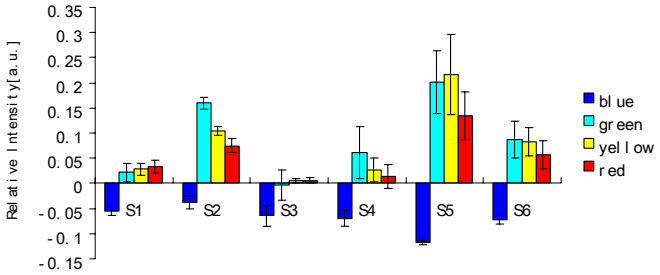


Nitrate

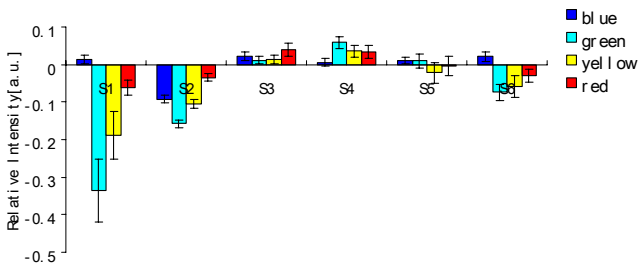


Dihydrogen phosphate

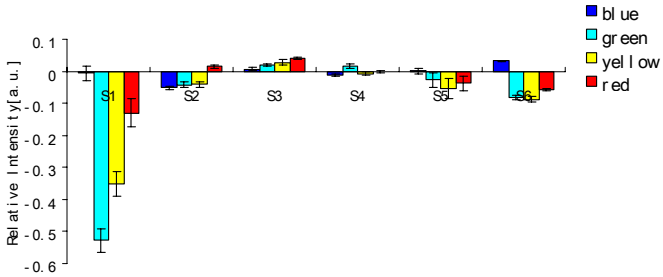


Anions analysis at pH 8

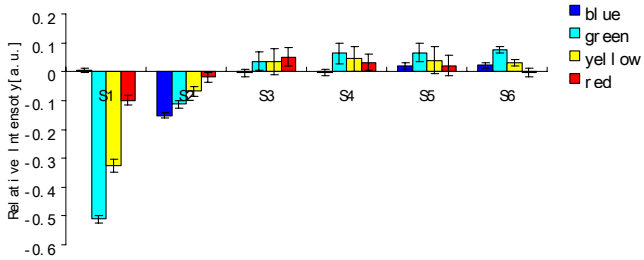
Fluoride



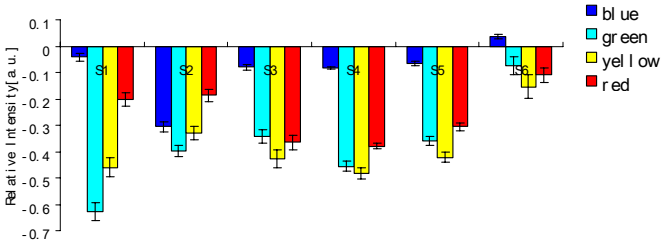
Chloride



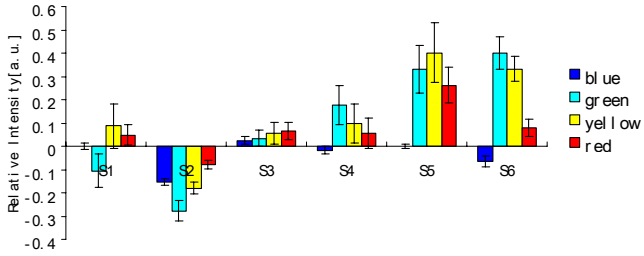
Bromide



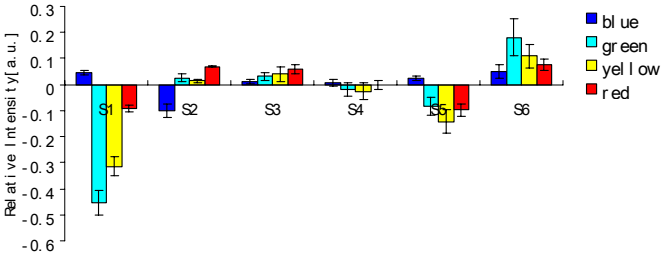
Iodine



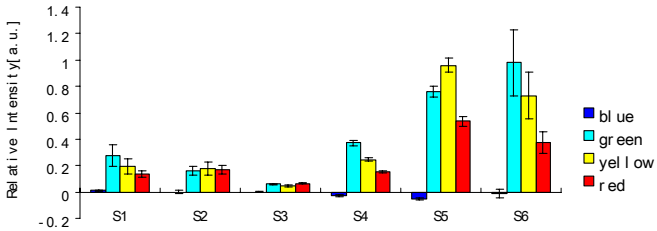
Acetate



Nitrate

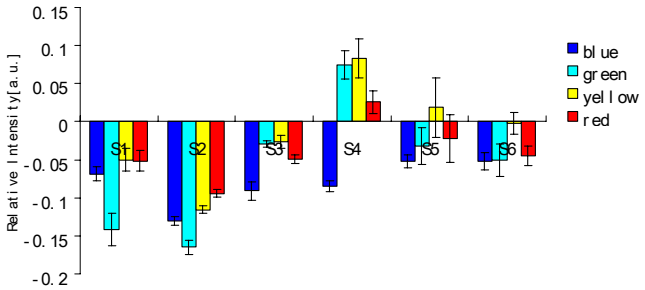


Dihydrogen phosphate

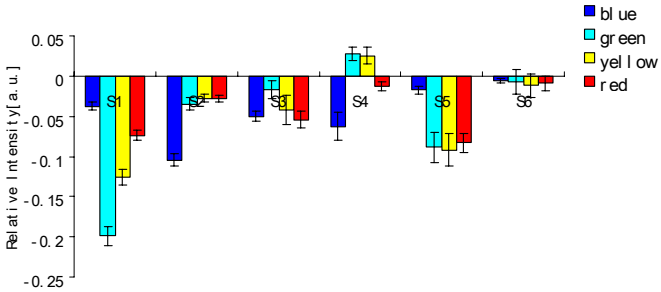


Anions analysis at pH 9

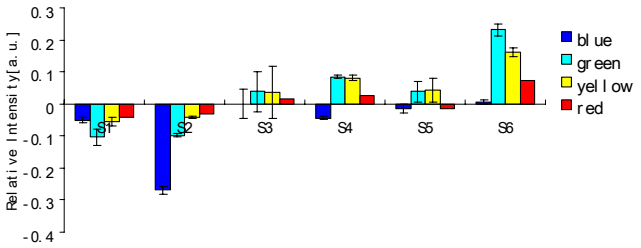
Fluoride



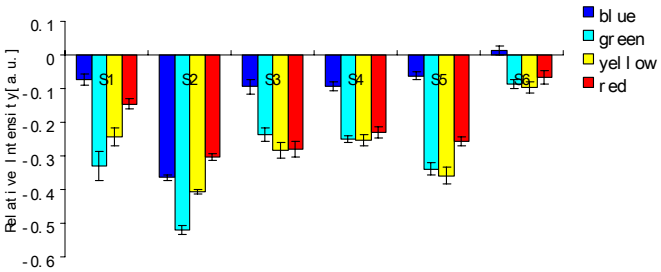
Chloride



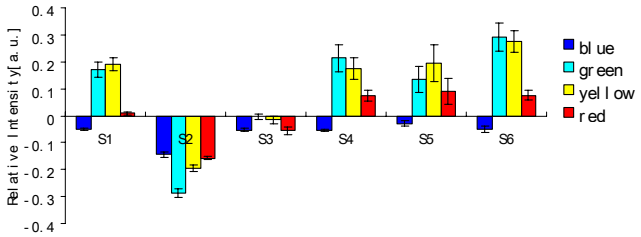
Bromide



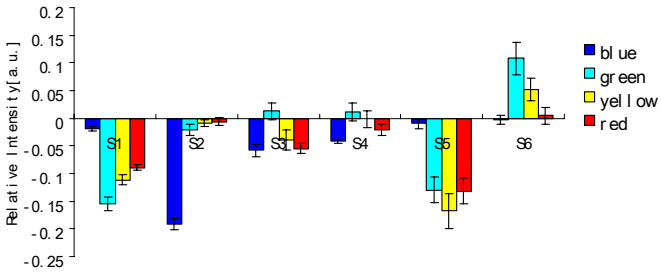
Iodine



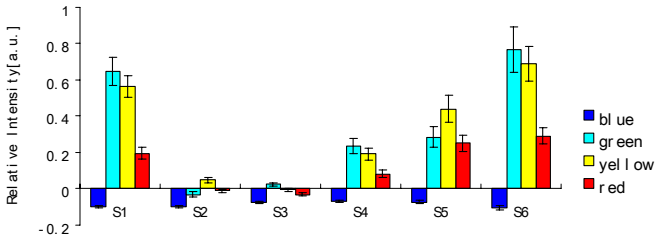
Acetate



Nitrate



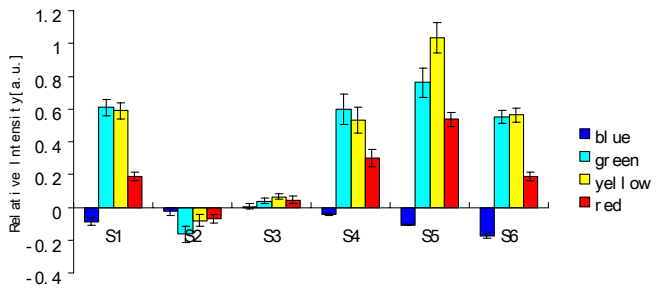
Dihydrogen phosphate



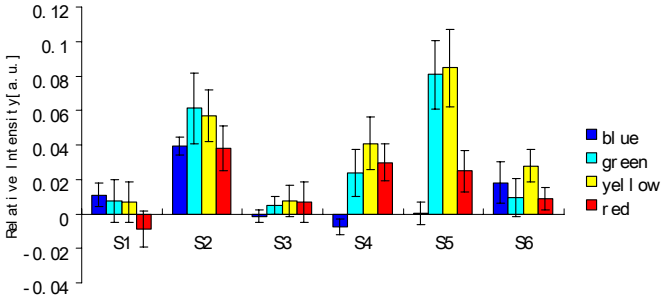
Potassium series anions analysis in the pH range of 5-9

Anions analysis at pH 5

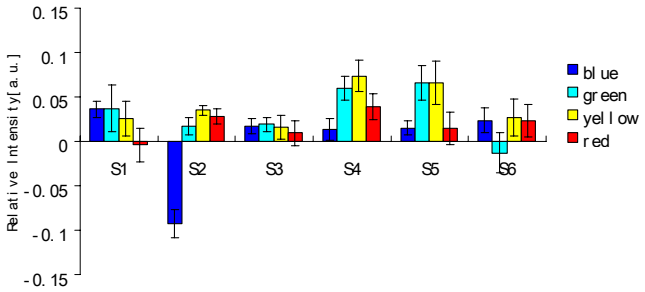
Fluoride



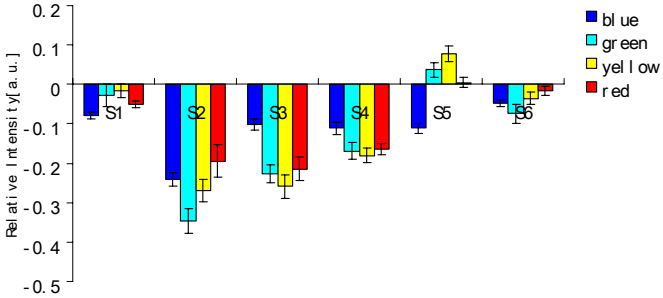
Chloride



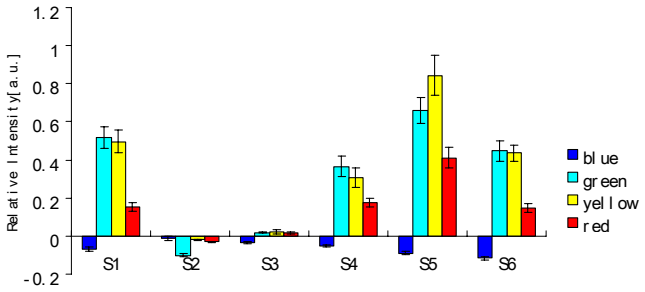
Bromide



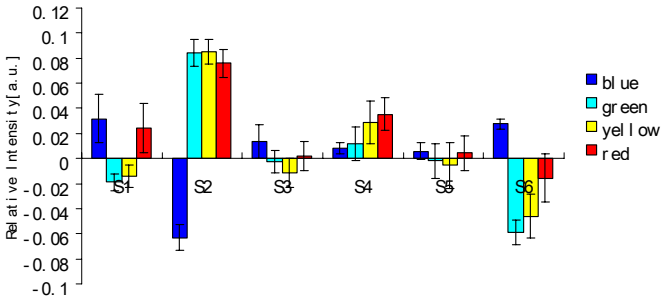
Iodine



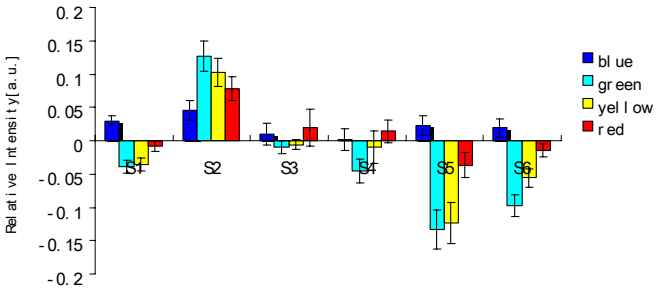
Acetate



Nitrate

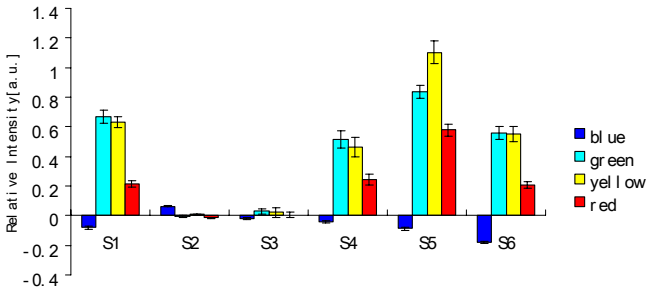


Dihydrogen phosphate

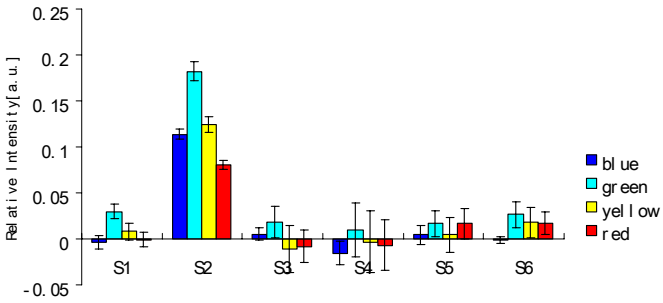


Anions analysis at pH 6

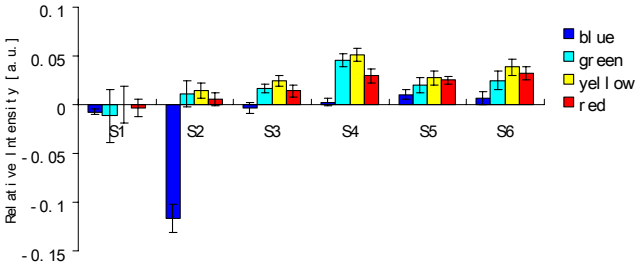
Fluoride



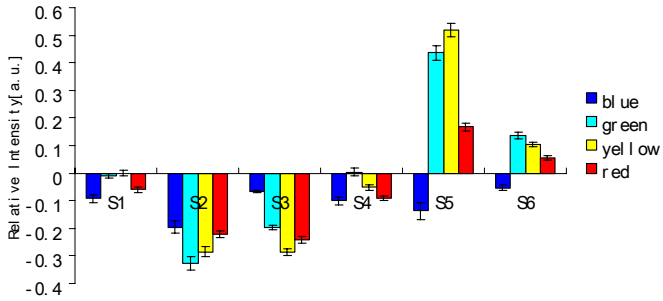
Chloride



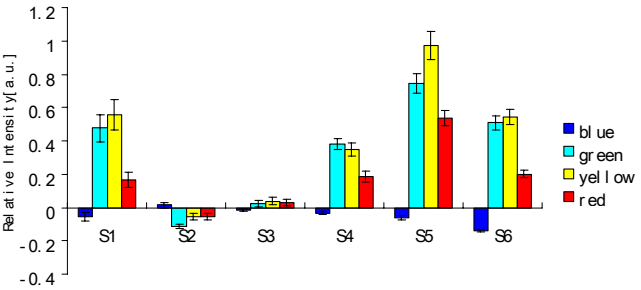
Bromide



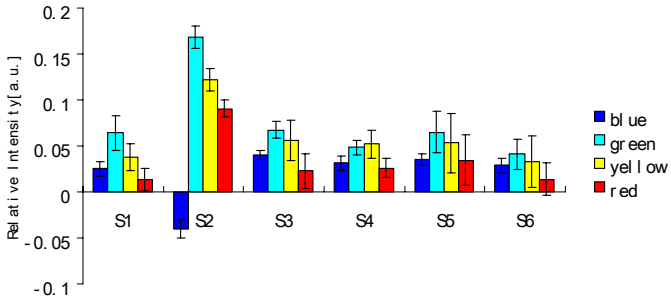
Iodine



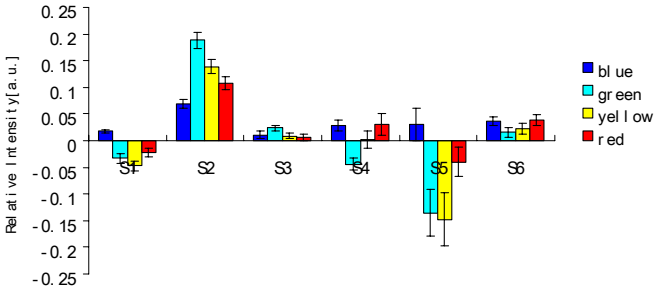
Acetate



Nitrate

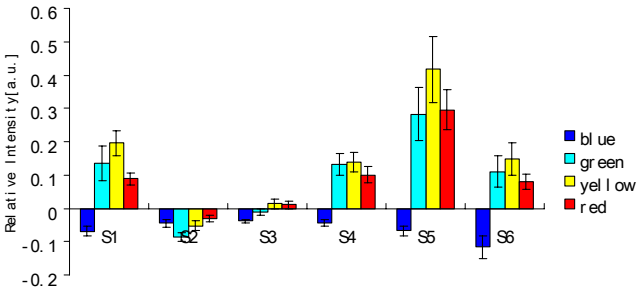


Dihydrogen phosphate

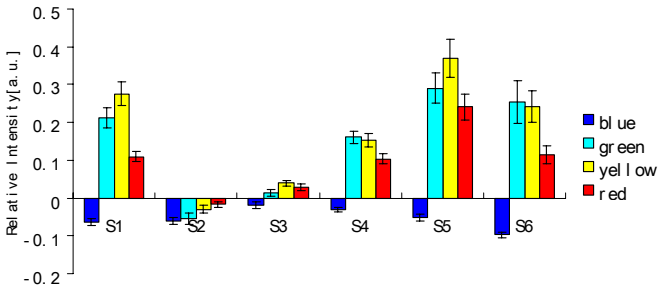


Anions analysis at pH 7

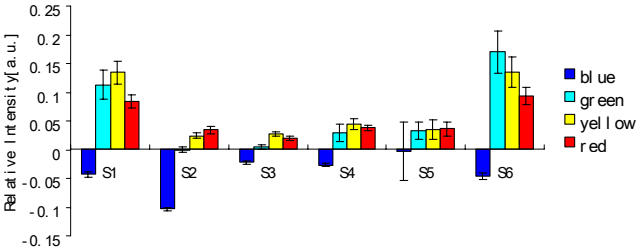
Fluoride



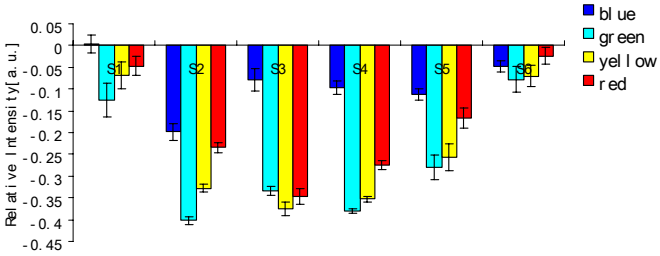
Chloride



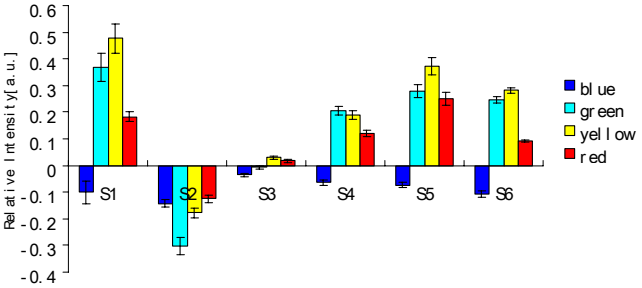
Bromide



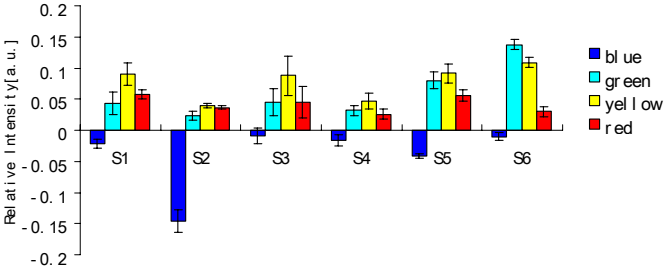
Iodine



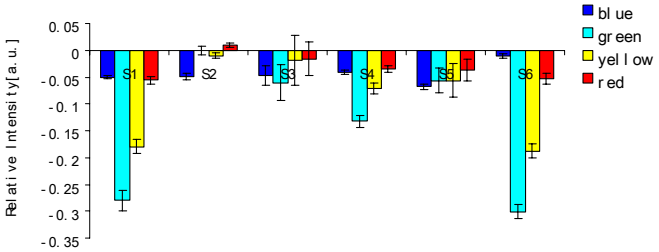
Acetate



Nitrate

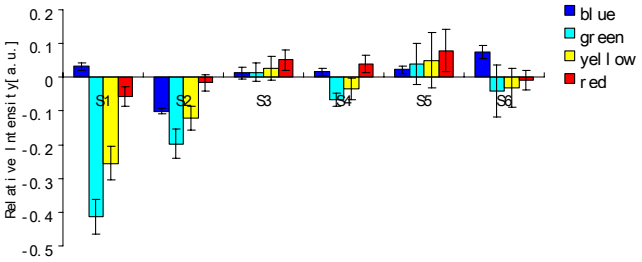


Dihydrogen phosphate

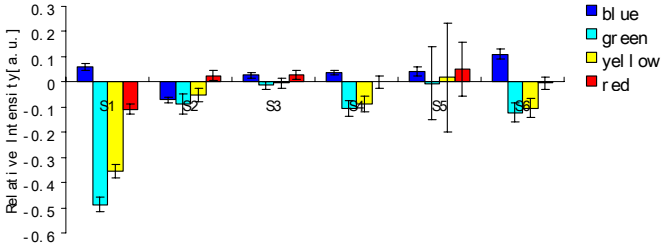


Anions analysis at pH 8

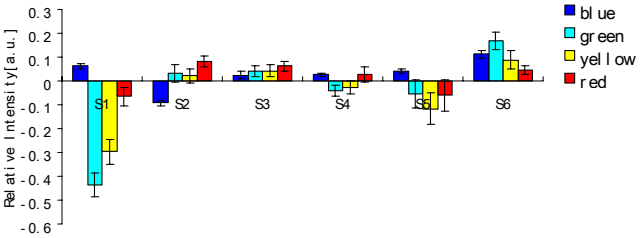
Fluoride



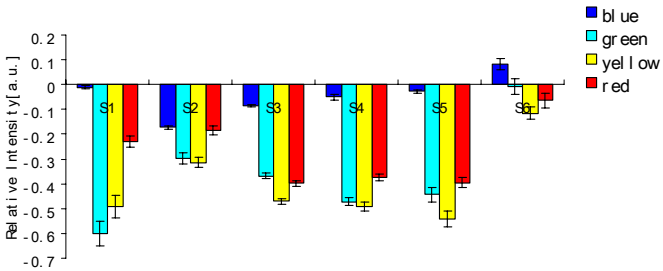
Chloride



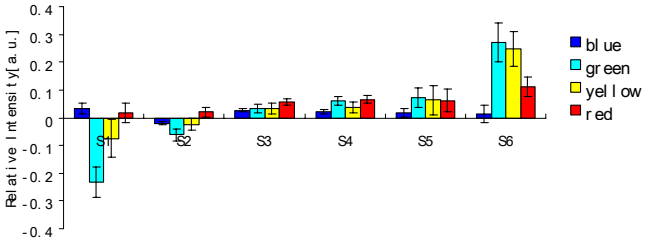
Bromide



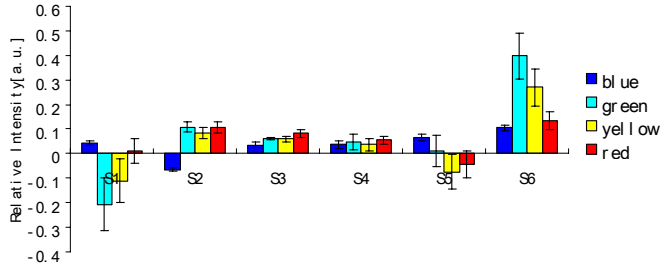
Iodine



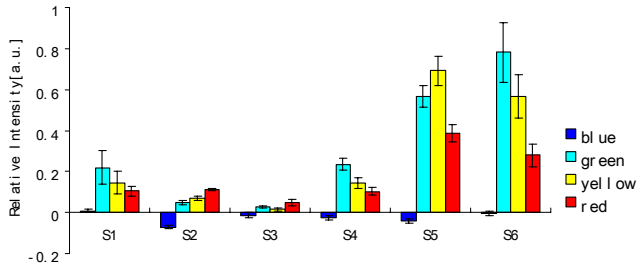
Acetate



Nitrate

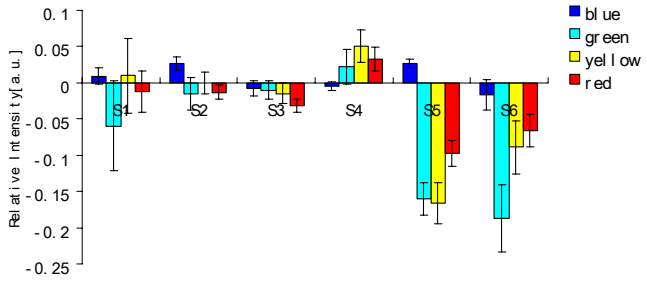


Dihydrogen phosphate

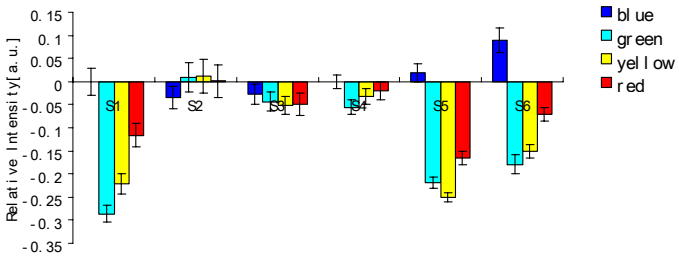


Anions analysis at pH 9

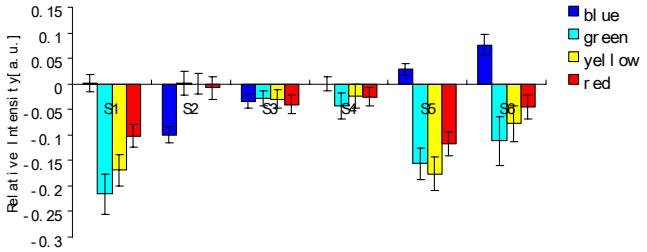
Fluoride



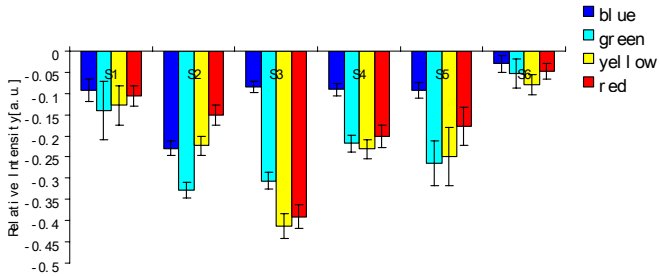
Chloride



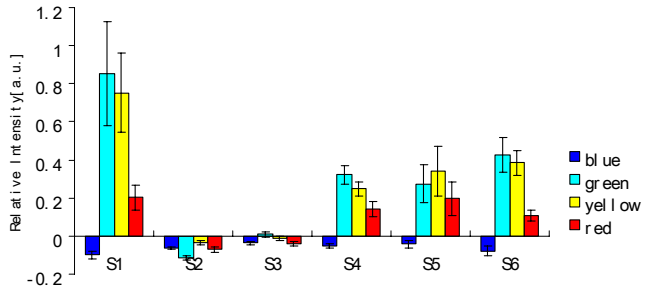
Bromide



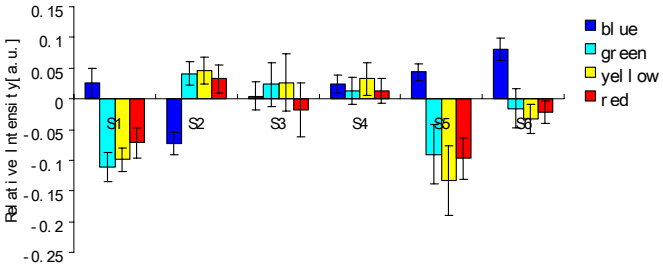
Iodine



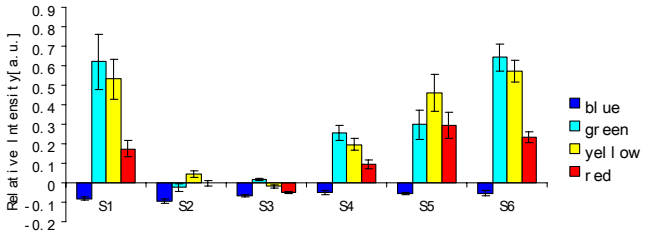
Acetate



Nitrate



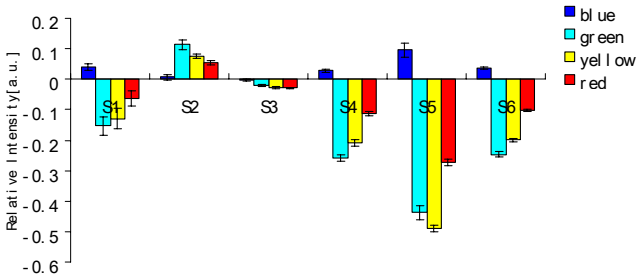
Dihydrogen phosphate



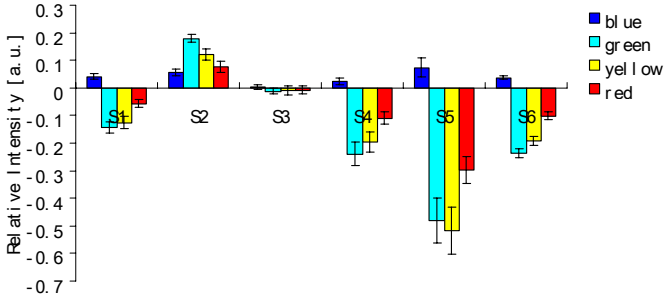
Ammonium series anions analysis in the pH range of 5-9

Anions analysis at pH 5

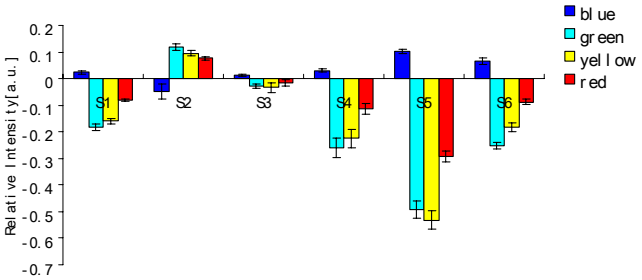
Fluoride



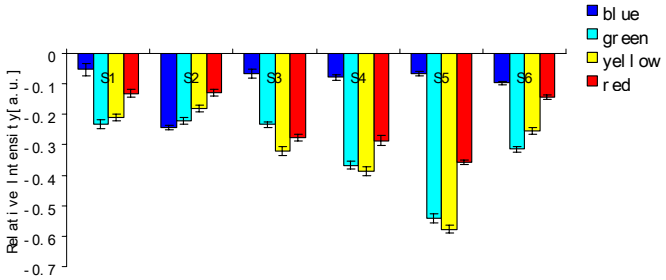
Chloride



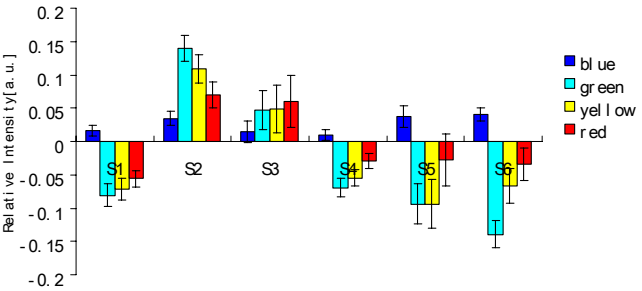
Bromide



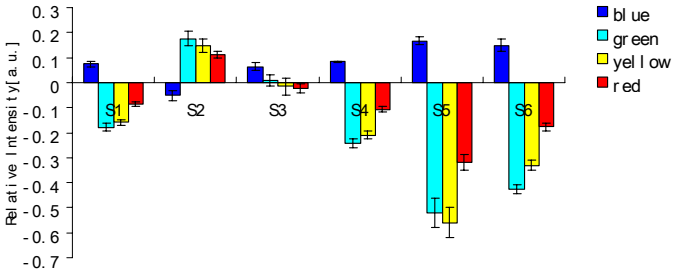
Iodine



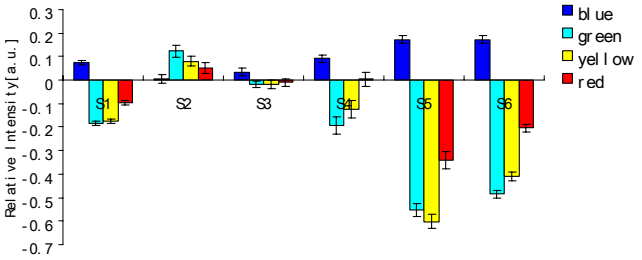
Acetate



Nitrate

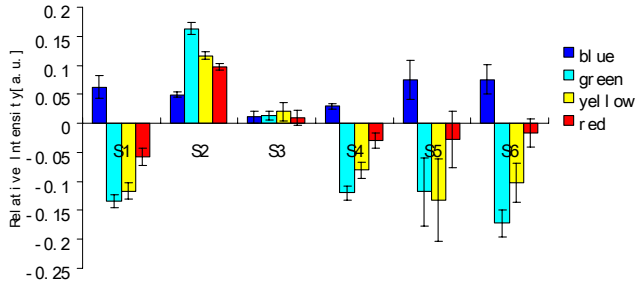


Dihydrogen phosphate

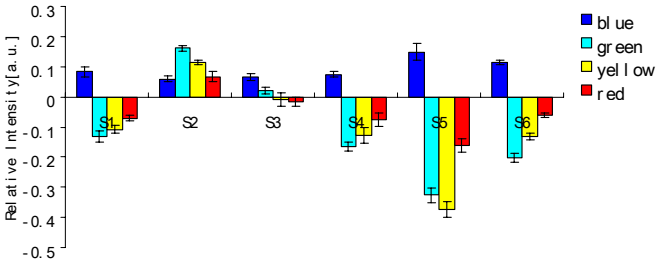


Anions analysis at pH 6

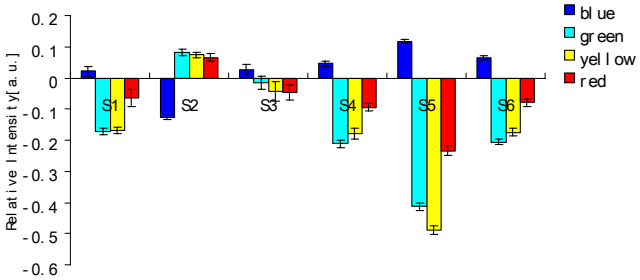
Fluoride



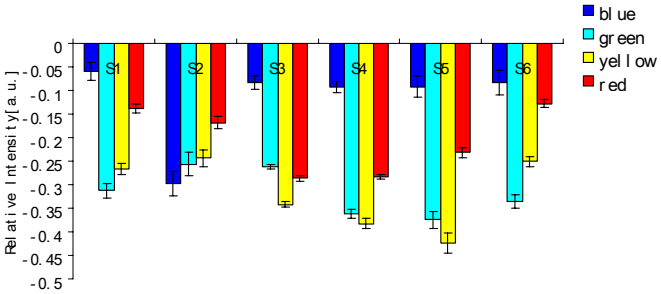
Chloride



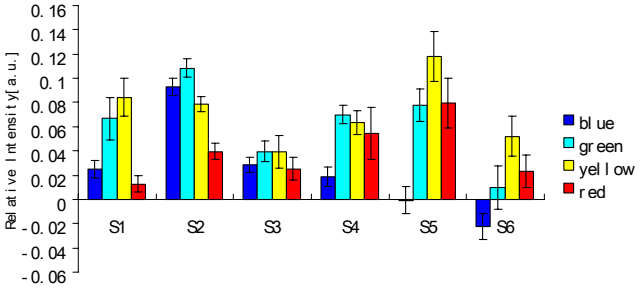
Bromide



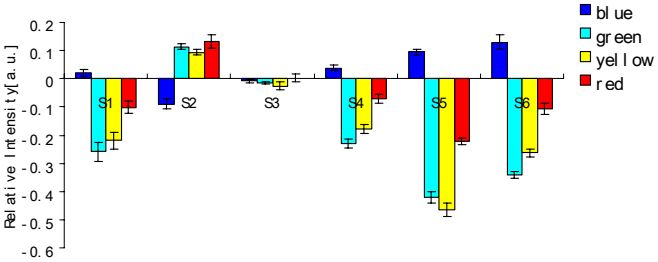
Iodine



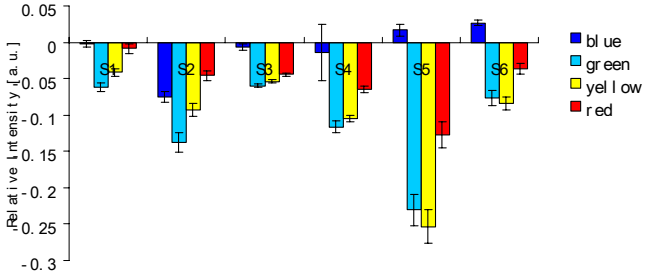
Acetate



Nitrate

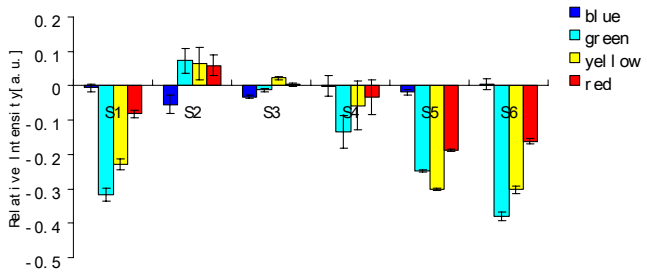


Dihydrogen phosphate

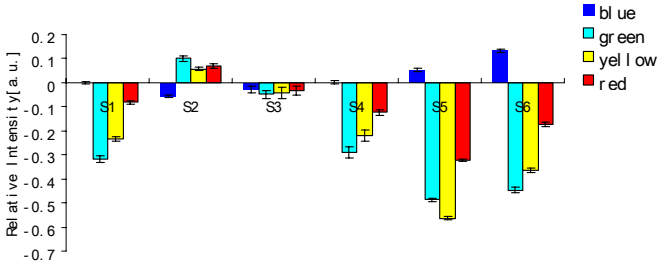


Anions analysis at pH 7

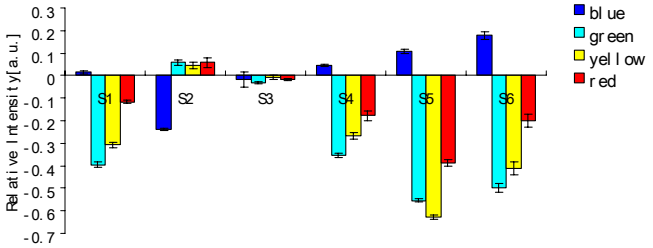
Fluoride



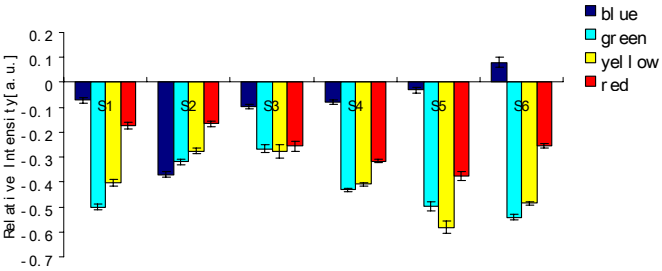
Chloride



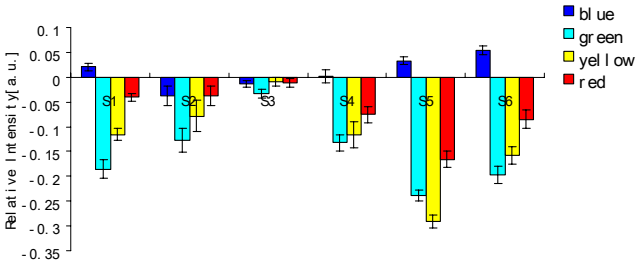
Bromide



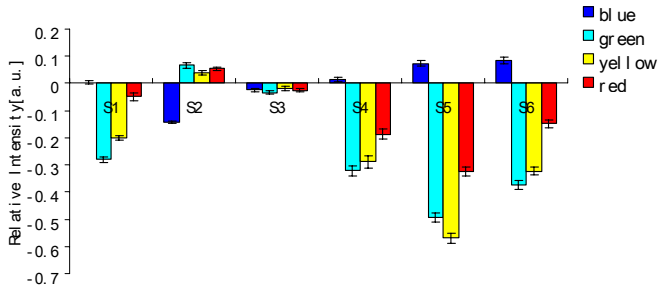
Iodine



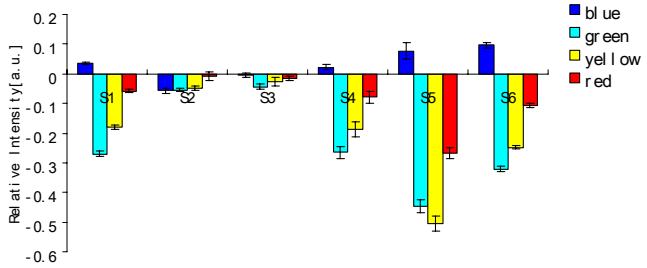
Acetate



Nitrate

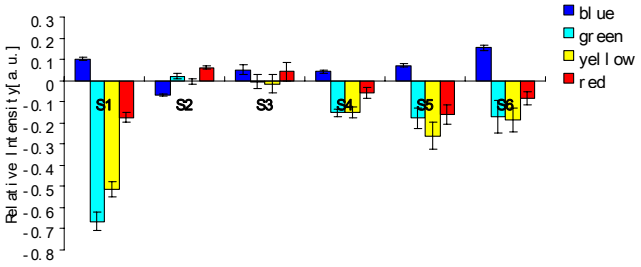


Dihydrogen phosphate

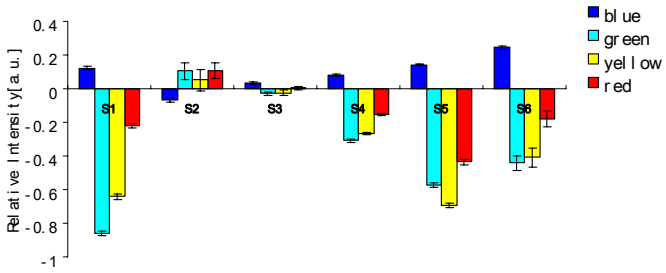


Anions analysis at pH 8

Fluoride



Chloride



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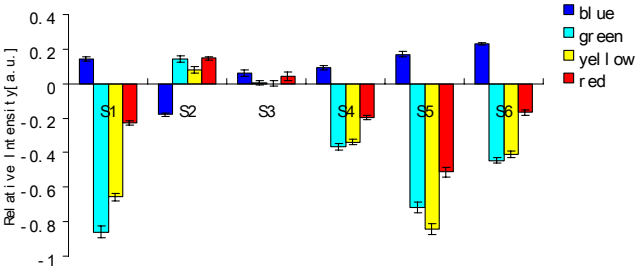

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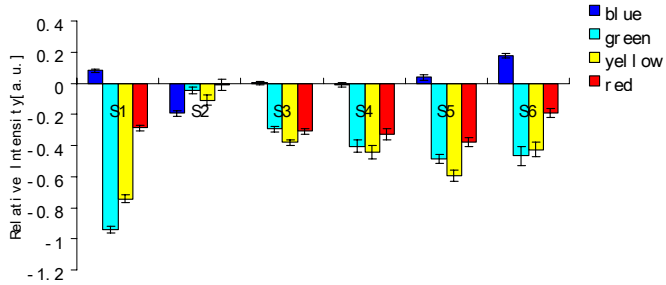
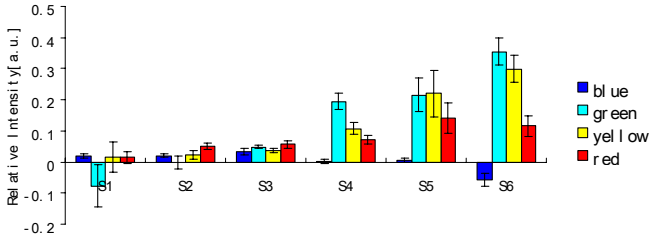
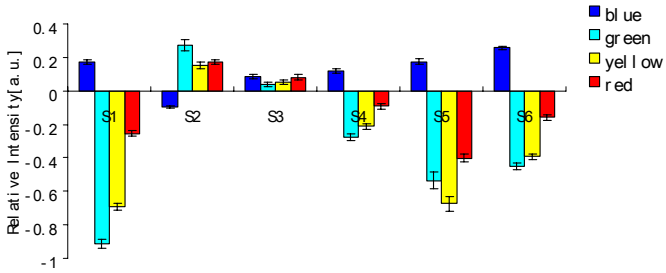


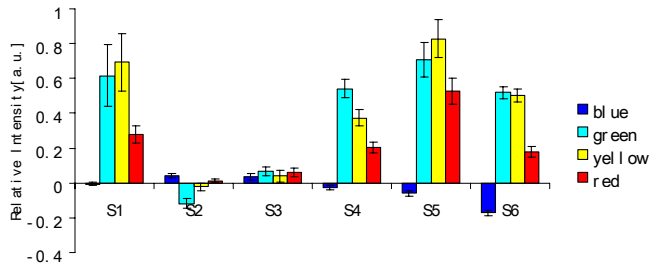
Acetate



Nitrate

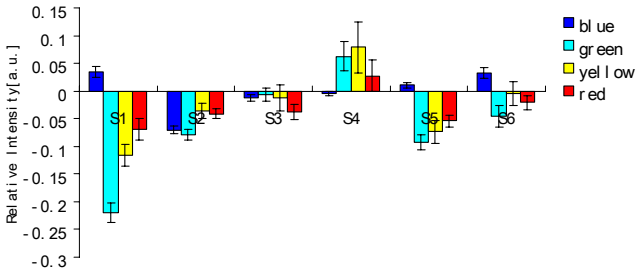


Dihydrogen phosphate

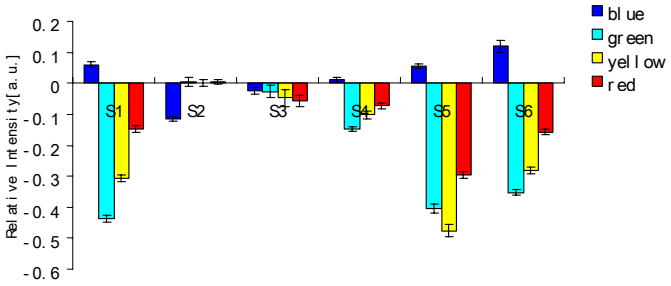


Anions analysis at pH 9

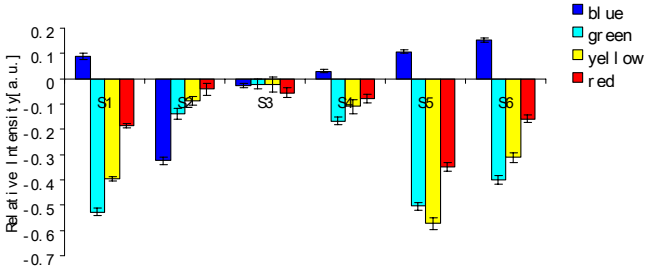
Fluoride



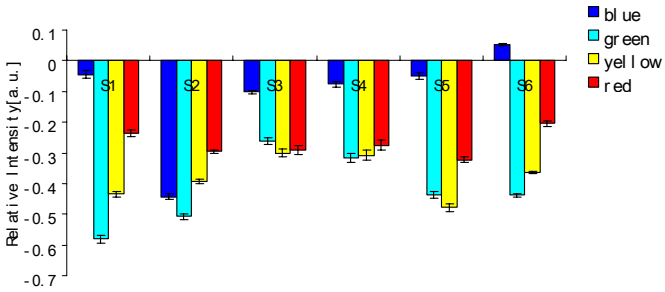
Chloride



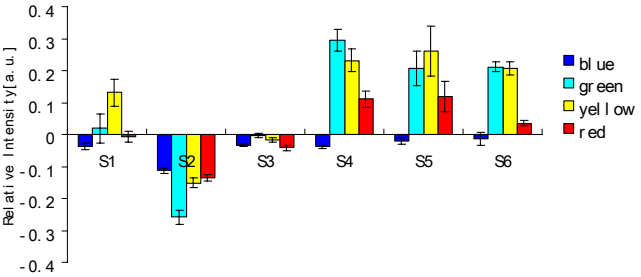
Bromide



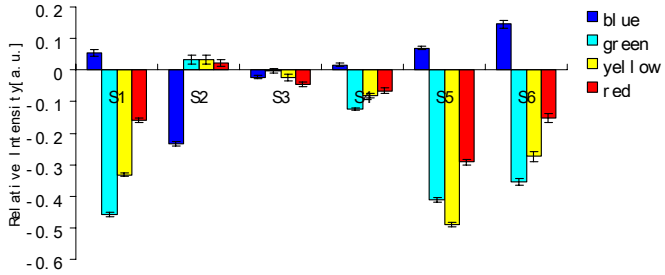
Iodine



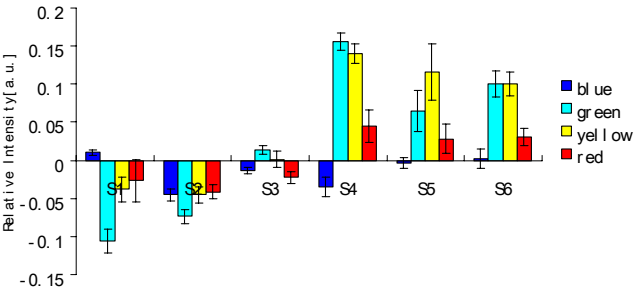
Acetate



Nitrate



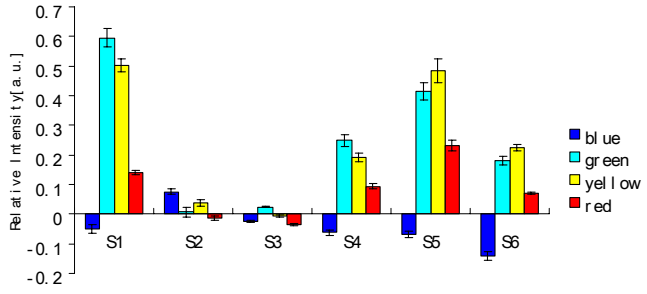
Dihydrogen phosphate



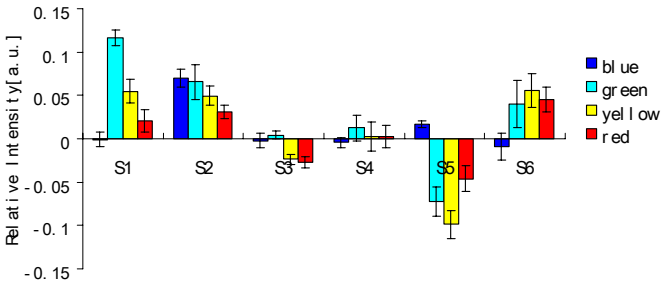
Tetrabutylmmonium series anions analysis in the pH range of 5-9

Anions analysis at pH 5

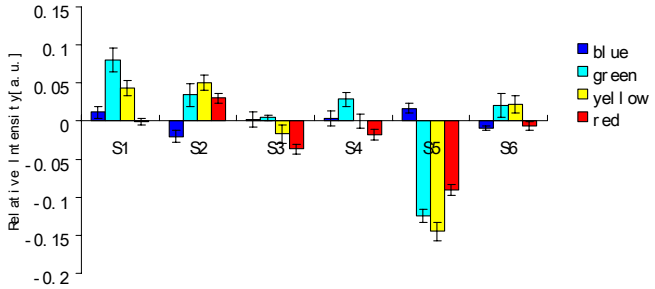
Fluoride



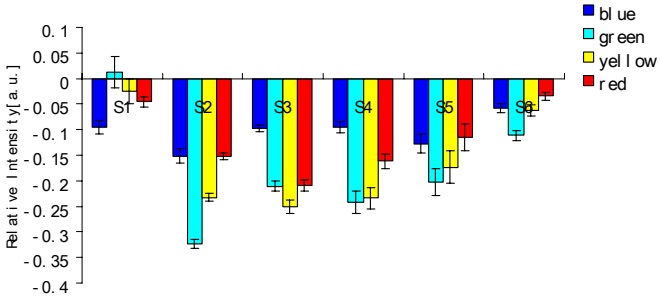
Chloride



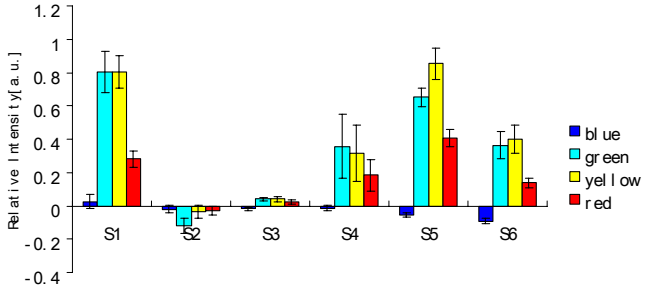
Bromide



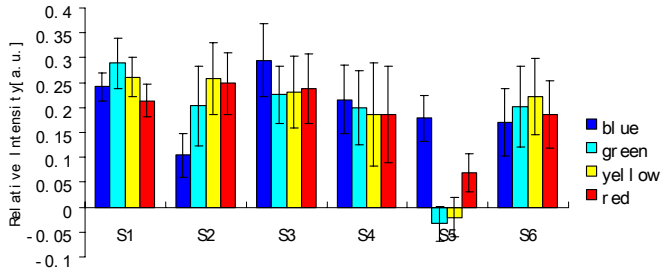
Iodine



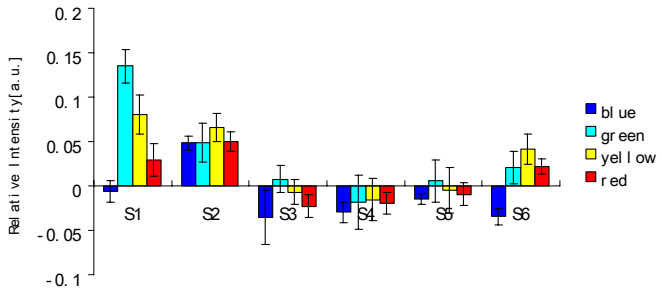
Acetate



Nitrate

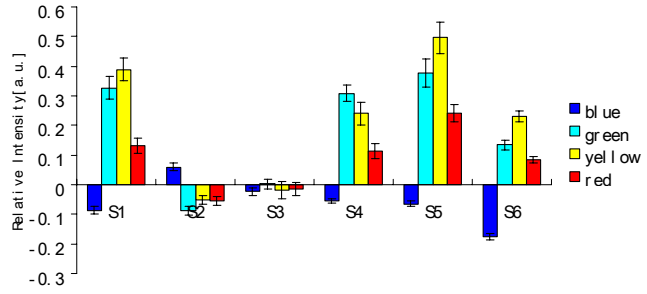


Dihydrogen phosphate

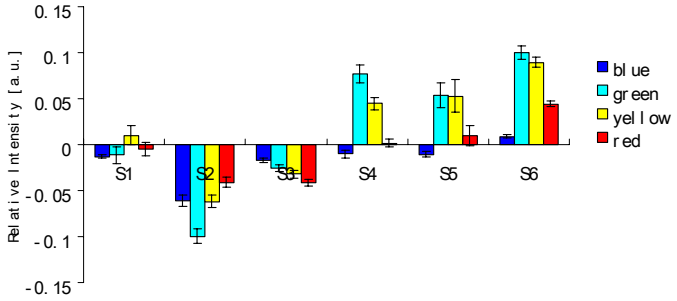


Anions analysis at pH 6

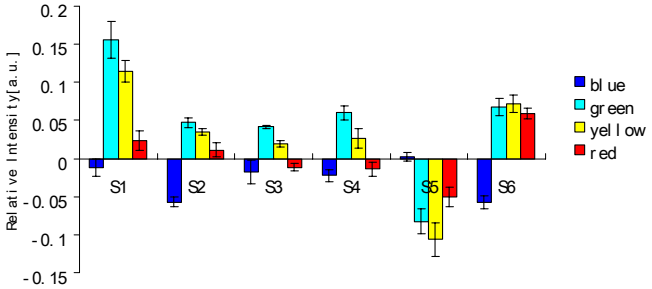
Fluoride



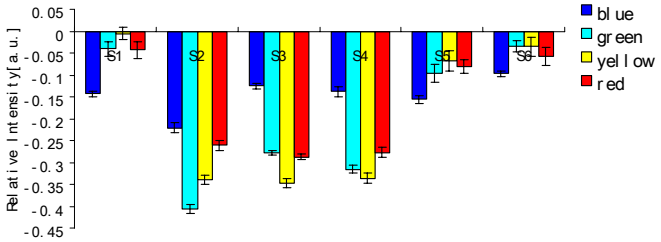
Chloride



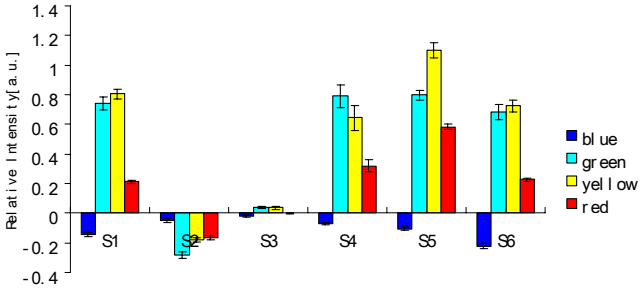
Bromide



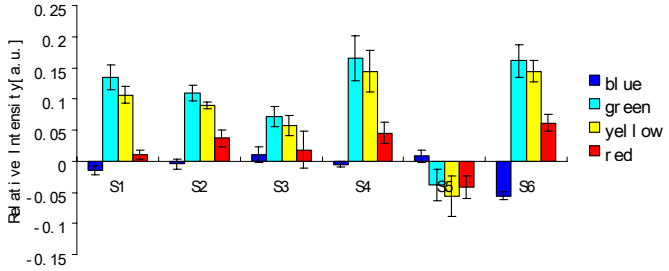
Iodine



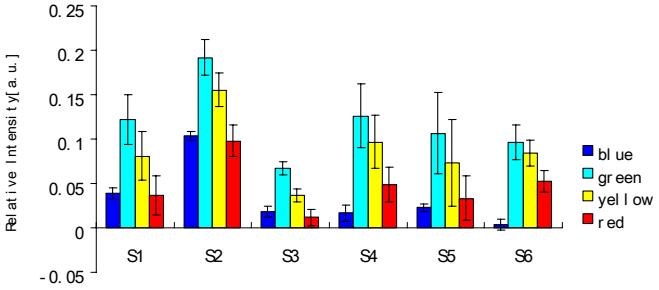
Acetate



Nitrate

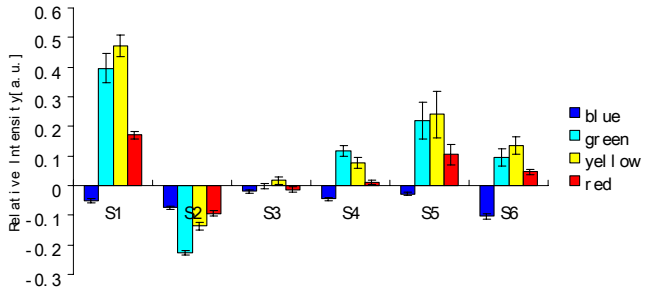


Dihydrogen phosphate

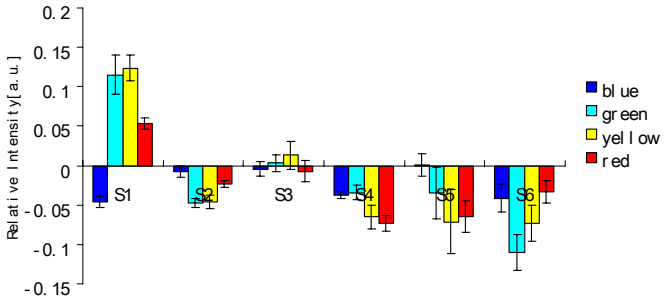


Anions analysis at pH 7

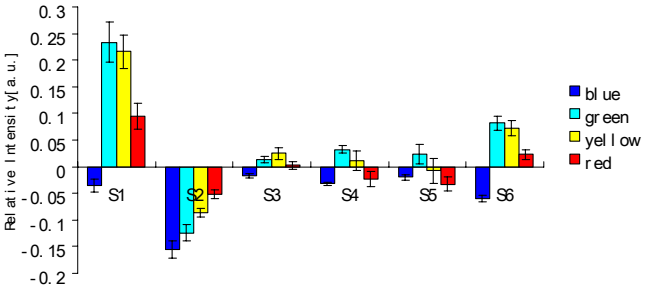
Fluoride



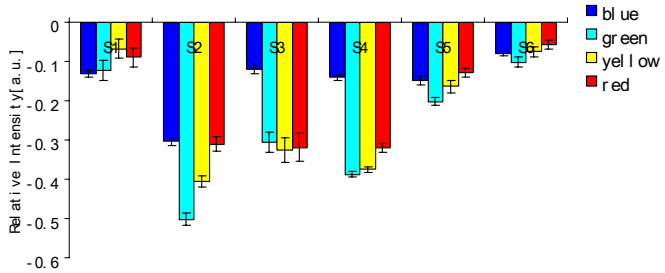
Chloride



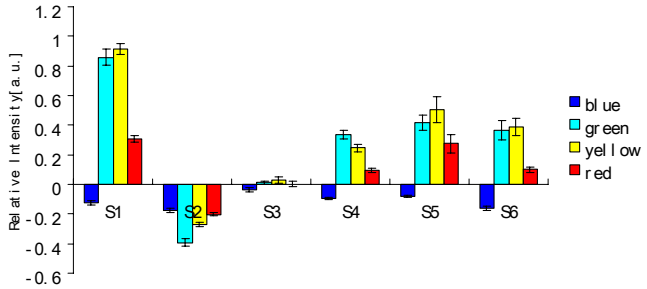
Bromide



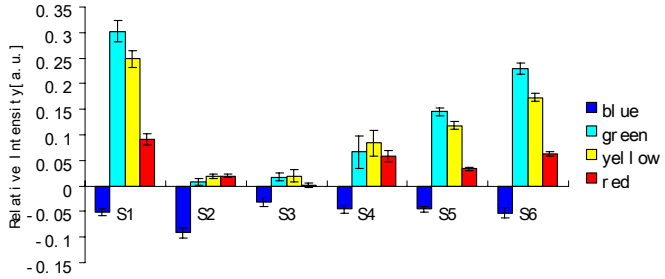
Iodine



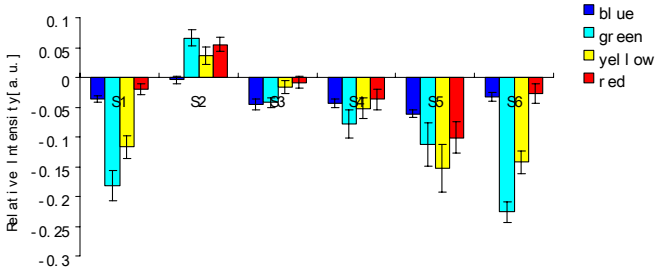
Acetate



Nitrate

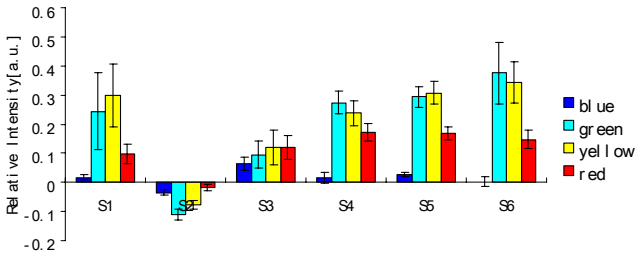


Dihydrogen phosphate

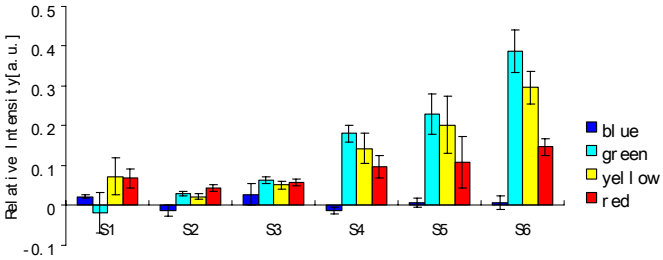


Anions analysis at pH 8

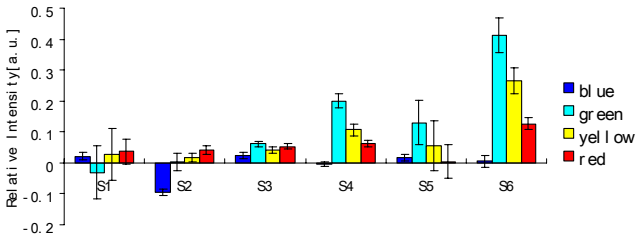
Fluoride



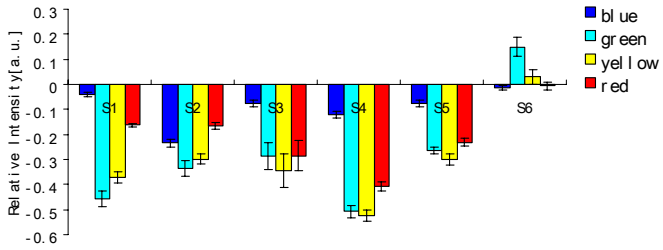
Chloride



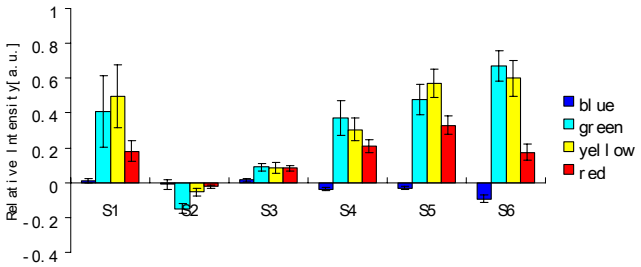
Bromide



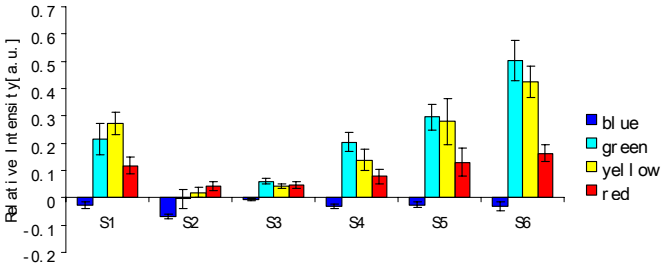
Iodine



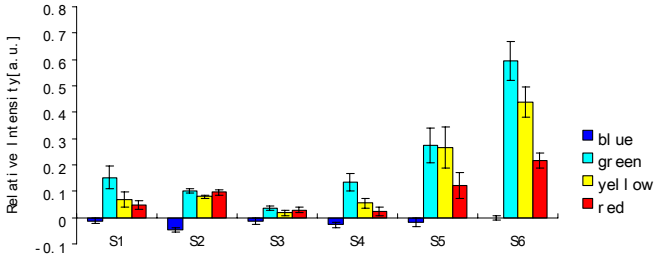
Acetate



Nitrate

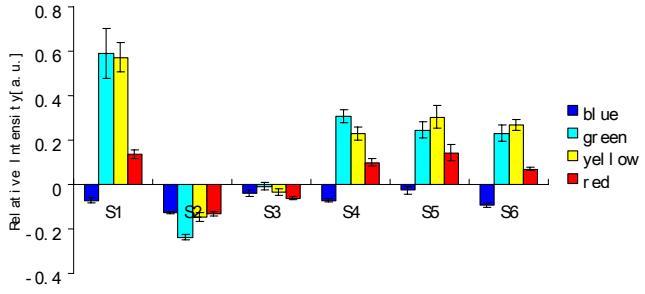


Dihydrogen phosphate

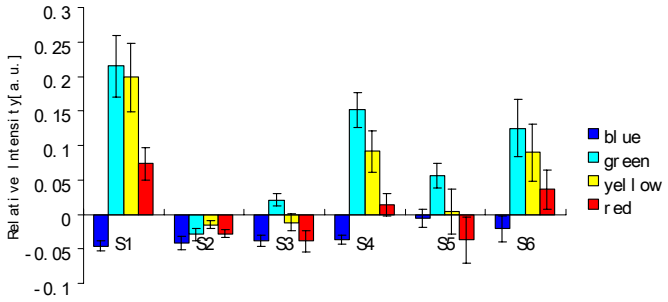


Anions analysis at pH 9

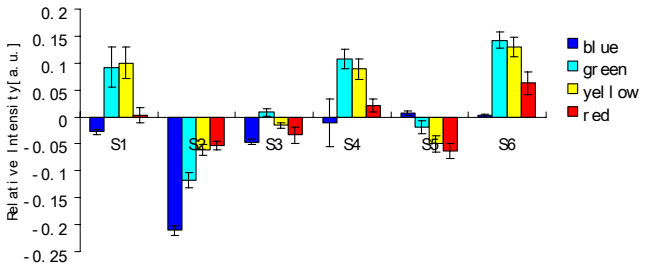
Fluoride



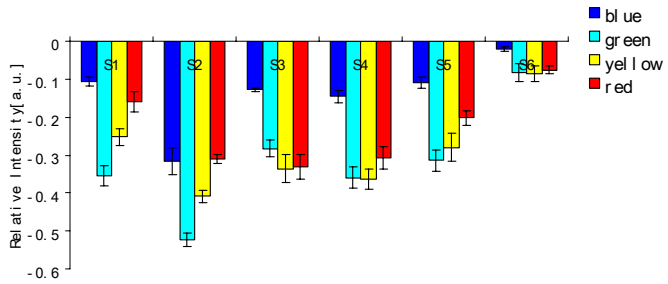
Chloride



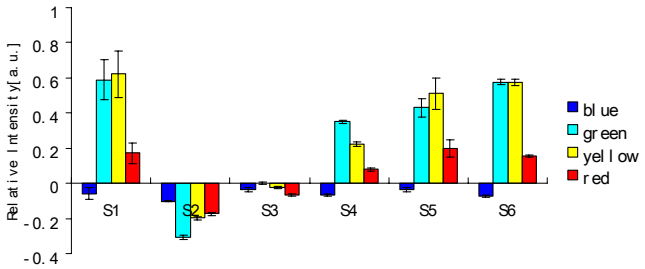
Bromide



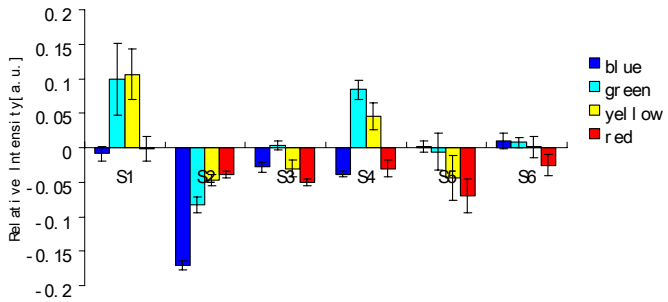
Iodine



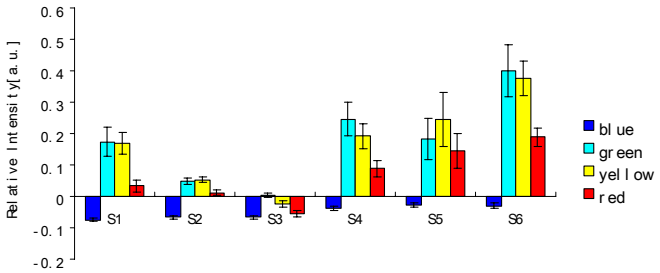
Acetate



Nitrate

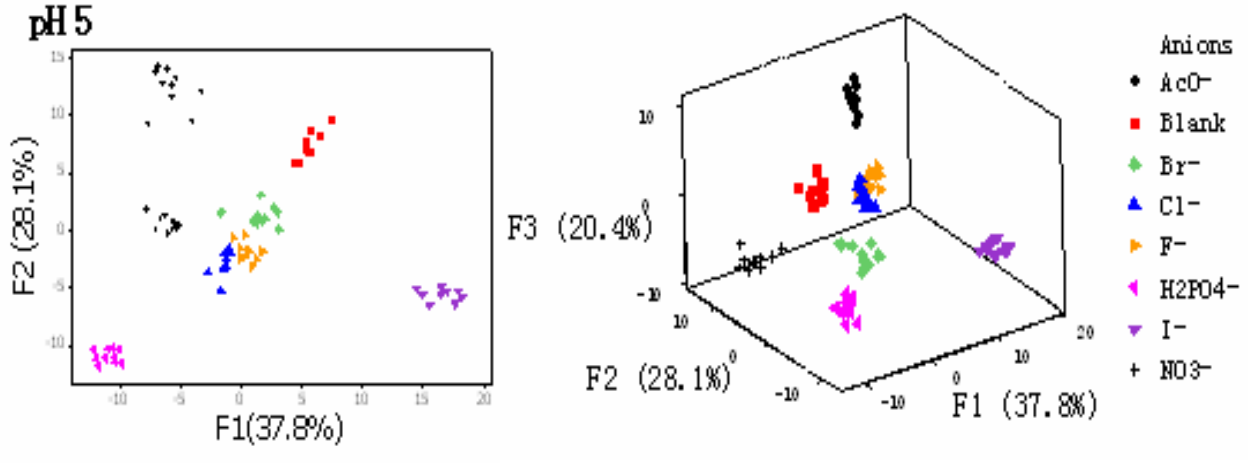


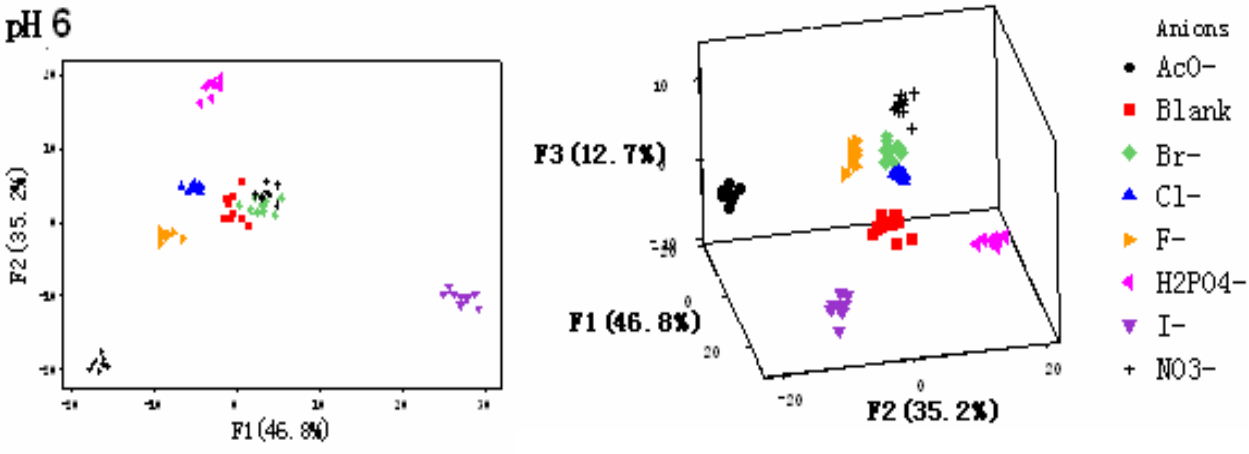
Dihydrogen phosphate

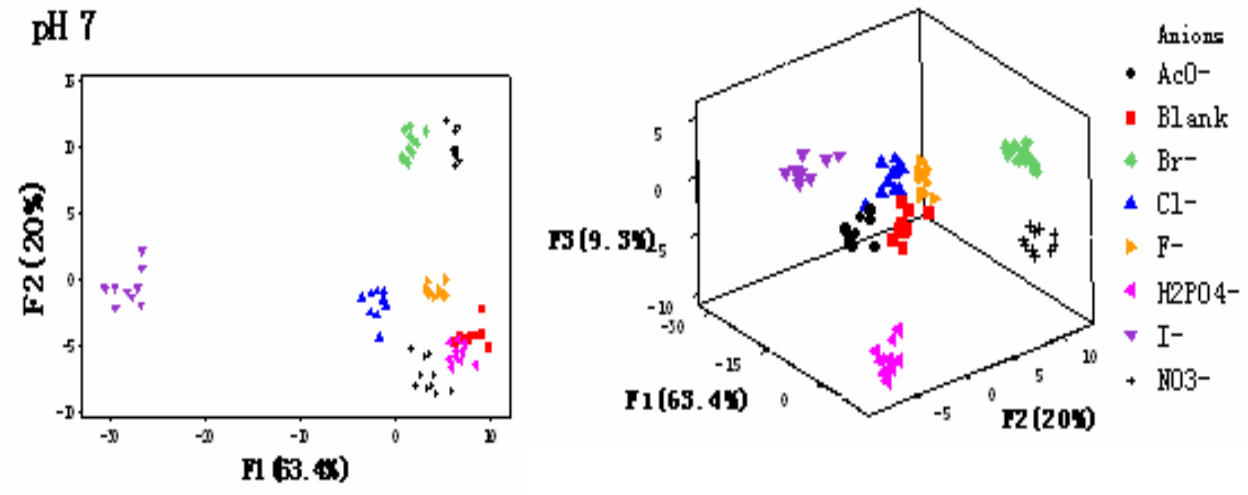


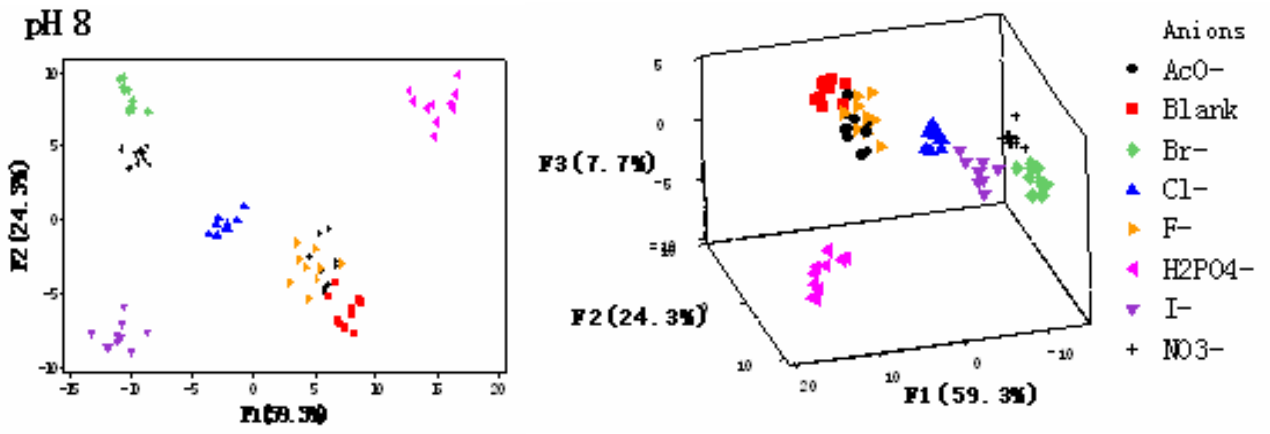
Linear Discriminant Analysis for anions in the form of their lithium salts at different pH values

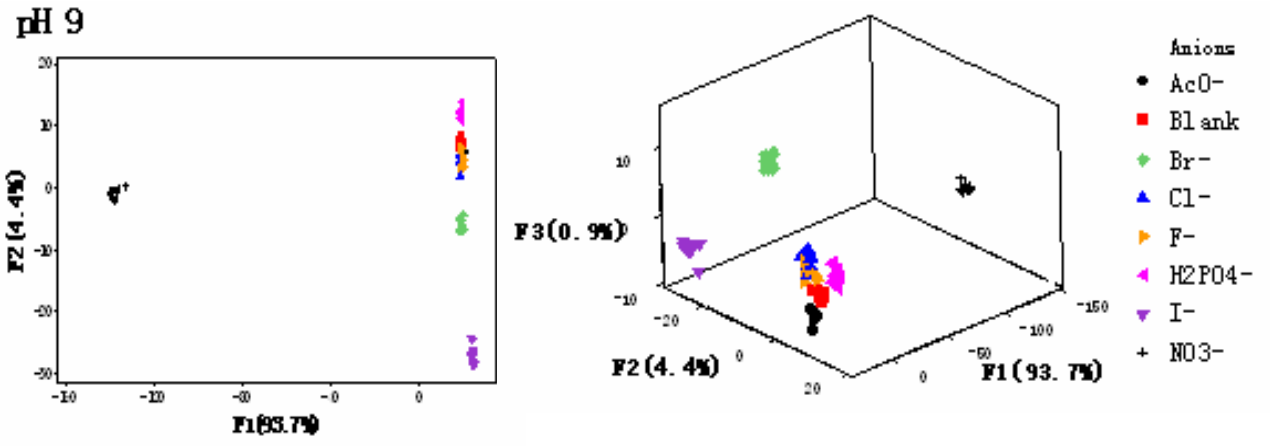
LDA for anions in the form of their lithium salts at different pH values



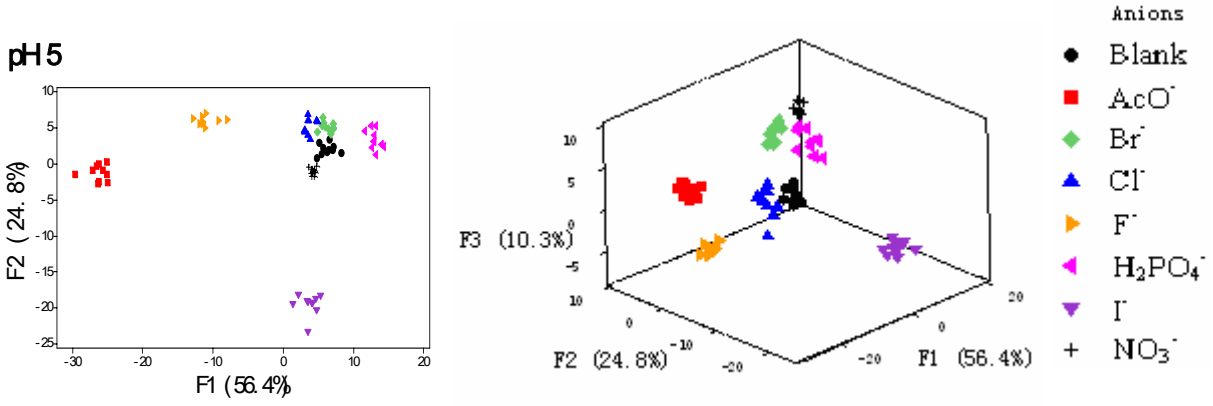


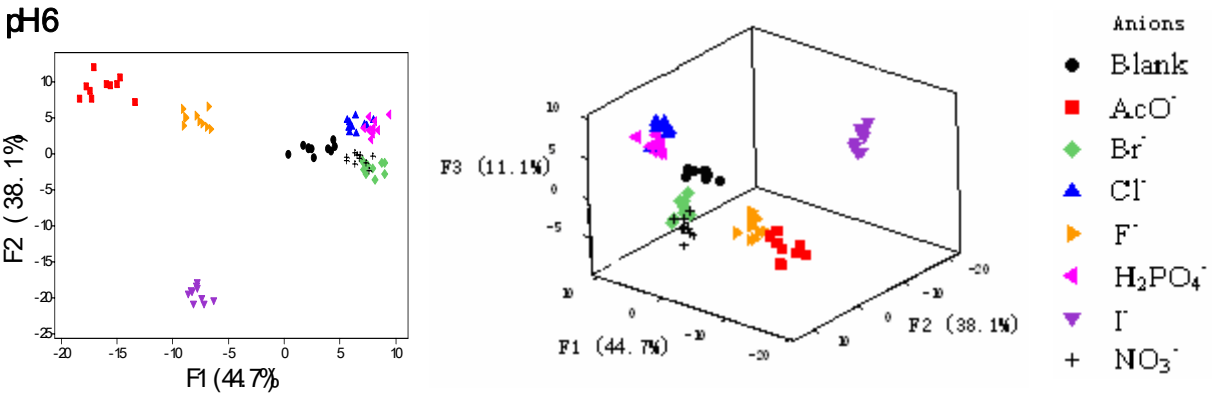


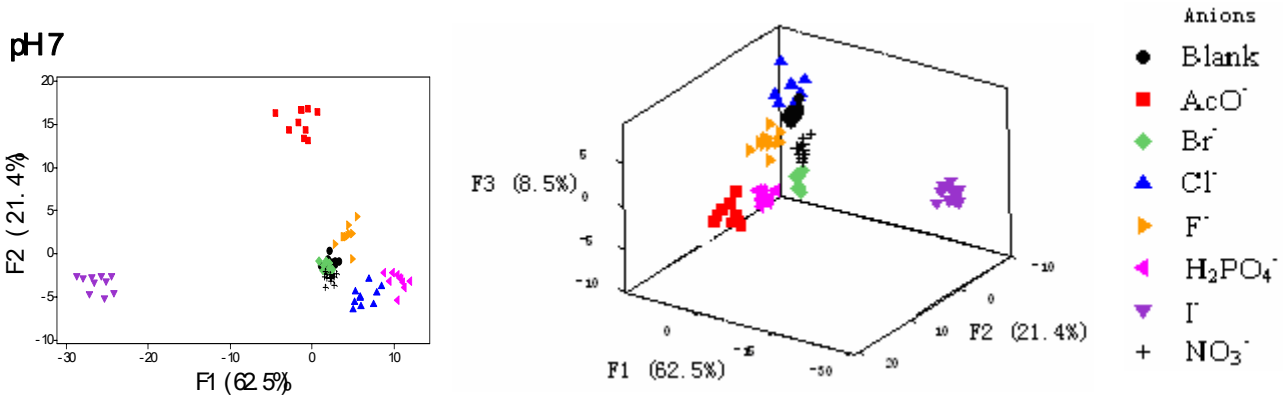

pH 8
F2 (24.3%)
F1(59.3%)
F3 (7.7%)
F2 (24.3%)
F1 (59.3%)
Anions
AcO-
Blank
Br-
Cl-
F-
H2PO4-
I-
NO3-


pH 9
F2 (4.4%)
F1(93.7%)
F3(0.9%)
F2(4.4%)
F1 (93.7%)
Anions
AcO-
Blank
Br-
Cl-
F-
H2PO4-
I-
NO3-

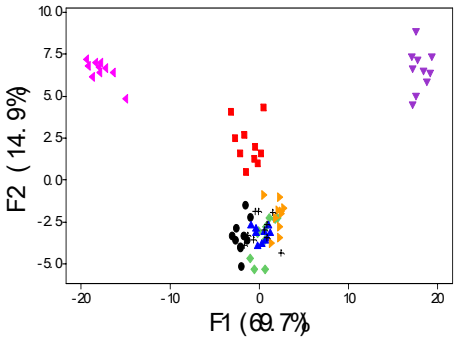
LDA for anions in the form of their sodium salts at different pH values

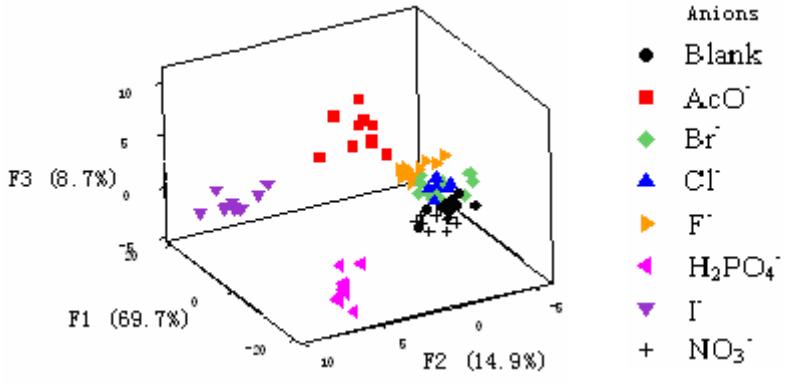




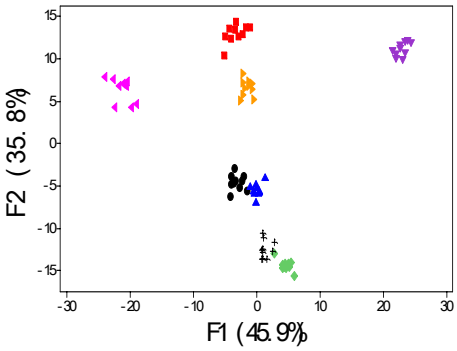


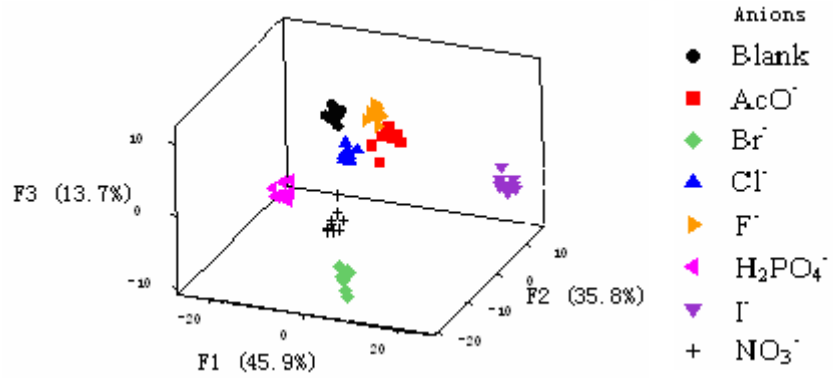
pH 8


F2 (14. 9%)
F1 (69. 7%)

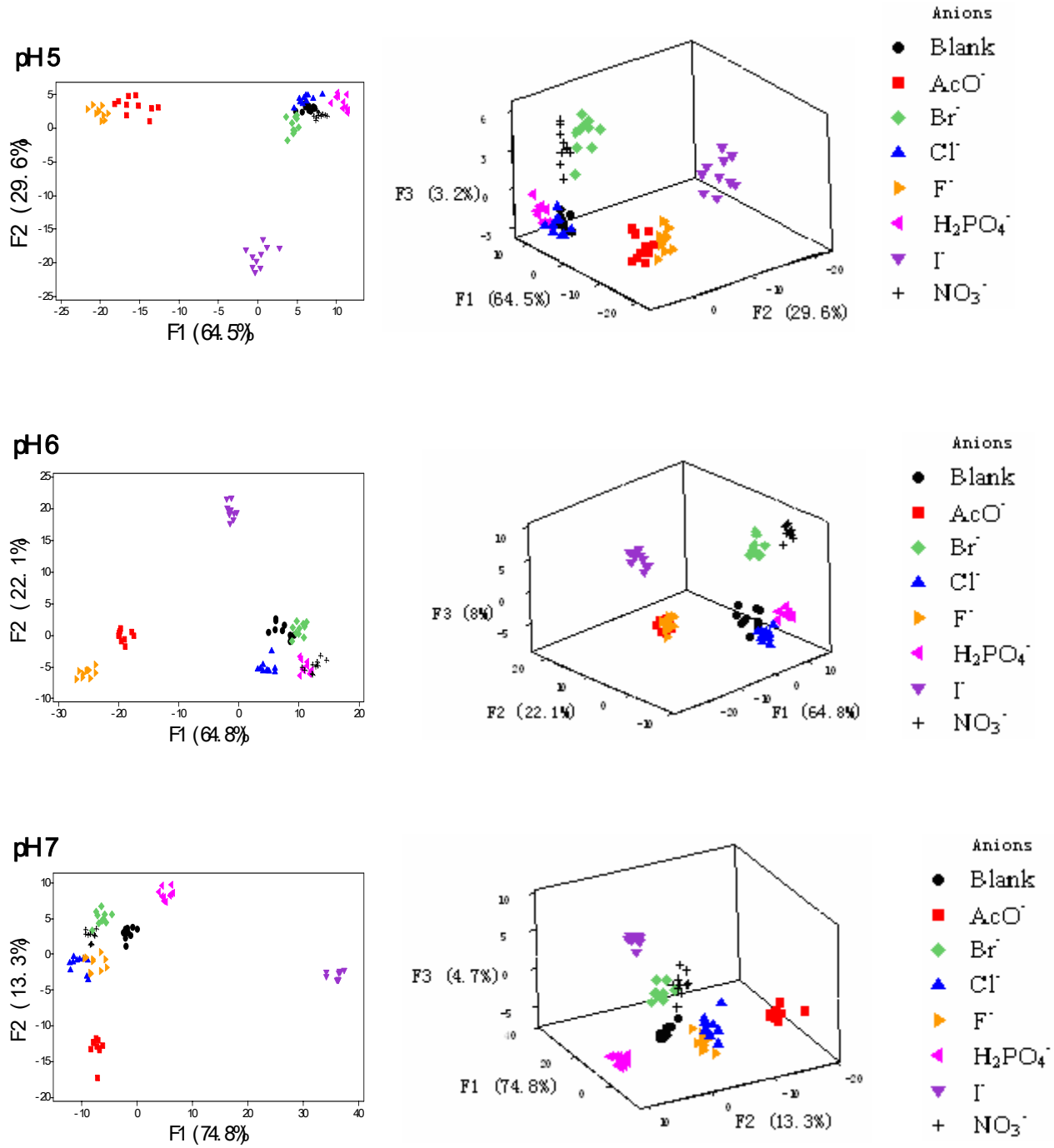

F3 (8.7%)
F1 (69.7%)
F2 (14.9%)
Anions
Blank
AcO-
Br-
Cl-
F-
H2PO4-
I-
NO3-

pH 9

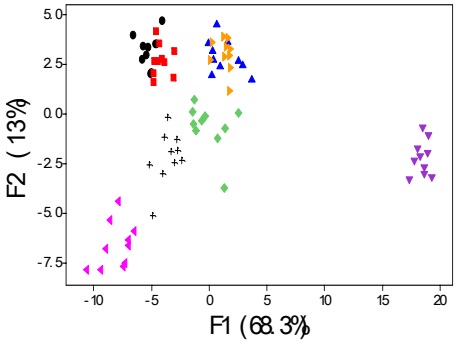

F2 (35. 8%)
F1 (45. 9%)

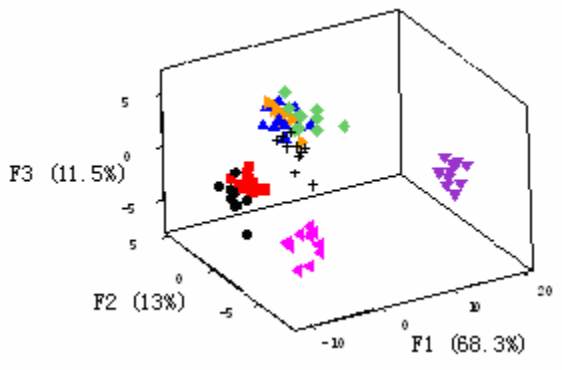

F3 (13.7%)
F1 (45.9%)
F2 (35.8%)
Anions
Blank
AcO-
Br-
Cl-
F-
H2PO4-
I-
NO3-

LDA for anions in form of their potassium salts at different pH values

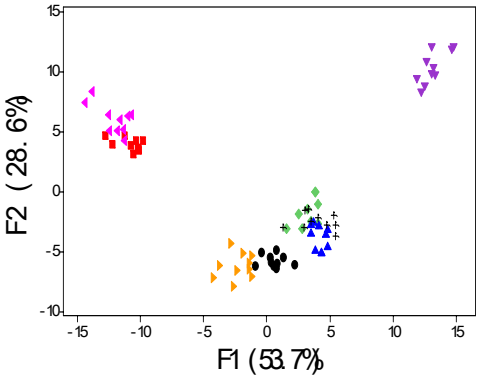


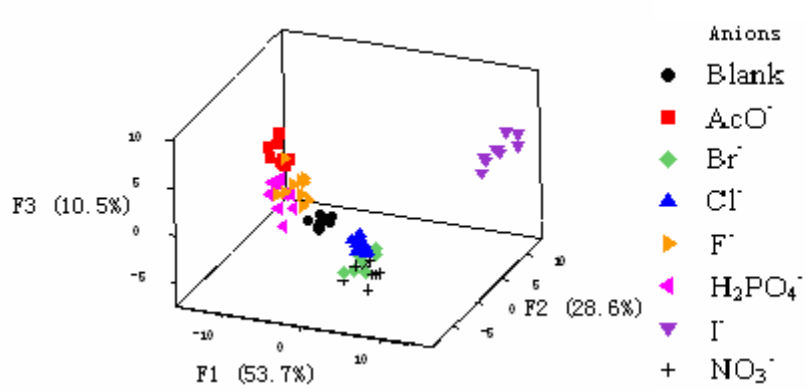
pH 8


F2 (13%)
F1 (68.3%)

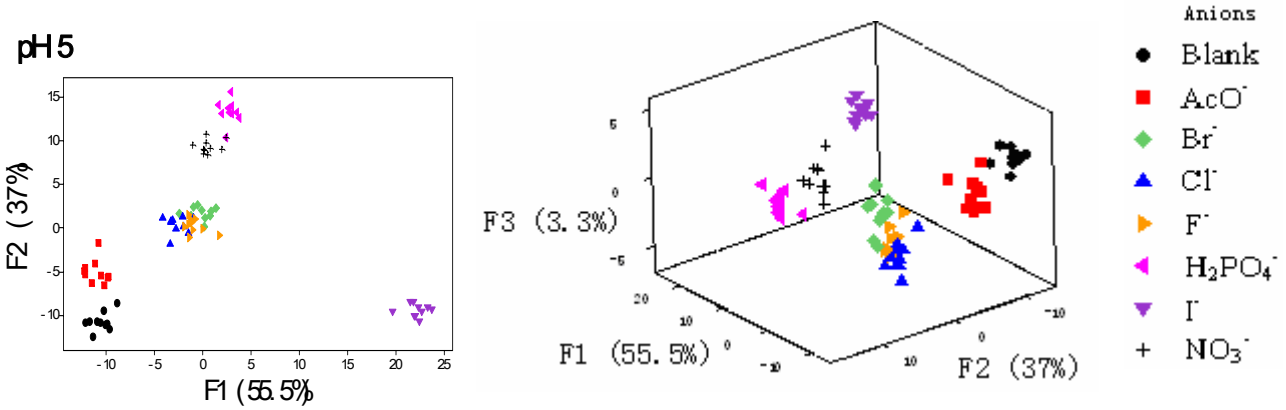

F3 (11.5%)
F2 (13%)
F1 (68.3%)
Anions
Blank
AcO⁻
Br⁻
Cl⁻
F⁻
H2PO4⁻
I⁻
NO3⁻

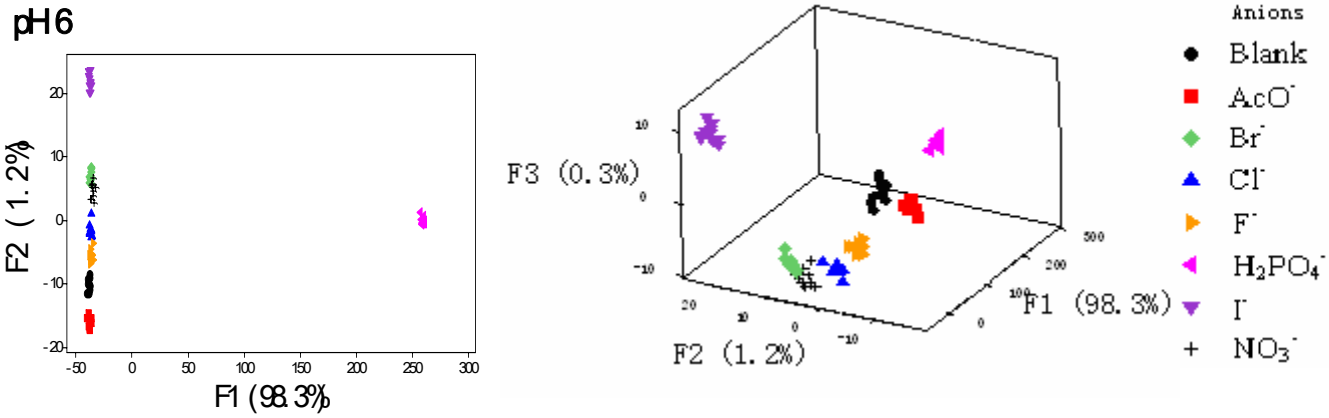
pH 9

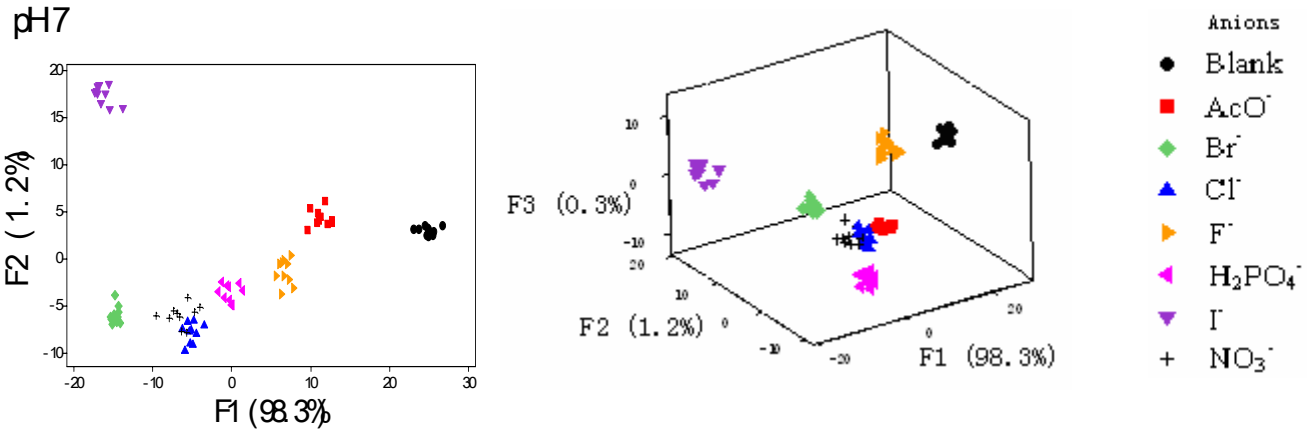

F2 (28.6%)
F1 (53.7%)


F3 (10.5%)
F2 (28.6%)
F1 (53.7%)
Anions
Blank
AcO⁻
Br⁻
Cl⁻
F⁻
H2PO4⁻
I⁻
NO3⁻

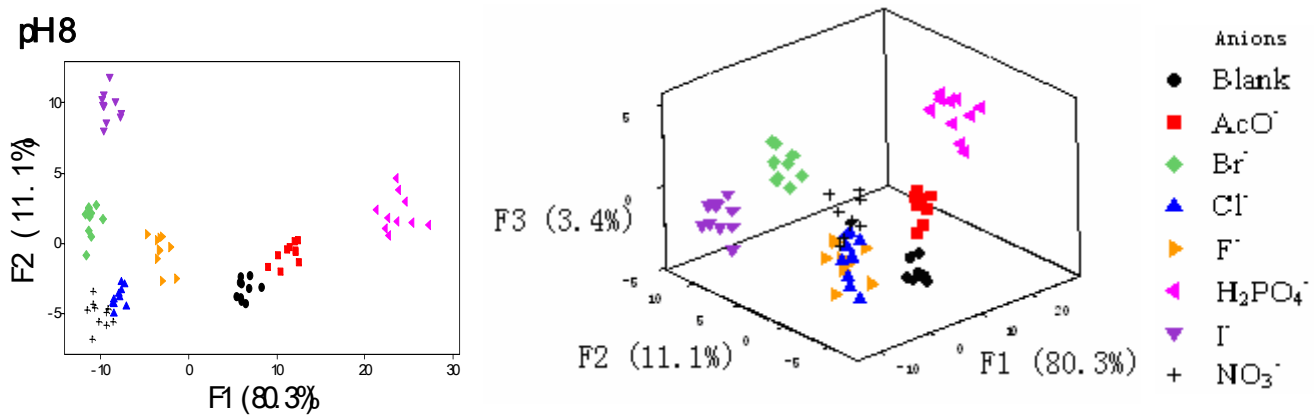
LDA for anions in form of their ammonium salts at different pH values



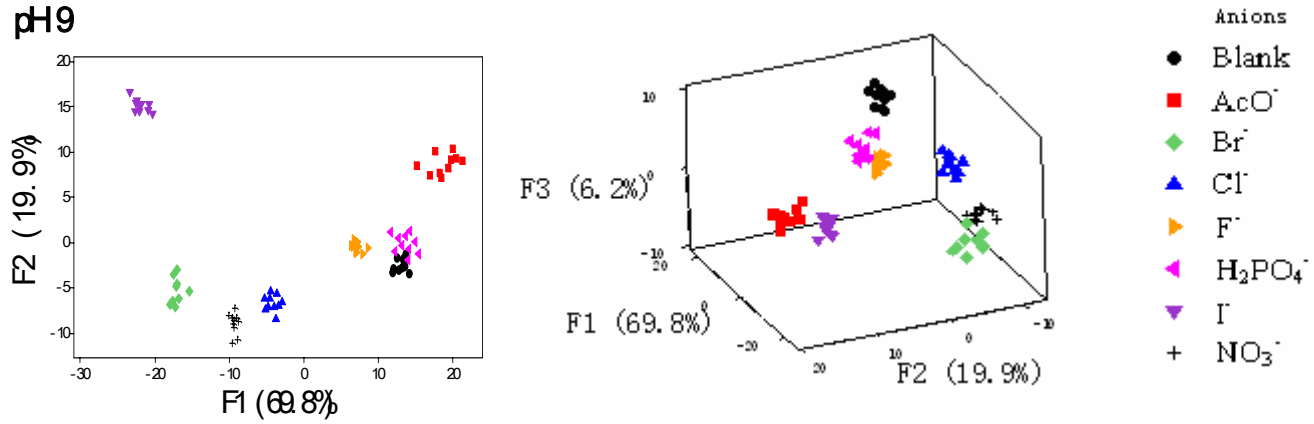




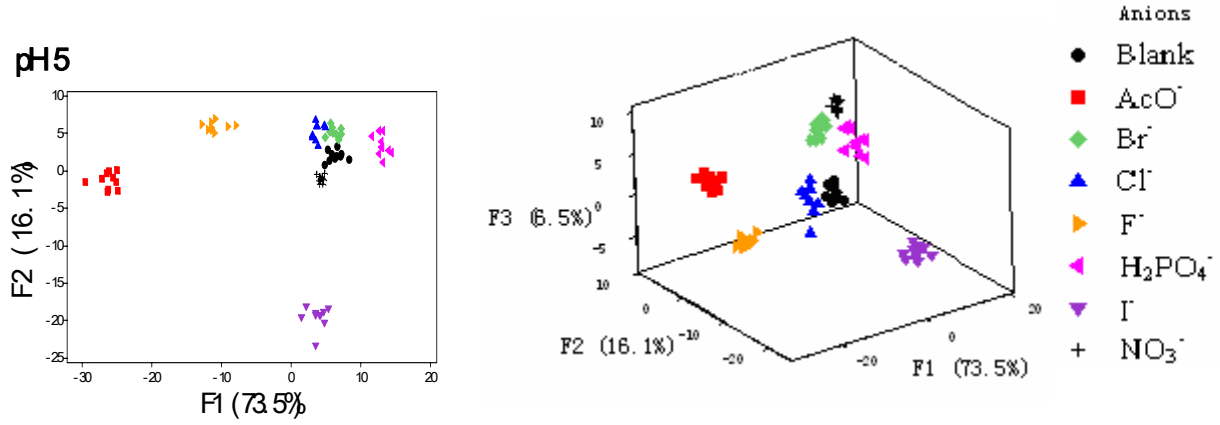
pH8

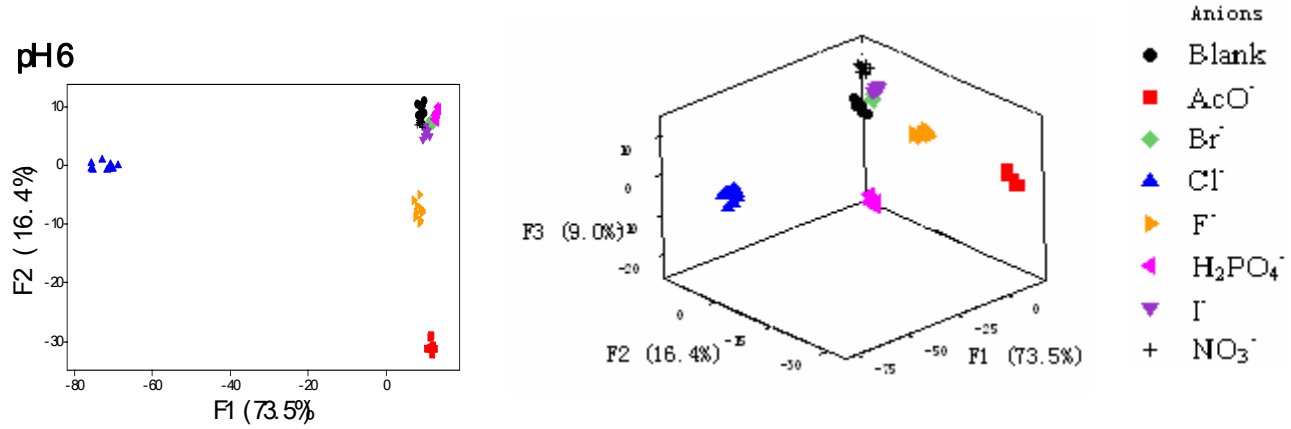

F2 (11.1%)
F1 (80.3%)
F3 (3.4%)
F2 (11.1%)
F1 (80.3%)
Anions
Blank
AcO⁻
Br⁻
Cl⁻
F⁻
H2PO4⁻
I⁻
NO3⁻

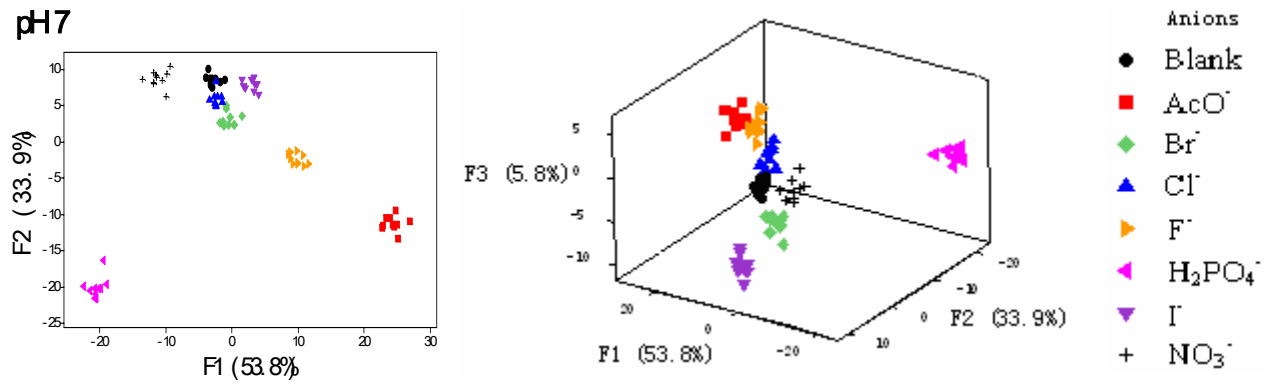
pH9


F2 (19.9%)
F1 (69.8%)
F3 (6.2%)
F1 (69.8%)
F2 (19.9%)
Anions
Blank
AcO⁻
Br⁻
Cl⁻
F⁻
H2PO4⁻
I⁻
NO3⁻

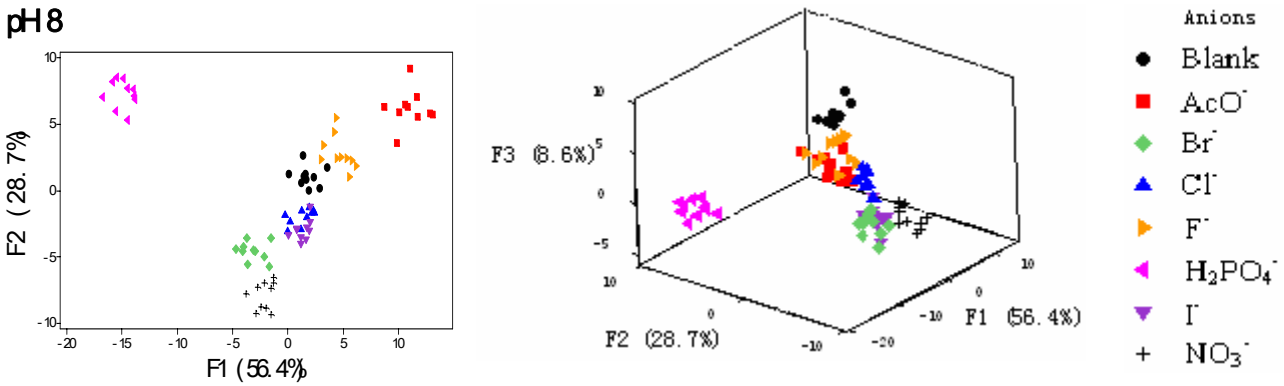
LDA for anions in form of their tetrabutylammonium salts at different pH values



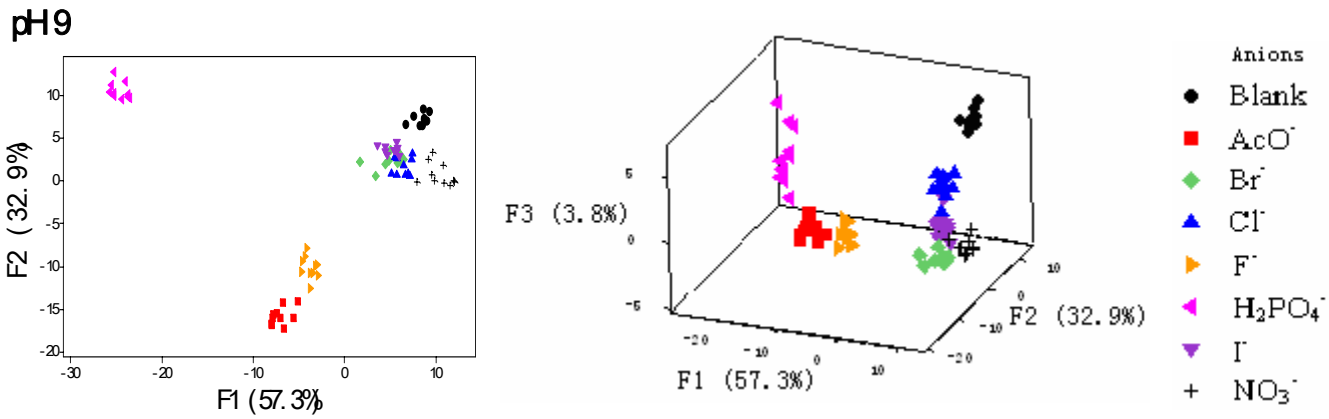




pH 8

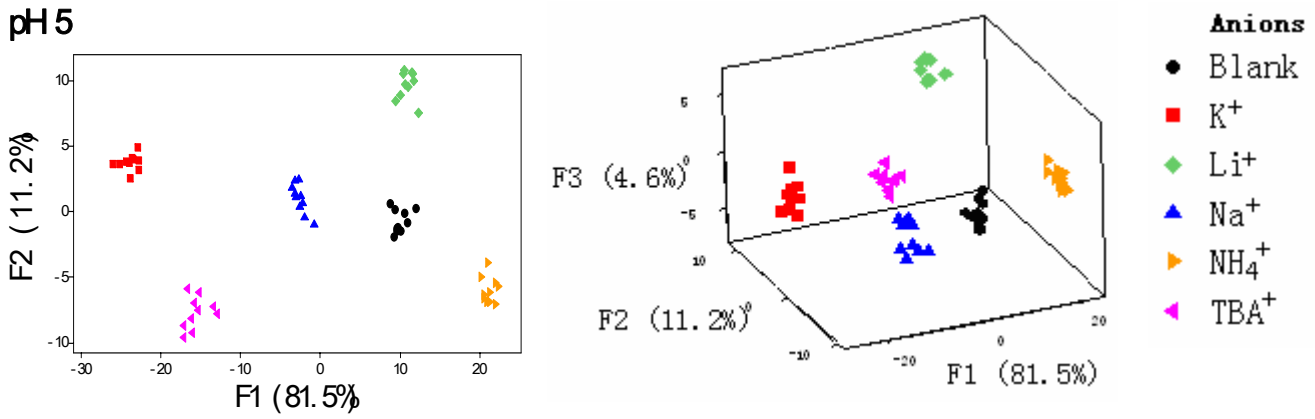

F2 (28.7%)
F1 (56.4%)
F3 (8.6%)
F2 (28.7%)
F1 (56.4%)
Anions
Blank
AcO-
Br-
Cl-
F-
H2PO4-
I-
NO3-

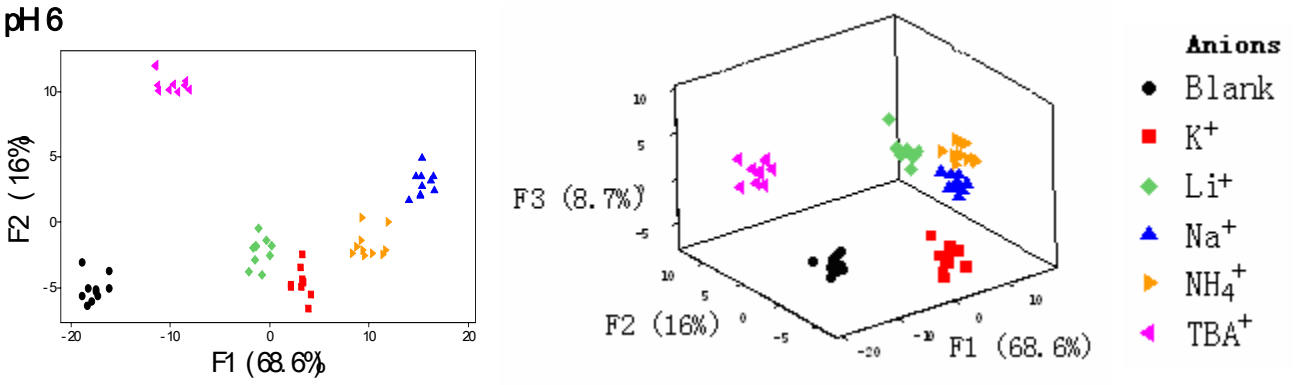
pH 9

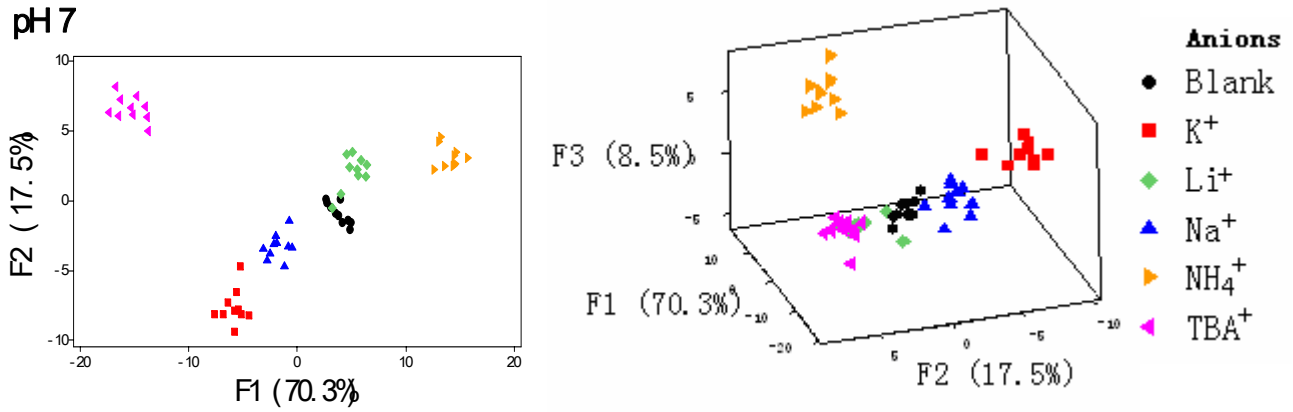

F2 (32.9%)
F1 (57.3%)
F3 (3.8%)
F2 (32.9%)
F1 (57.3%)
Anions
Blank
AcO-
Br-
Cl-
F-
H2PO4-
I-
NO3-

Linear Discriminant Analysis for all cations in form of their different salts at different pH values

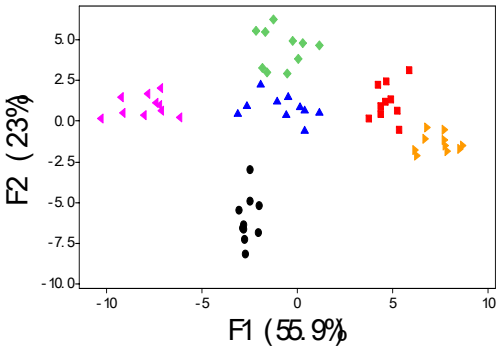
LDA for cations in the form of their fluoride salts at different pH values

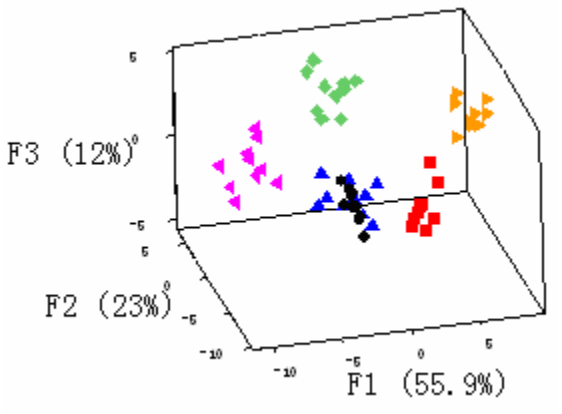




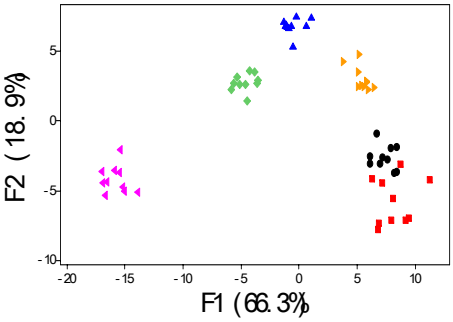


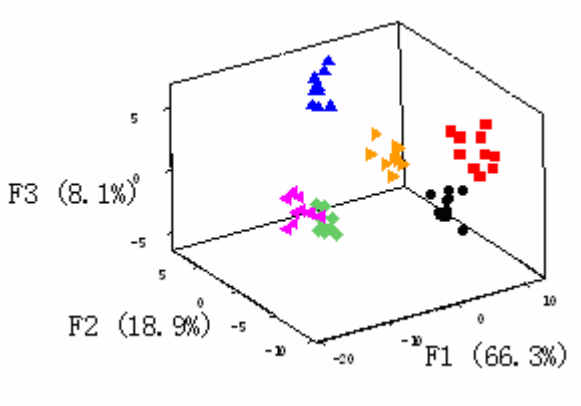
pH 8


F2 (23%)
F1 (55.9%)

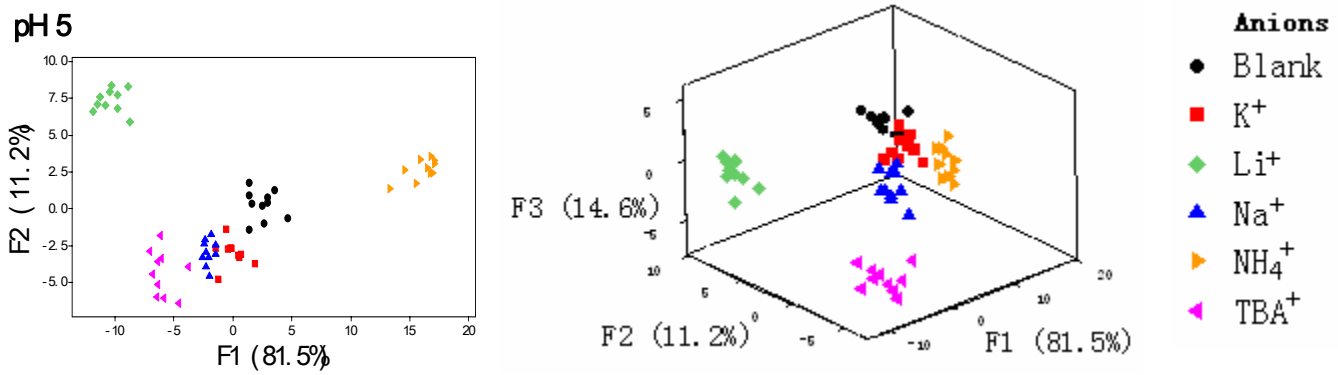

F3 (12%)
F2 (23%)
F1 (55.9%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

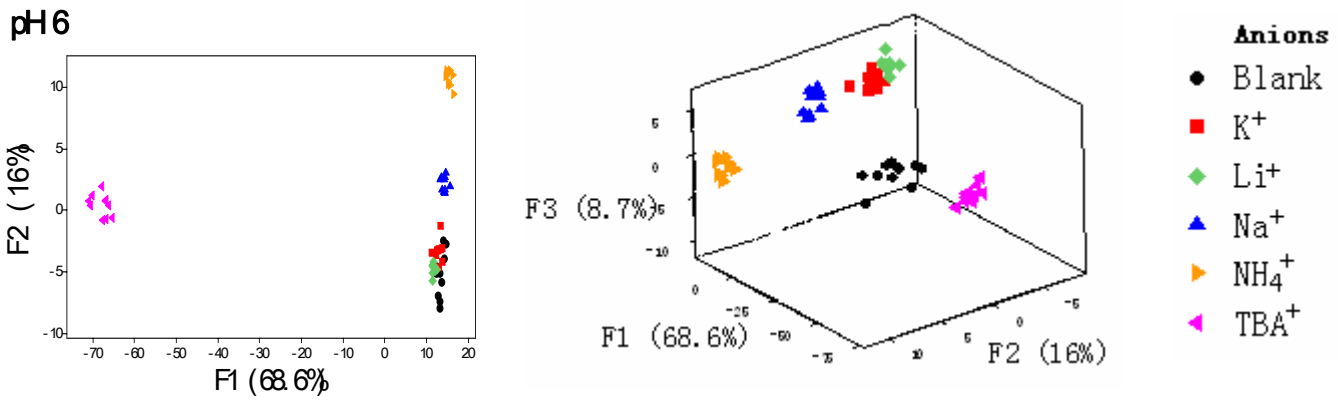
pH 9

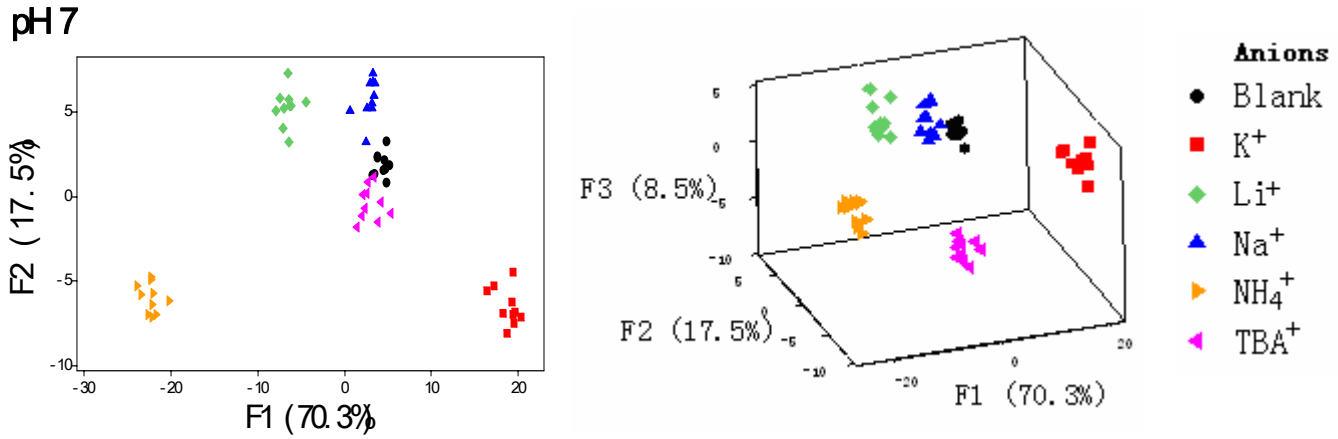

F2 (18.9%)
F1 (66.3%)


F3 (8.1%)
F2 (18.9%)
F1 (66.3%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

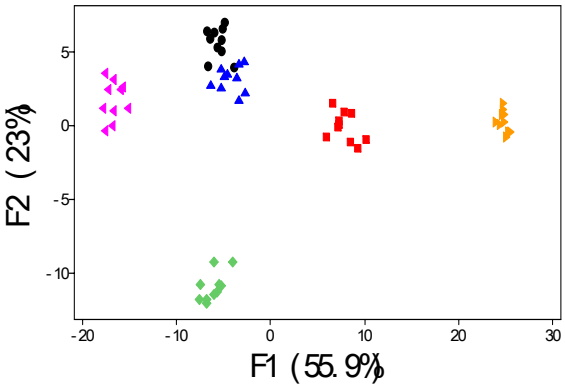
LDA for cations in the form of their chloride salts at different pH values

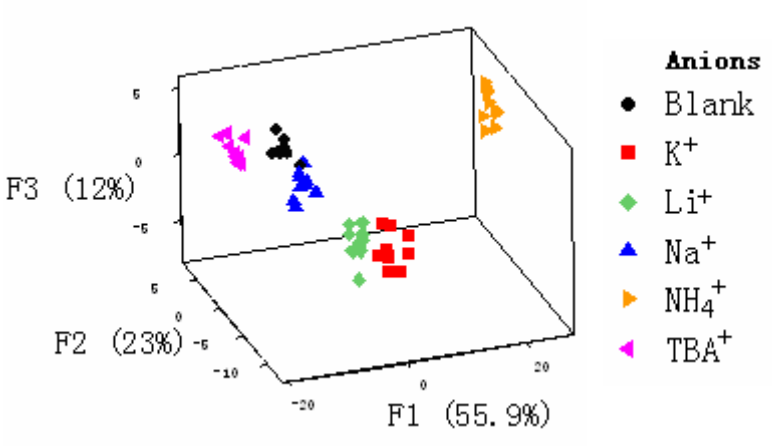




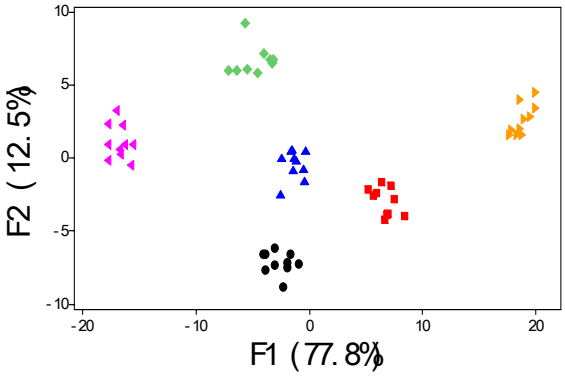


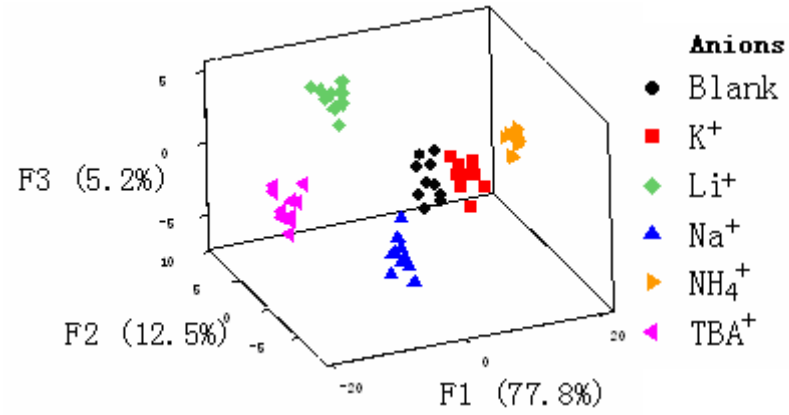
pH 8


F2 (23%)
F1 (55.9%)


F3 (12%)
F2 (23%)
F1 (55.9%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

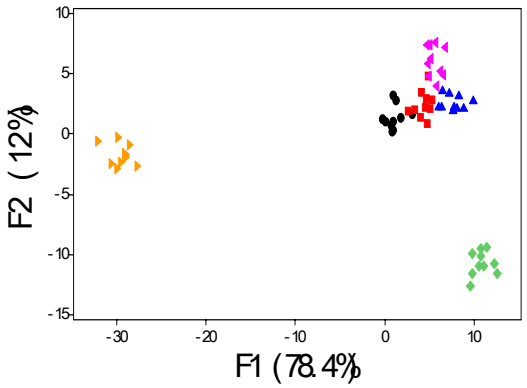
pH 9

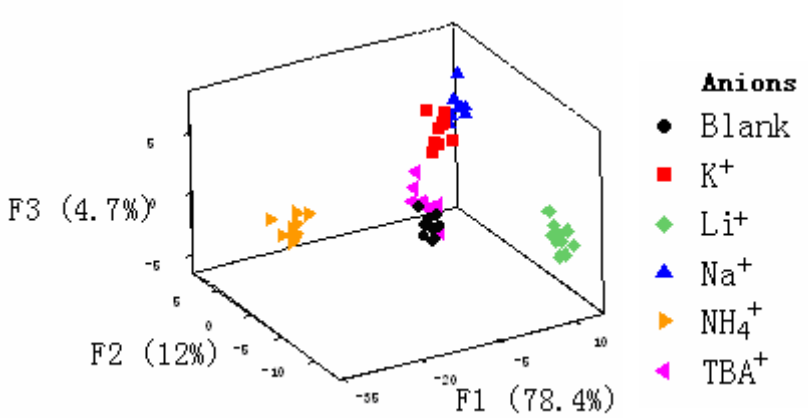

F2 (12.5%)
F1 (77.8%)


F3 (5.2%)
F2 (12.5%)
F1 (77.8%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

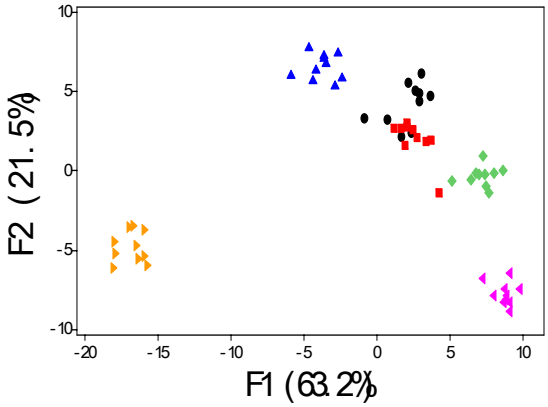
LDA for cations in the form of their bromide salts at different pH values

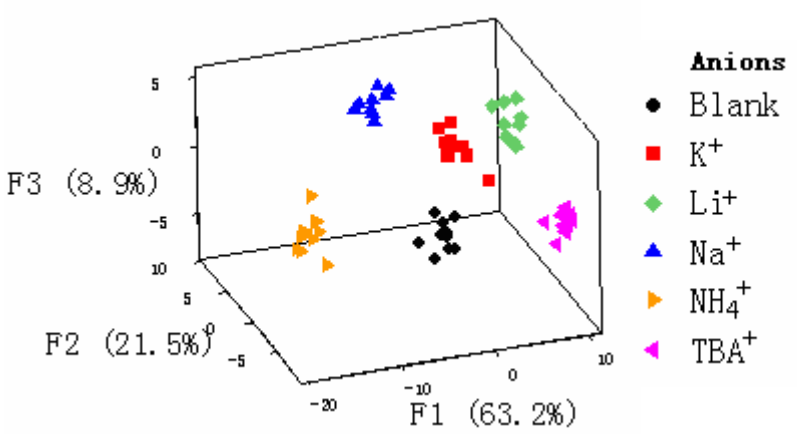
pH 5



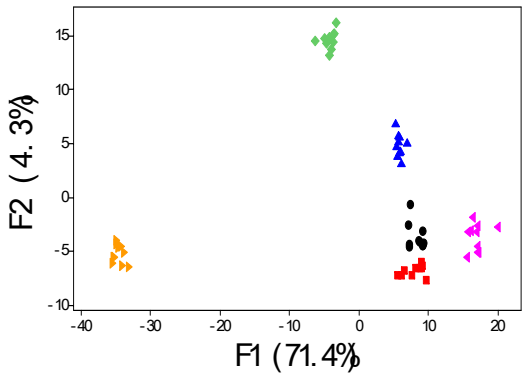


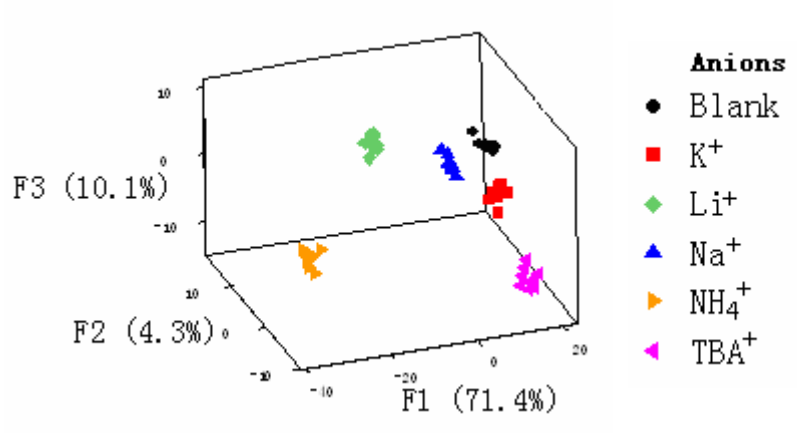
pH 6



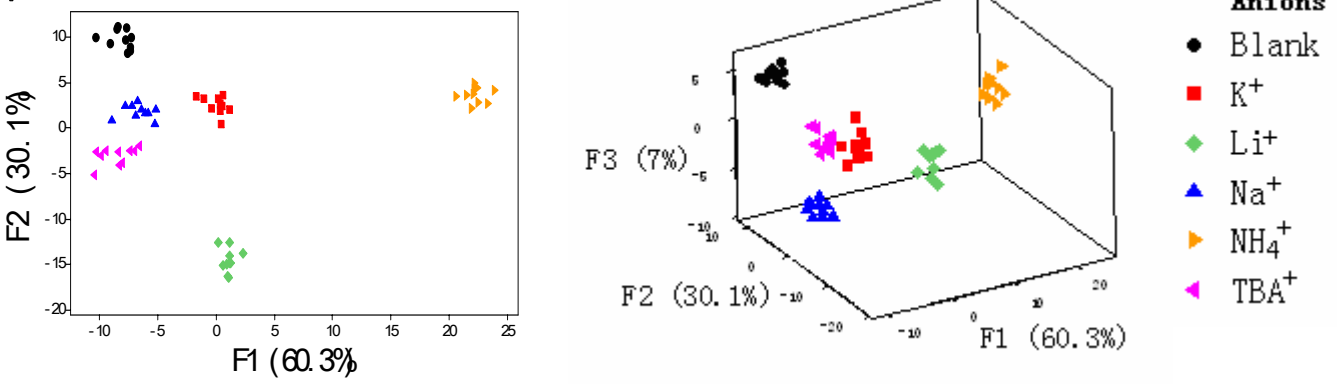


pH 7

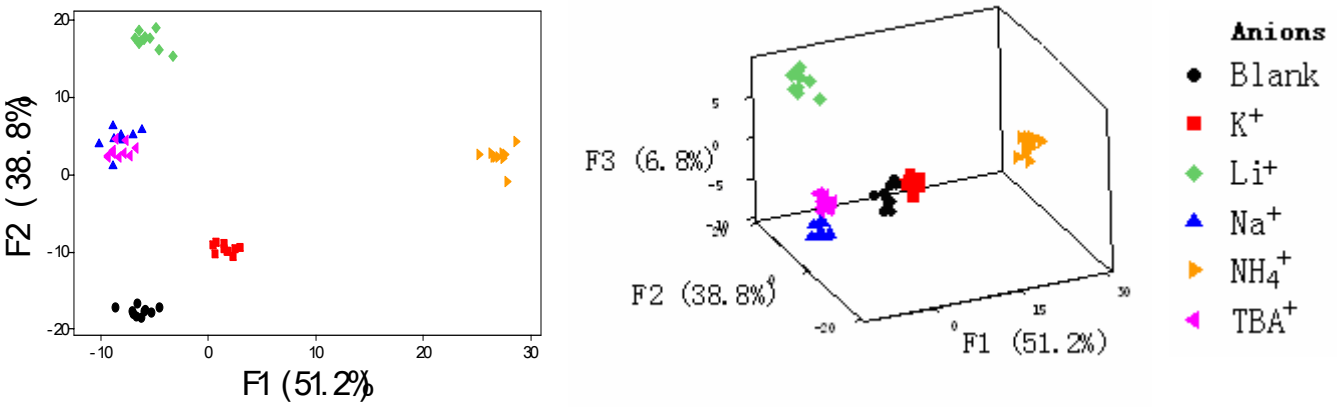




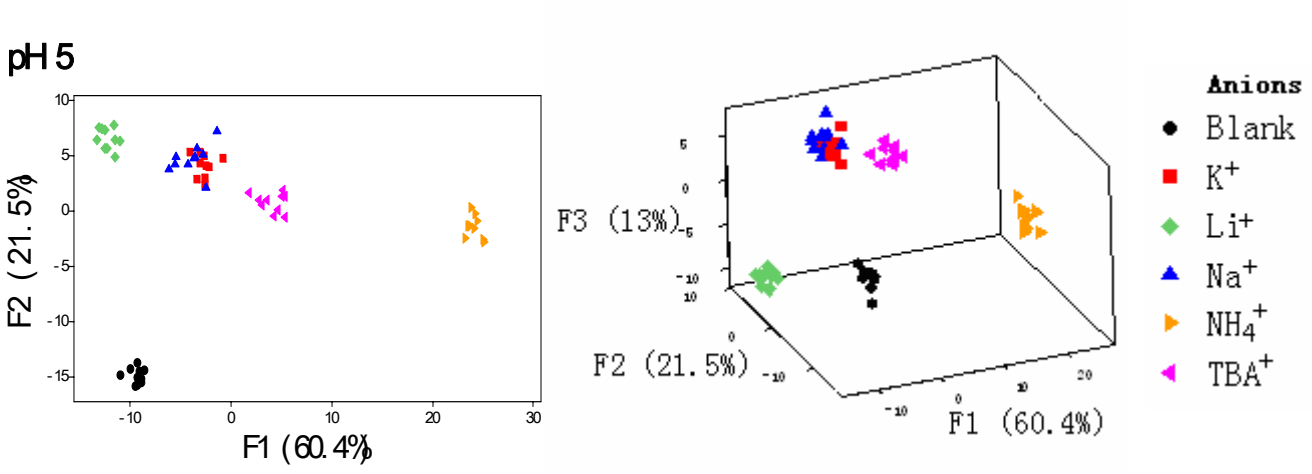
pH 8

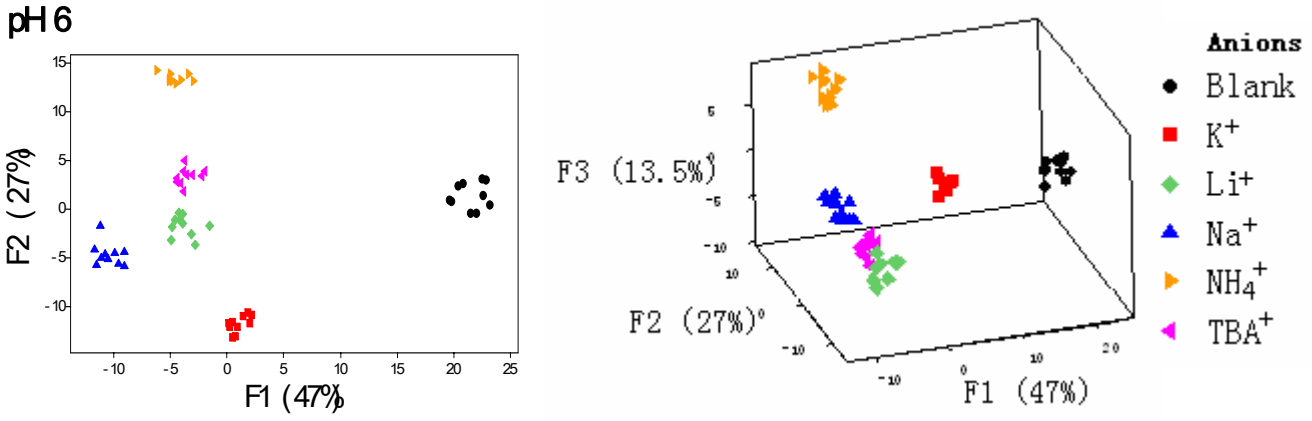

F2 (30.1%)
F1 (60.3%)
F3 (7%)
F2 (30.1%)
F1 (60.3%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

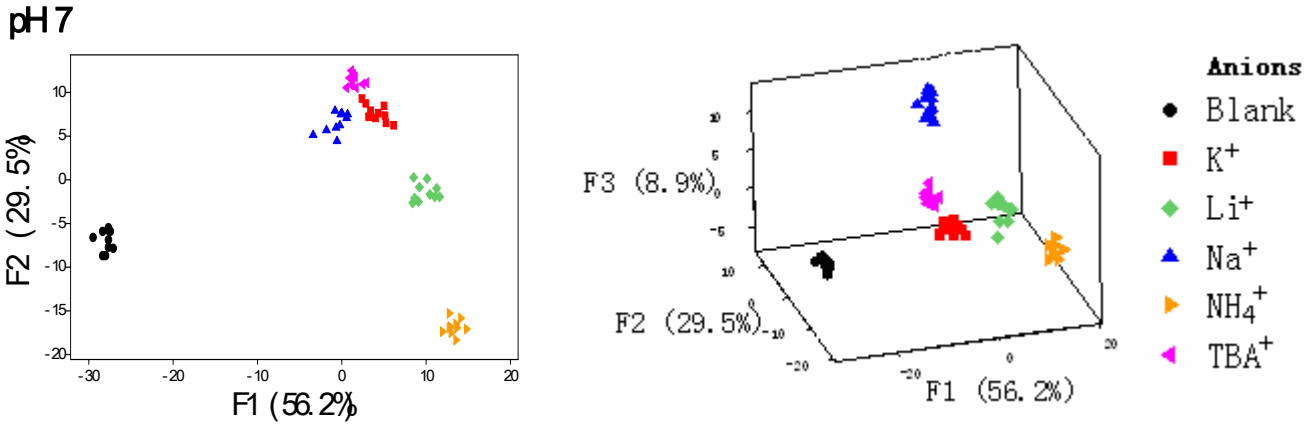
pH 9


F2 (38.8%)
F1 (51.2%)
F3 (6.8%)
F2 (38.8%)
F1 (51.2%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

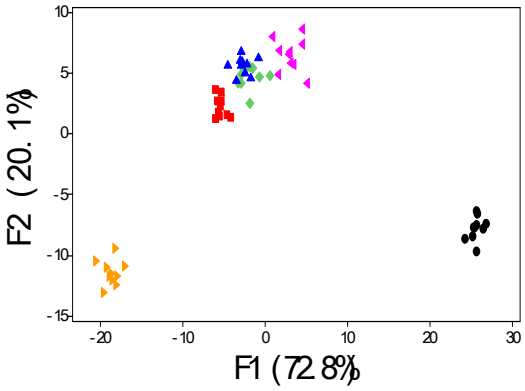
LDA for cations in the form of their iodine salts at different pH values

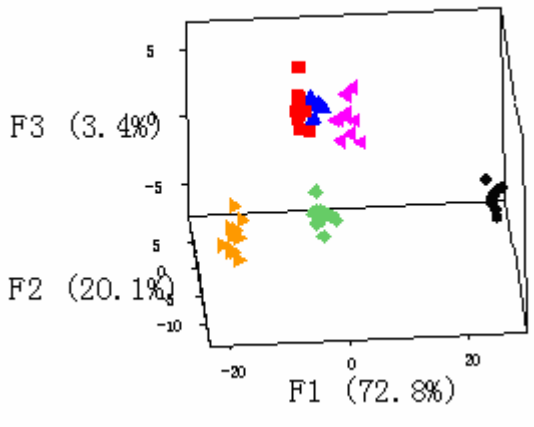






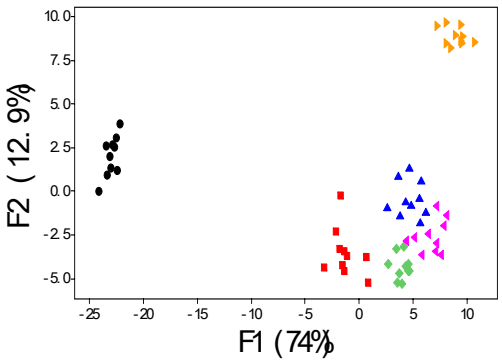
pH 8

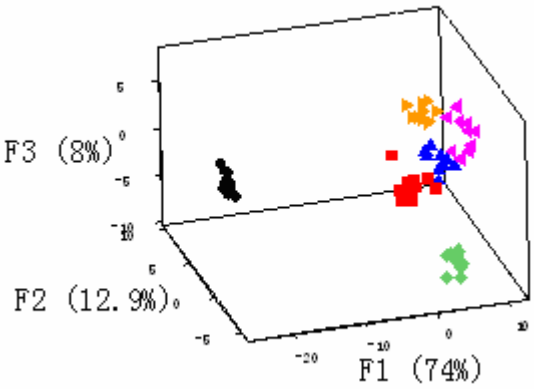

F2 (20.1%)
F1 (72.8%)


F3 (3.4%)
F2 (20.1%)
F1 (72.8%)


Anions
Blank
K+
Li+
Na+
NH4+
TBA+

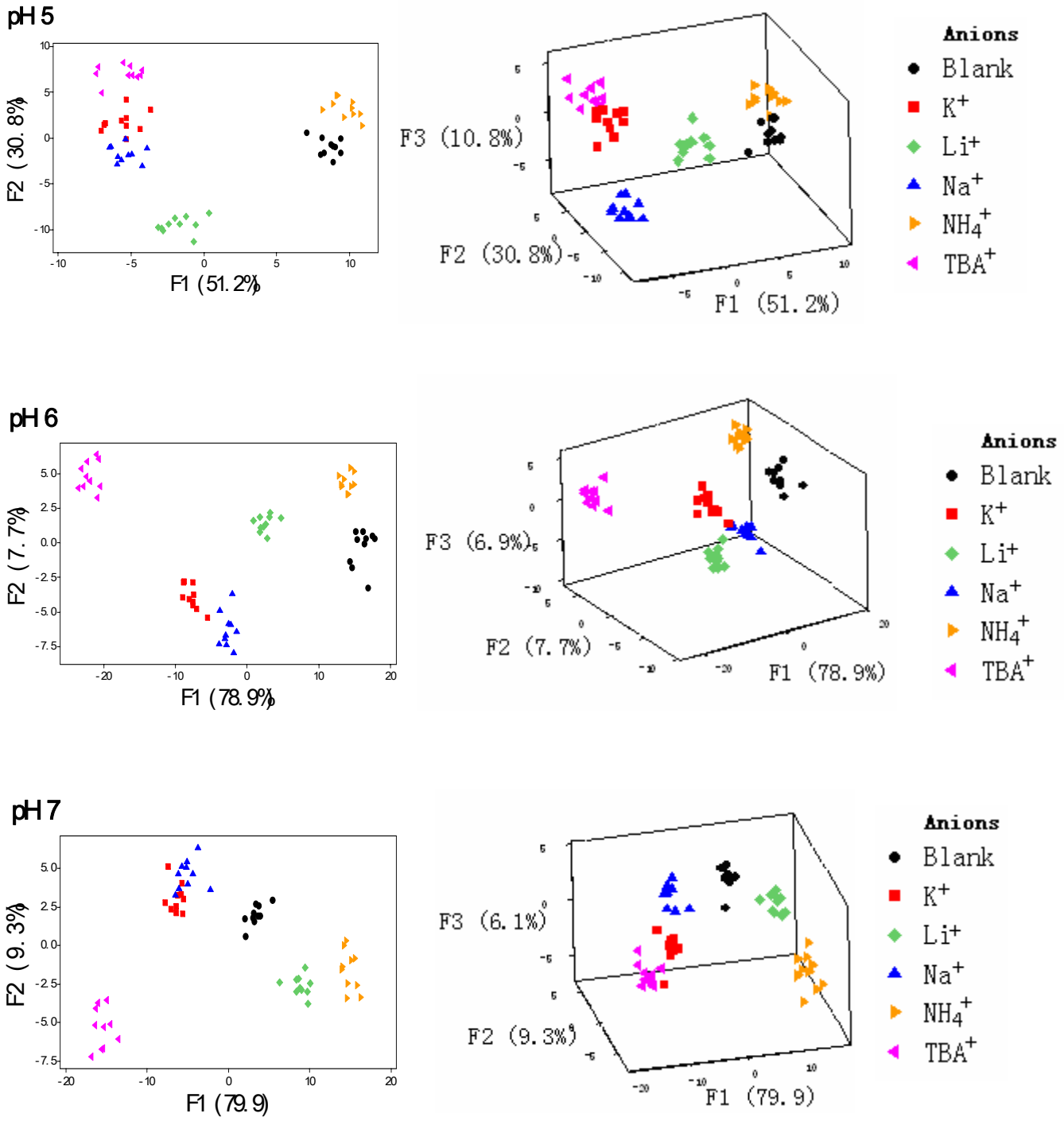
pH 9


F2 (12.9%)
F1 (74%)

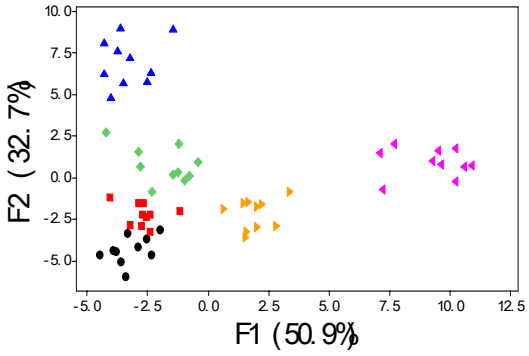

F3 (8%)
F2 (12.9%)
F1 (74%)

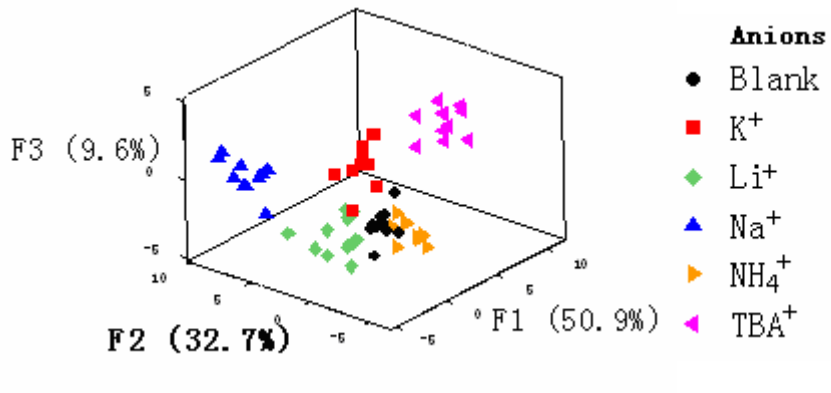

Anions
Blank
K+
Li+
Na+
NH4+
TBA+

LDA for cations in the form of their acetate salts at different pH values

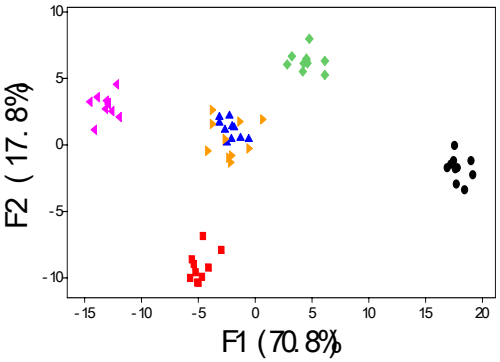


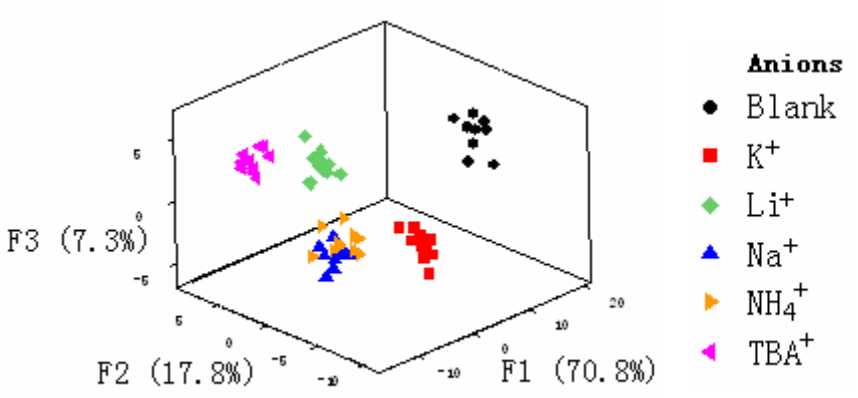
pH 8


F2 (32.7%)
F1 (50.9%)


F3 (9.6%)
F2 (32.7%)
F1 (50.9%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

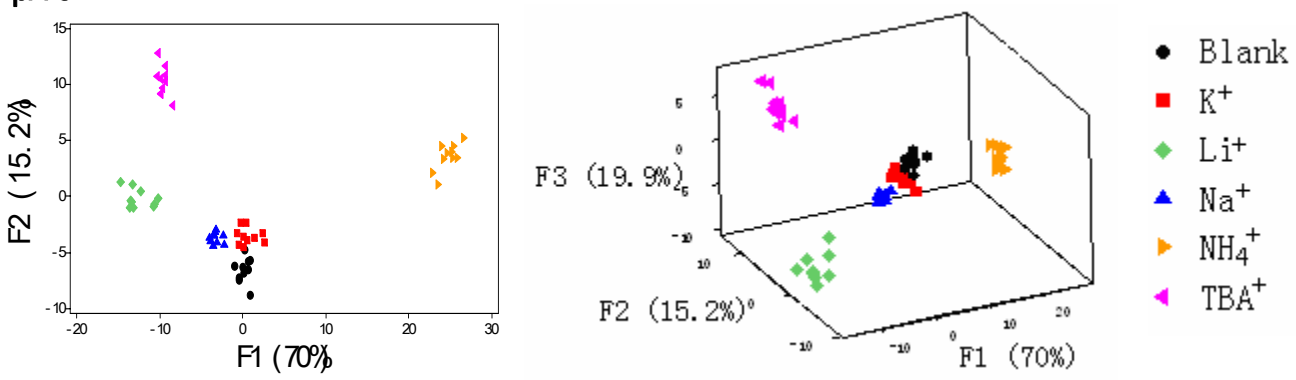
pH 9


F2 (17.8%)
F1 (70.8%)

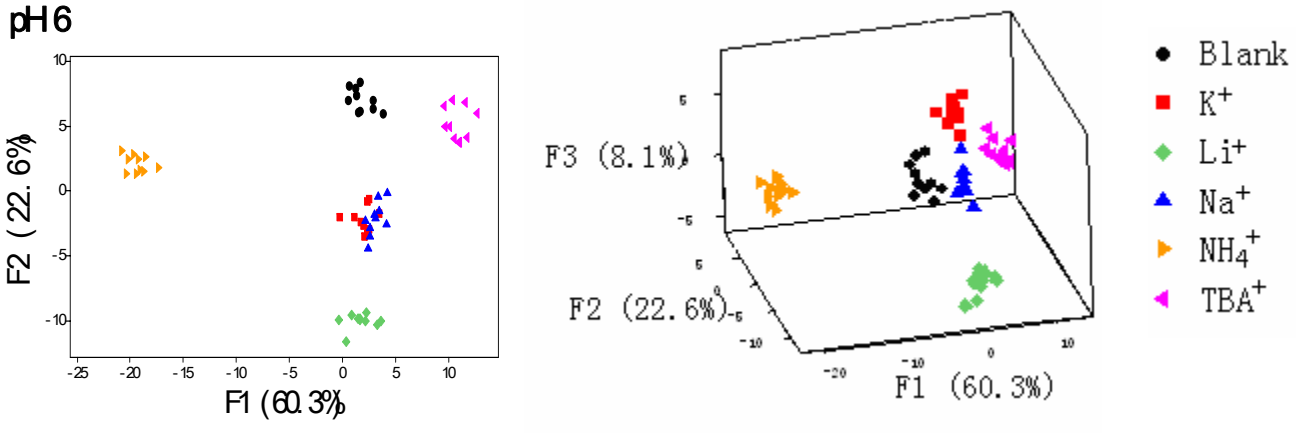

F3 (7.3%)
F2 (17.8%)
F1 (70.8%)
Anions
Blank
K+
Li+
Na+
NH4+
TBA+

LDA for cations in the form of their nitrate salts at different pH values

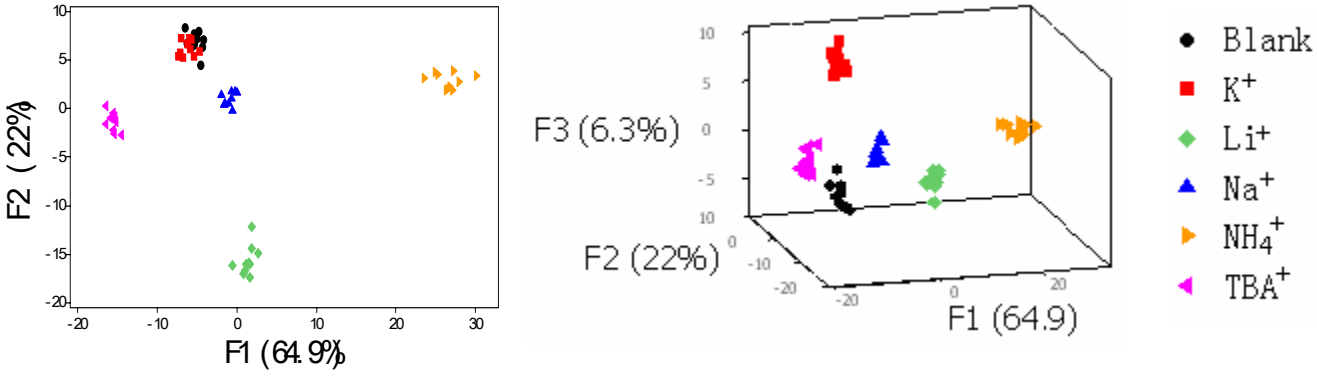
pH 5



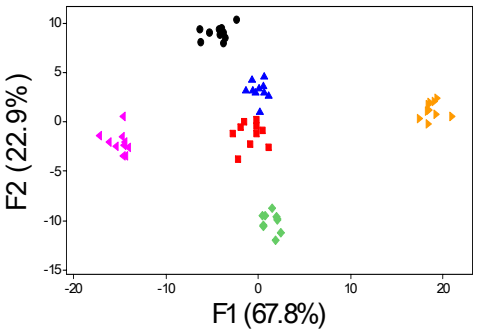
pH 6

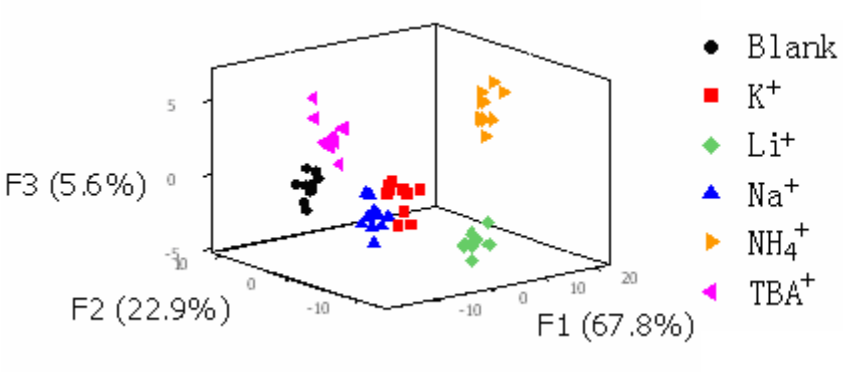


pH 7

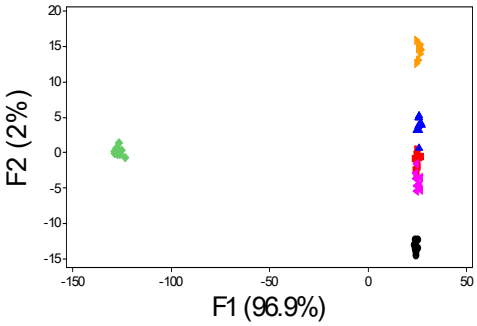


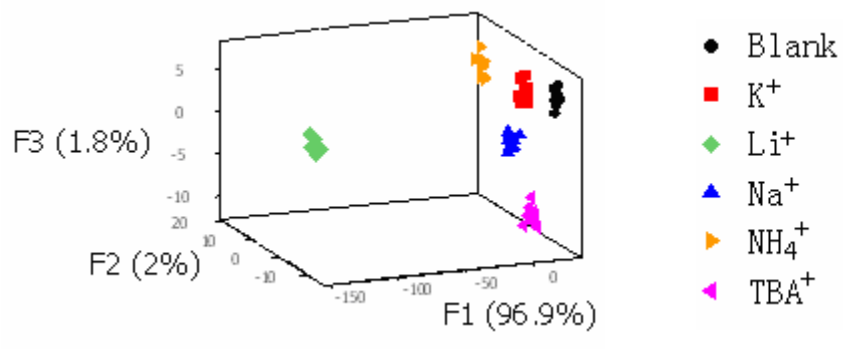
pH 8


F2 (22.9%)
F1 (67.8%)


F3 (5.6%)
F2 (22.9%)
F1 (67.8%)
Blank
K+
Li+
Na+
NH4+
TBA+

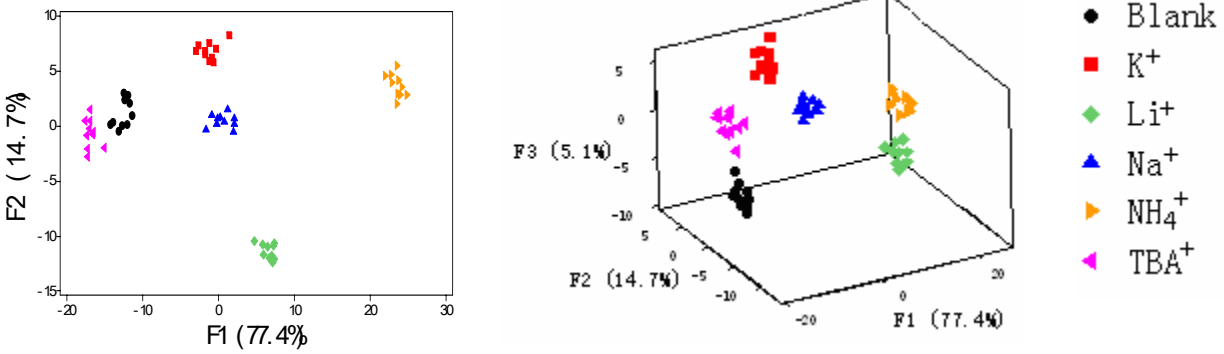
pH 9


F2 (2%)
F1 (96.9%)

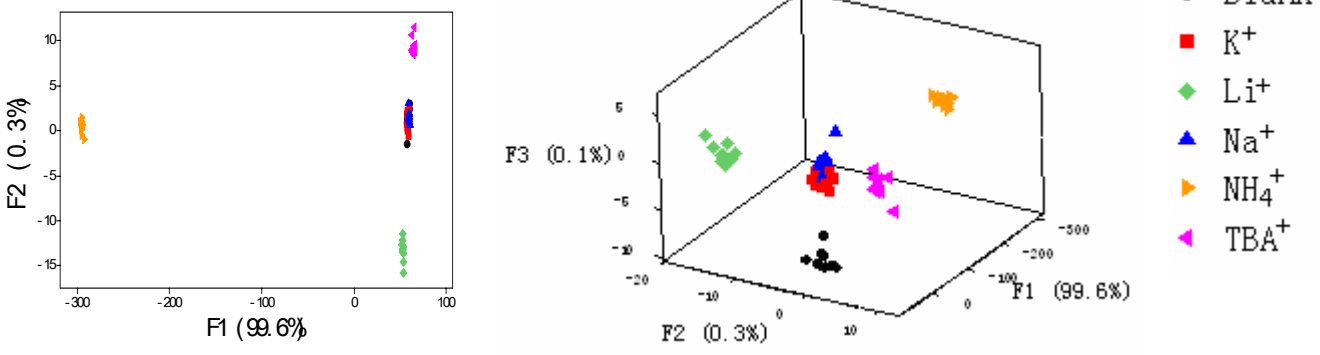

F3 (1.8%)
F2 (2%)
F1 (96.9%)
Blank
K+
Li+
Na+
NH4+
TBA+

LDA for cations in the form of their dihydrogenphosphate salts at different pH values

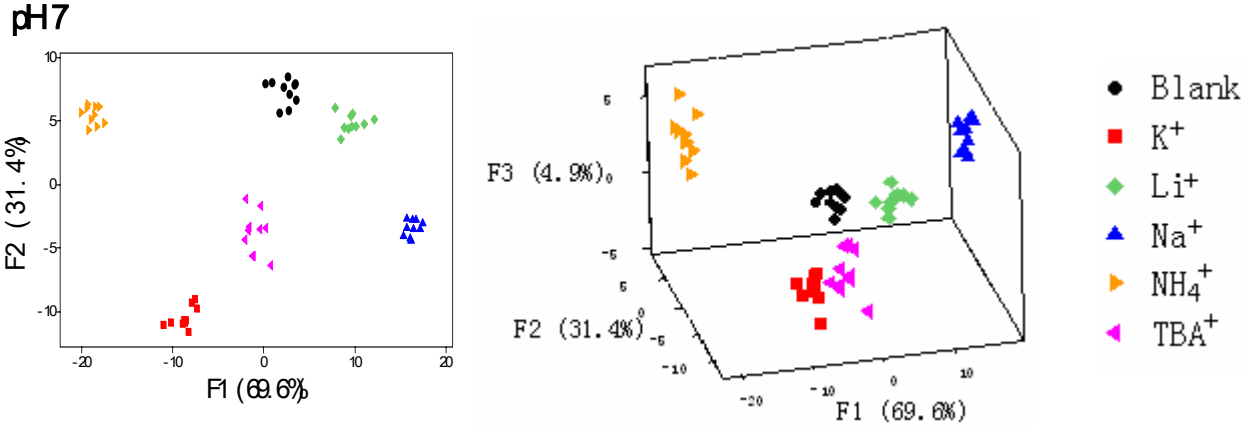
pH5



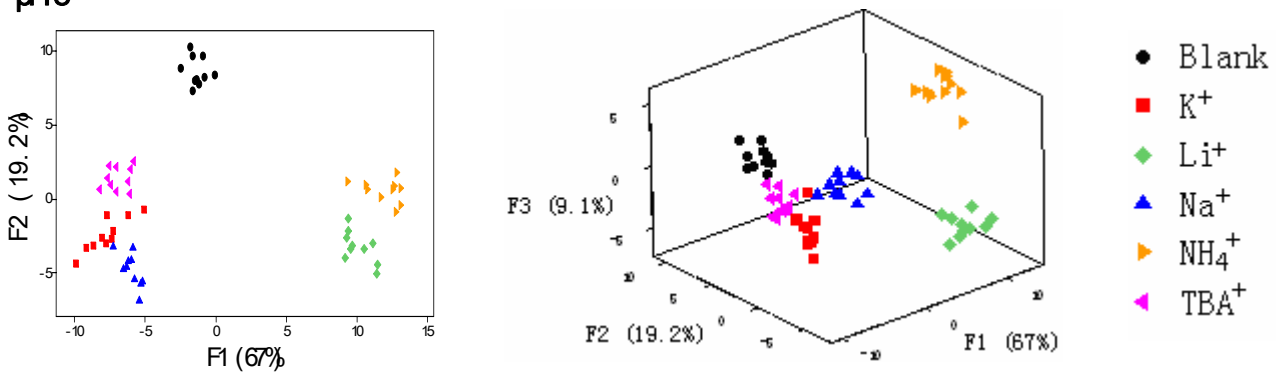
pH6



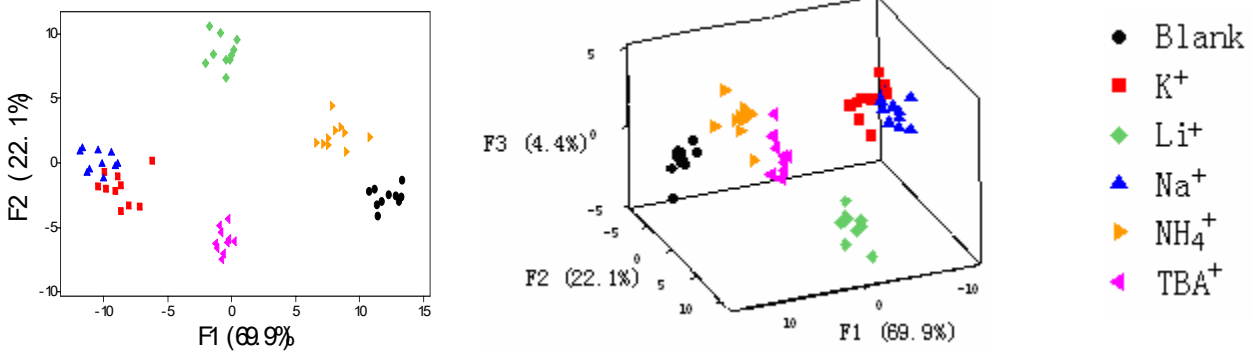
pH7



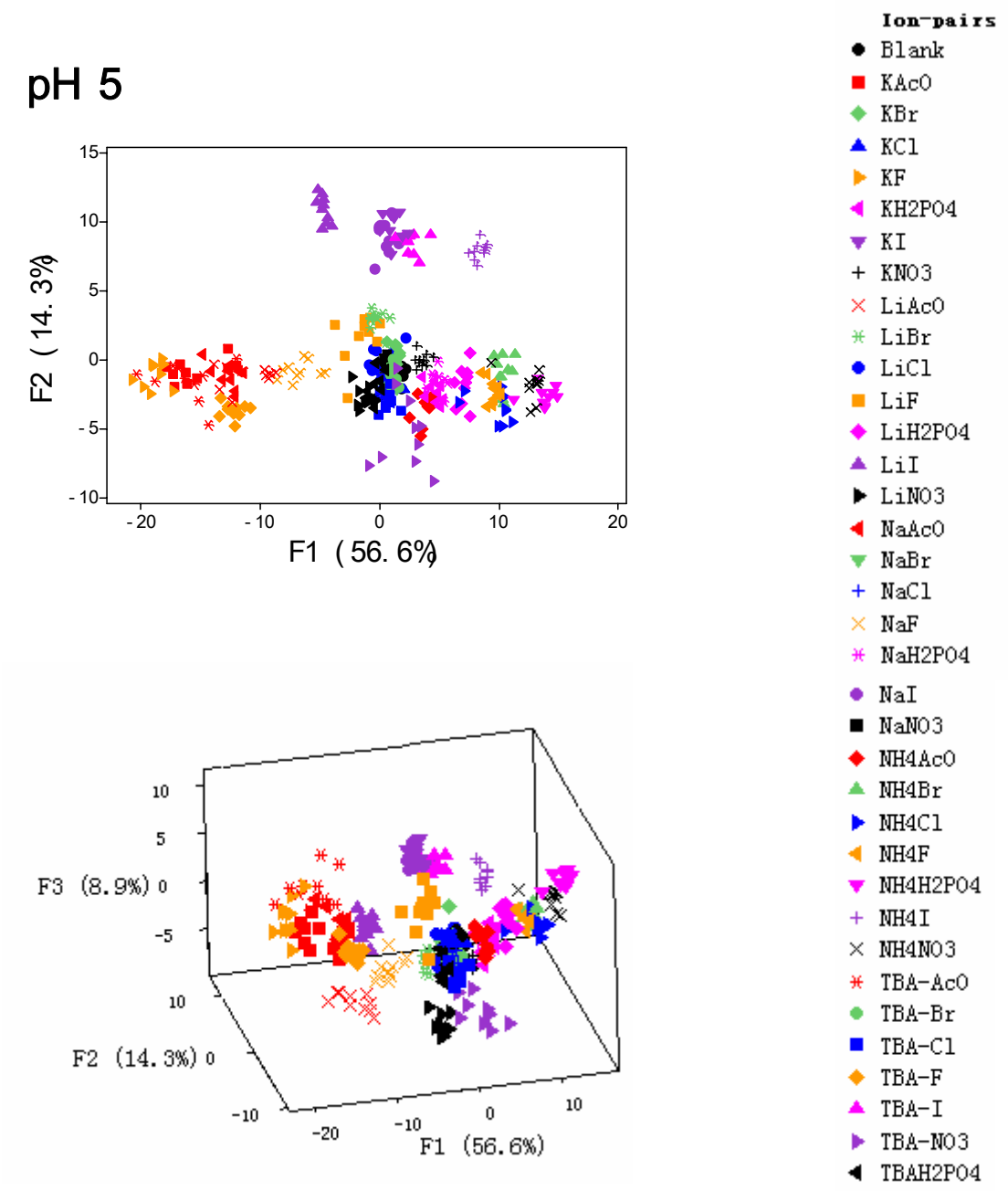
pH8


F2 (19.2%)
F1 (67%)
F3 (9.1%)
F2 (19.2%)
F1 (67%)
Blank
K+
Li+
Na+
NH4+
TBA+

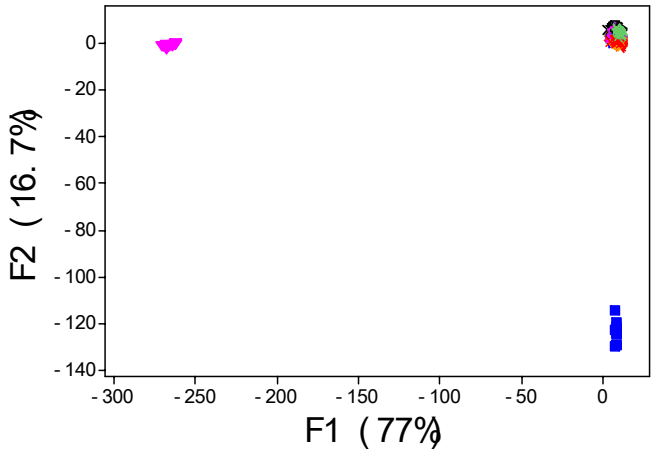
pH9

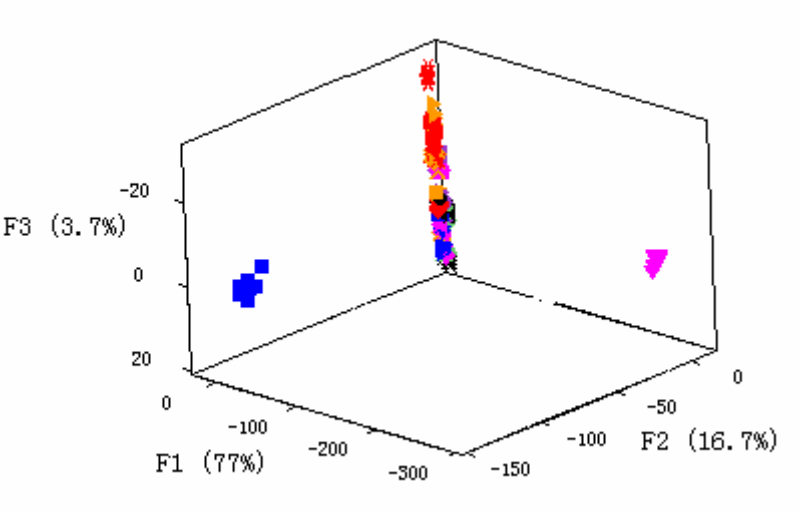

F2 (22.1%)
F1 (69.9%)
F3 (4.4%)
F2 (22.1%)
F1 (69.9%)
Blank
K+
Li+
Na+
NH4+
TBA+

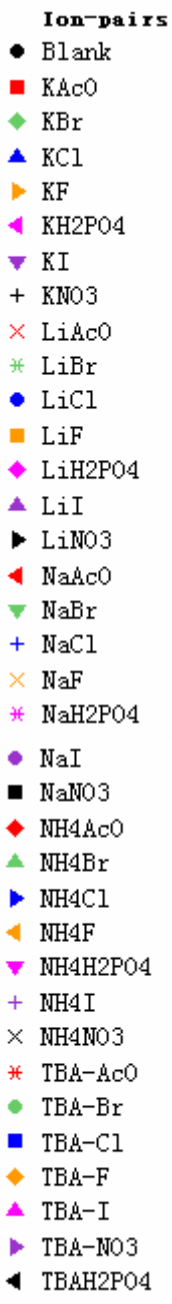
Linear Discriminant Analysis for Ion-pairs at different pH values



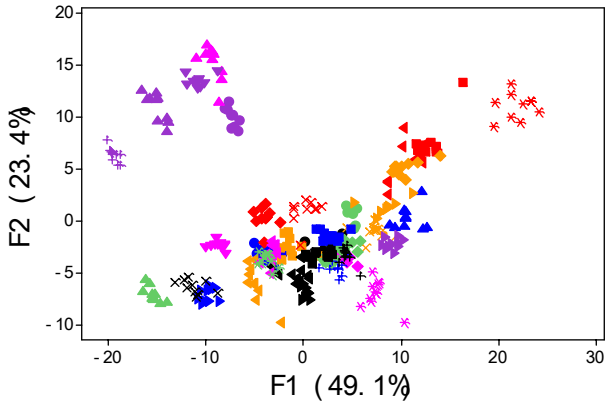
pH 6

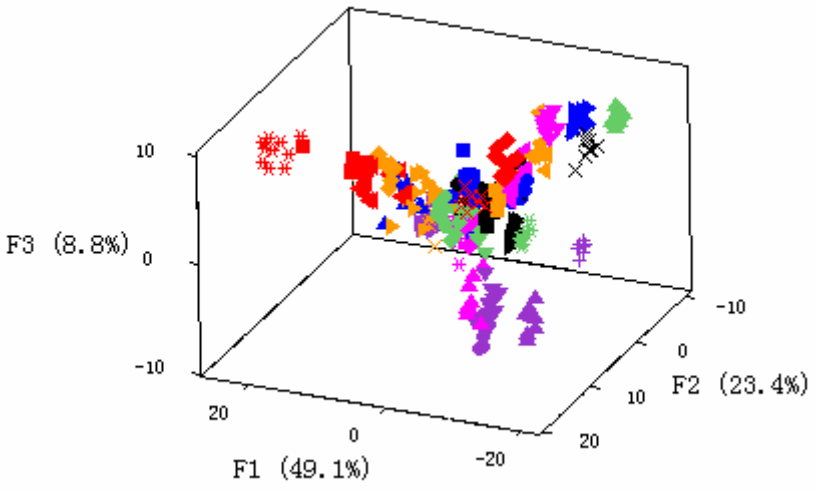

0
-20
-40
-60
-80
-100
-120
-140
-300
-250
-200
-150
-100
-50
0
F2 (16. 7%)
F1 (77%)

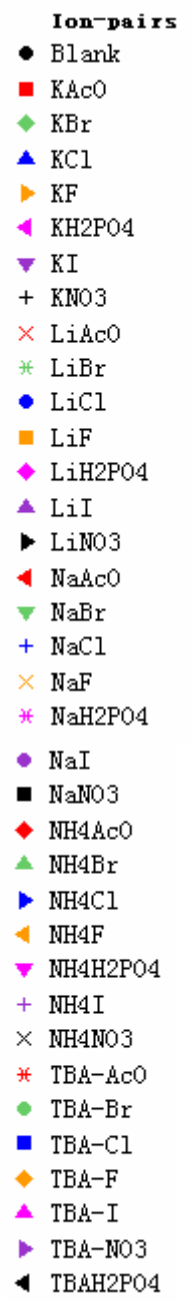

F3 (3.7%)
-20
0
20
0
-100
-200
-300
F1 (77%)
-150
-100
-50
0
F2 (16.7%)


Ion-pairs
Blank
KAcO
KBr
KCl
KF
KH2PO4
KI
KNO3
LiAcO
LiBr
LiCl
LiF
LiH2PO4
LiI
LiNO3
NaAcO
NaBr
NaCl
NaF
NaH2PO4
NaI
NaNO3
NH4AcO
NH4Br
NH4Cl
NH4F
NH4H2PO4
NH4I
NH4NO3
TBA-AcO
TBA-Br
TBA-Cl
TBA-F
TBA-I
TBA-NO3
TBAH2PO4

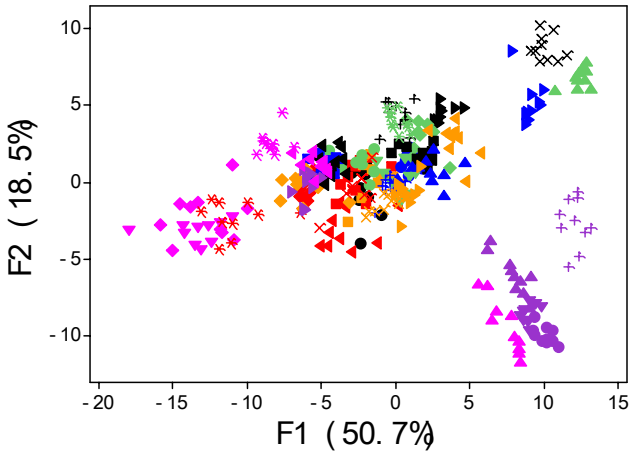
pH 7

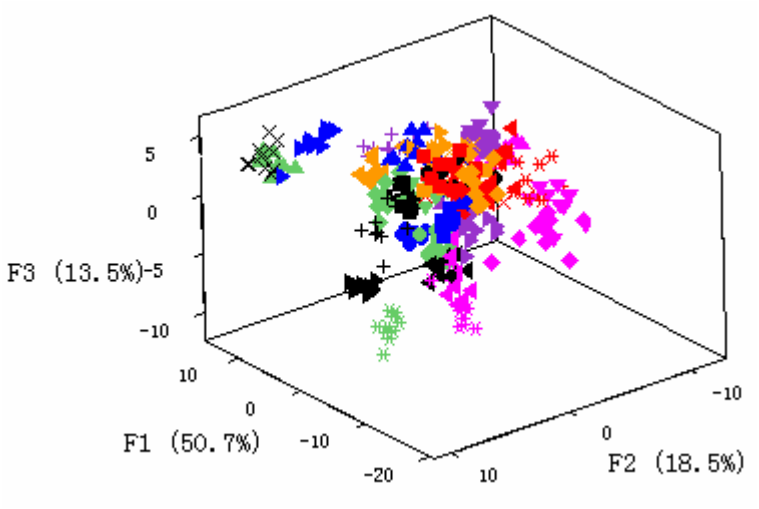

F2 (23.4%)
F1 (49.1%)
20
15
10
5
0
-5
-10
-20
-10
0
10
20
30


F3 (8.8%)
F1 (49.1%)
F2 (23.4%)
10
0
-10
20
0
-20
-10
0
10
20

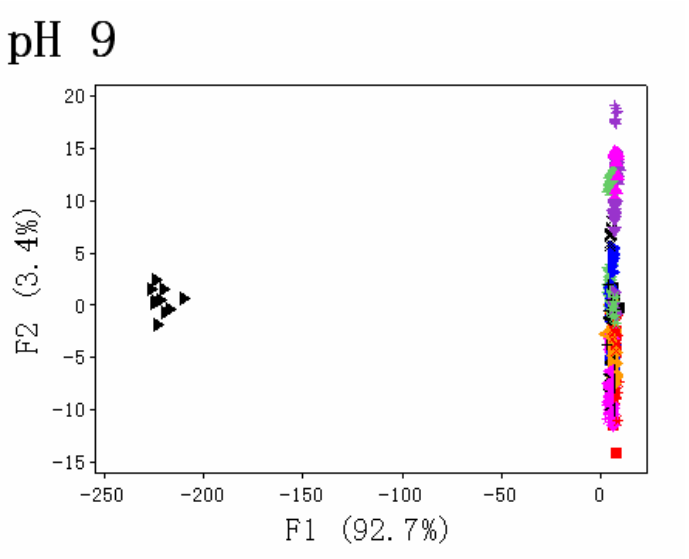

Ion-pairs
Blank
KAcO
KBr
KCl
KF
KH2PO4
KI
KNO3
LiAcO
LiBr
LiCl
LiF
LiH2PO4
LiI
LiNO3
NaAcO
NaBr
NaCl
NaF
NaH2PO4
NaI
NaNO3
NH4AcO
NH4Br
NH4Cl
NH4F
NH4H2PO4
NH4I
NH4NO3
TBA-AcO
TBA-Br
TBA-Cl
TBA-F
TBA-I
TBA-NO3
TBAH2PO4

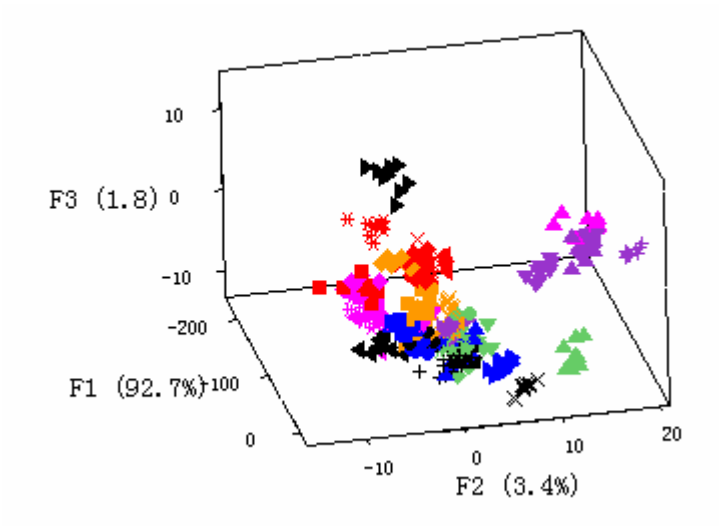
pH 8

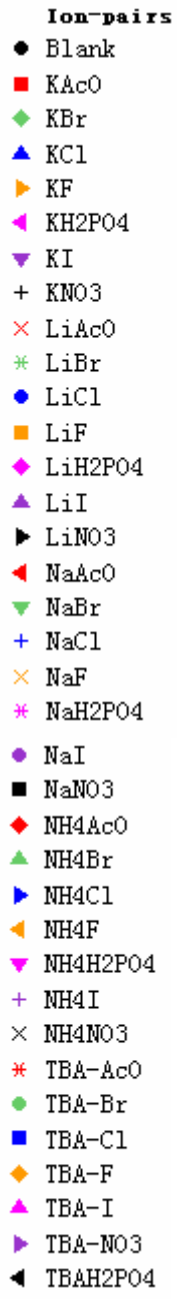




Ion-pairs
- Blank
- KAcO
- KBr
- KCl
- KF
- KH2PO4
- KI
- KNO3
- LiAcO
- LiBr
- LiCl
- LiF
- LiH2PO4
- LiI
- LiNO3
- NaAcO
- NaBr
- NaCl
- NaF
- NaH2PO4
- NaI
- NaNO3
- NH4AcO
- NH4Br
- NH4Cl
- NH4F
- NH4H2PO4
- NH4I
- NH4NO3
- TBA-AcO
- TBA-Br
- TBA-Cl
- TBA-F
- TBA-I
- TBA-NO3
- TBAH2PO4


pH 9
F2 (3.4%)
F1 (92.7%)
20
15
10
5
0
-5
-10
-15
-250
-200
-150
-100
-50
0


F3 (1.8)
F1 (92.7%)
F2 (3.4%)
10
0
-10
-200
-100
0
-10
0
10
20


Ion-pairs
Blank
KAcO
KBr
KCl
KF
KH2PO4
KI
KNO3
LiAcO
LiBr
LiCl
LiF
LiH2PO4
LiI
LiNO3
NaAcO
NaBr
NaCl
NaF
NaH2PO4
NaI
NaNO3
NH4AcO
NH4Br
NH4Cl
NH4F
NH4H2PO4
NH4I
NH4NO3
TBA-AcO
TBA-Br
TBA-Cl
TBA-F
TBA-I
TBA-NO3
TBAH2PO4

Relative response (heat) map of the recorded 24×180 replica-averaged values illustrates the high output signal variability recorded from the array across the whole dataset

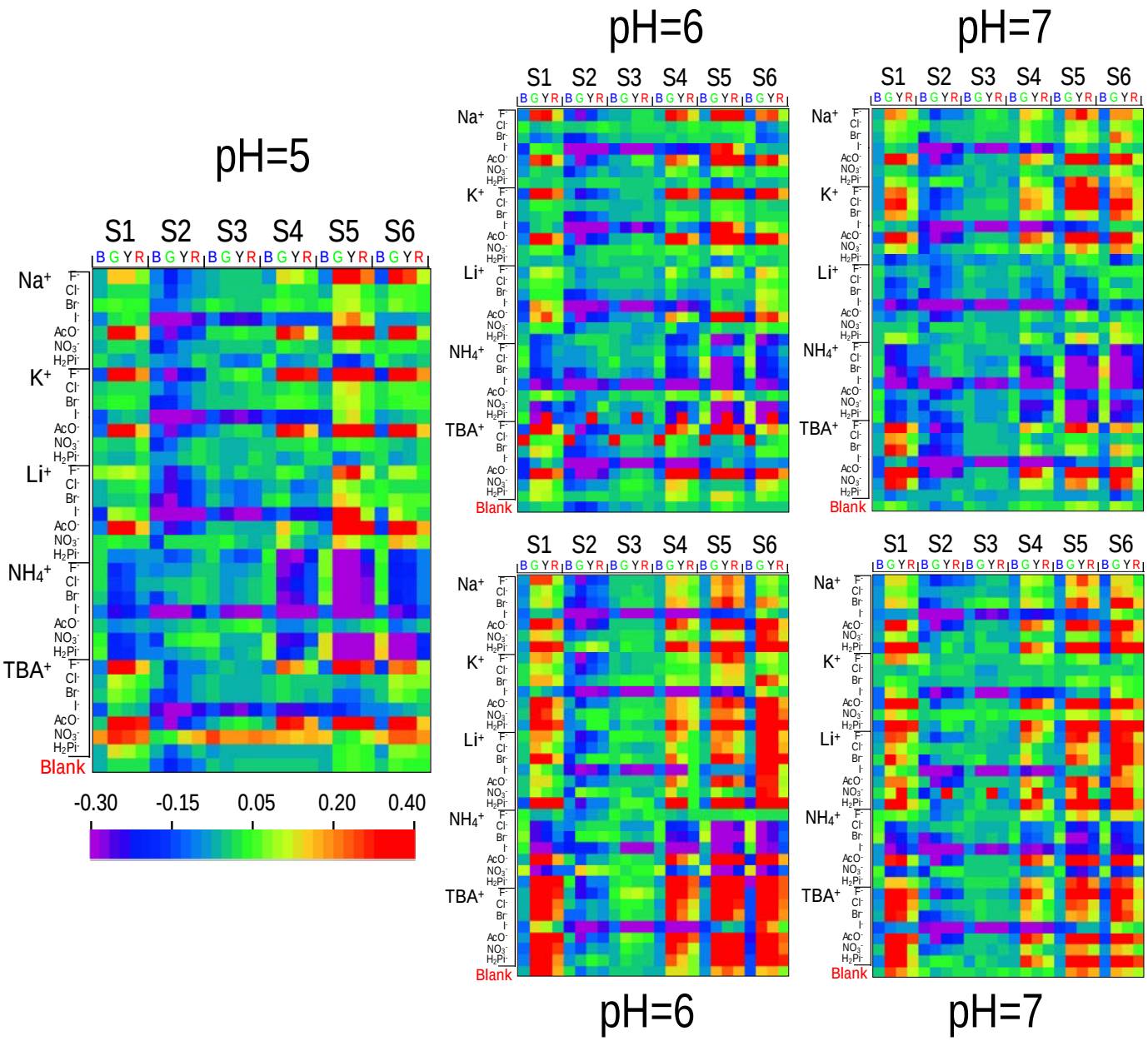


Table 1. Summary table of LDA cross-validated (leave-one-out) classification accuracy for anions in the presence of different cations at different pH values.

pH	Li^+	Na^+	K^+	NH_4^+	TBA^+
5	100%	98%	90%	86%	94%
6	99%	96%	100%	100%	100%
7	95%	96%	93%	100%	100%
8	100%	93%	94%	100%	94%
9	99%	99%	93%	98%	98%

Table 2. Summary table of LDA cross-validated (leave-one-out) classification accuracy for cations in the presence of different anions at different pH values.

pH	F^-	Cl^-	Br^-	I^-	AcO^-	NO_3^-	$H_2PO_4^-$
5	98%	97%	100%	93%	90%	92%	98%
6	100%	93%	97%	100%	97%	98%	92%
7	90%	98%	100%	98%	93%	100%	97%
8	95%	97%	100%	95%	92%	97%	95%
9	100%	100%	100%	93%	95%	97%	93%

Table 3. LDA cross-validated (leave-one-out) classification accuracy for **ion-pair** at different pH values.

pH	5	6	7	8	9
Classification accuracy (%)	89%	95%	94%	93%	93%

Reference
1 Zhuo Wang, Manuel A. Palacios, and Pavel Anzenbacher, Jr. *Anal. Chem.* 2008, 80, 7451-7459.
2 Palacios, M. A., Wang, Z., Montes, V. A., Zyryanov, G.V., Hausch, B. J., Jursikova, K., Anzenbacher, P., Jr. *Chem. Commun.* 2007, 3708-3710.