Supplementary Material

A Saccharide Chemosensor Array Developed Based on an Indicator Displacement Assay Using a Combination of Commercially Available Reagents

Yui Sasaki, Zhoujie Zhang and Tsuyoshi Minami[*]

_____

Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo, Japan
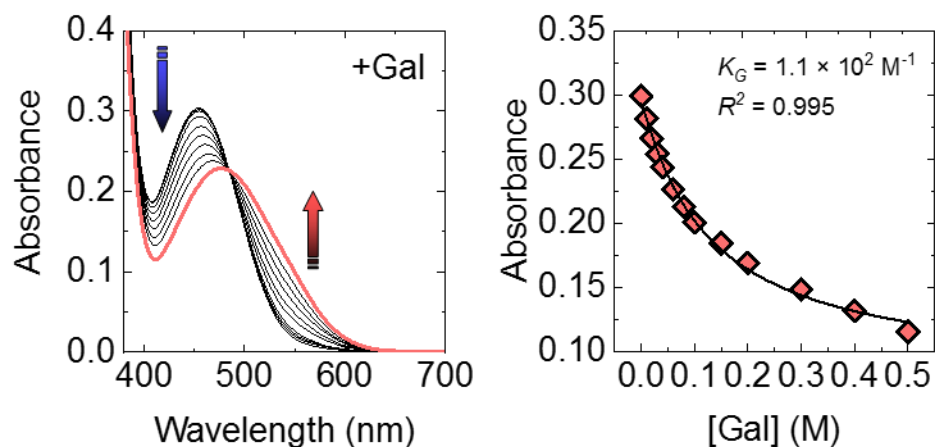
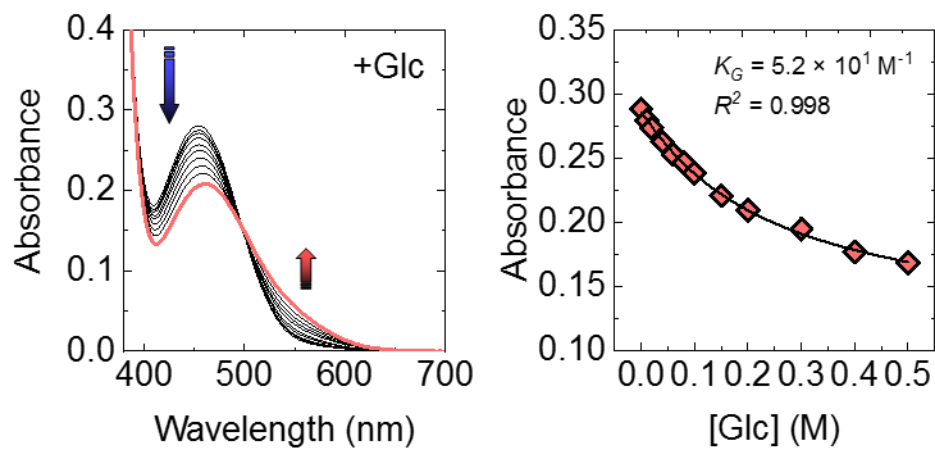*** Correspondence:**
Tsuyoshi Minami
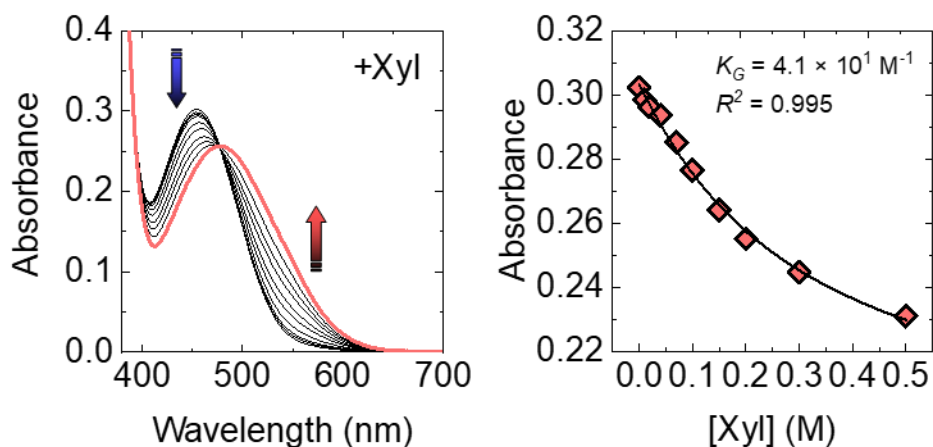tminami@iis.u-tokyo.ac.jp

Contents

1   UV-vis measurements for saccharides

Supplementary Figure 1. UV－vis spectra of the ARS (40 μM)－3-NPBA (6 mM) complex upon the addition of galactose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

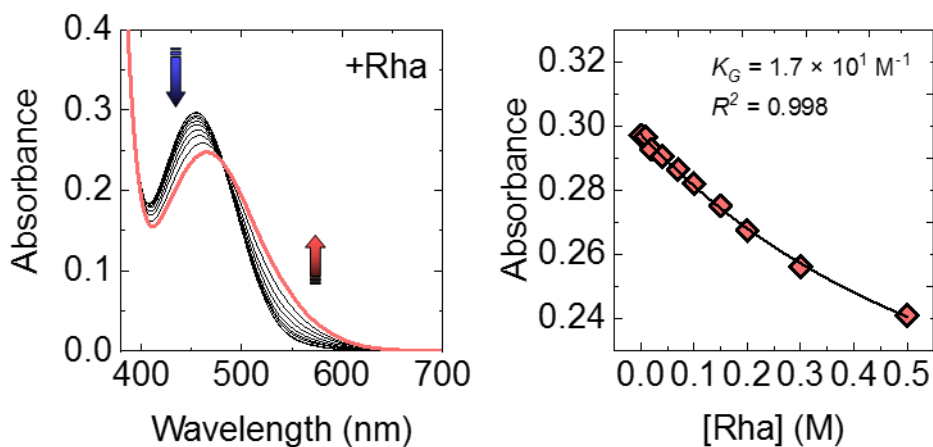**Supplementary Figure 2.** UV－vis spectra of the ARS (40 μM)－3-NPBA (6 mM) complex upon the addition of glucose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

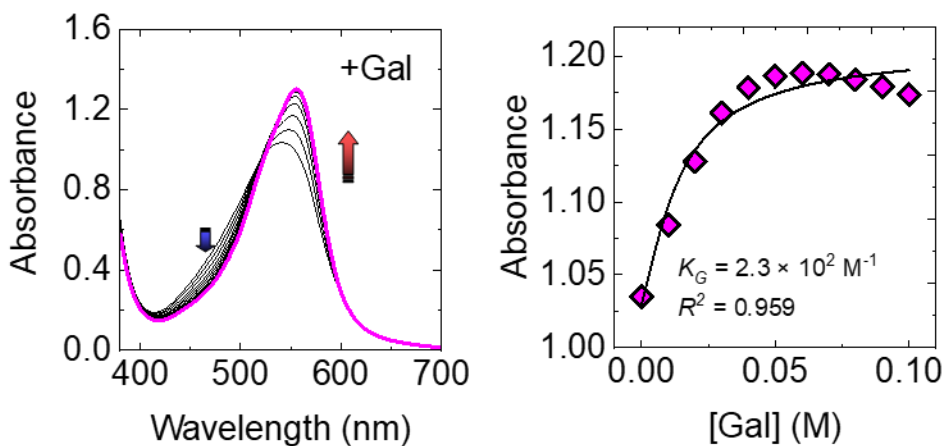**Supplementary Figure 3.** UV－vis spectra of the ARS (40 µM)－3-NPBA (6 mM) complex upon the addition of xylose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

Supplementary Figure 4. UV－vis spectra of the ARS (40 µM)－3-NPBA (6 mM) complex upon the addition of rhamnose in a phosphate buffer solution (100 mM) at at a pH of 7.4 at 25 °C.

Supplementary Figure 5. UV－vis spectra of the BPR (40 µM)－3-NPBA (6 mM) complex upon the addition of galactose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

Supplementary Figure 6. UV－vis spectra of the BPR (40 μM)－3-NPBA (6 mM) complex upon the addition of glucose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.
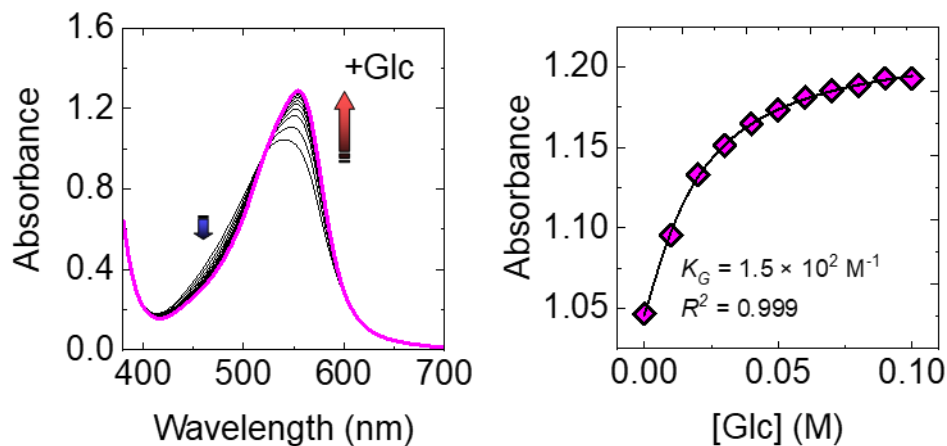

Supplementary Figure 7. UV－vis spectra of the BPR (40 μM)－3-NPBA (6 mM) complex upon the addition of xylose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.
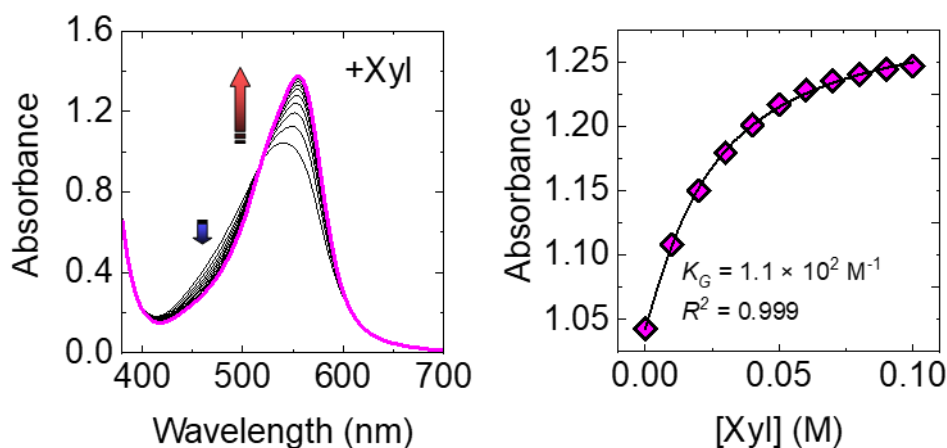

Supplementary Figure 8. UV－vis spectra of the BPR (40 μM)－3-NPBA (6 mM) complex upon the addition of mannose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

Supplementary Figure 9. UV－vis spectra of the BPR (40 μM)－3-NPBA (6 mM) complex upon the addition of rhamnose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.
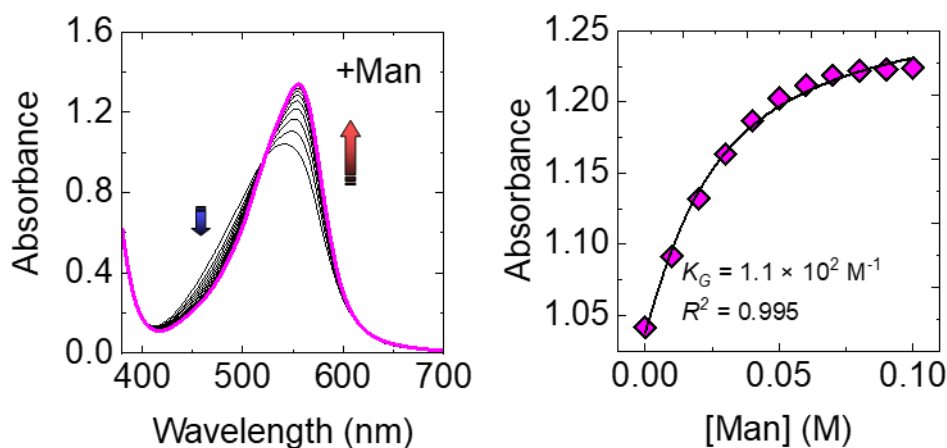

Supplementary Figure 10. UV－vis spectra of the PV (40 μM)－3-NPBA (6 mM) complex upon the addition of galactose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.
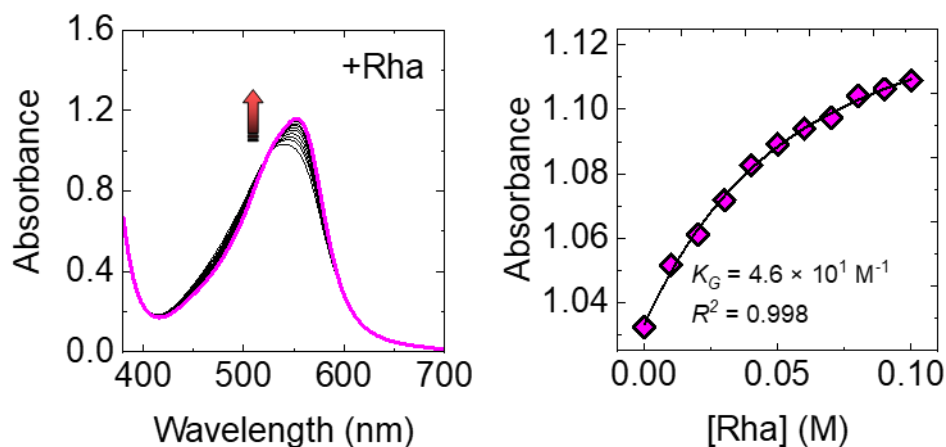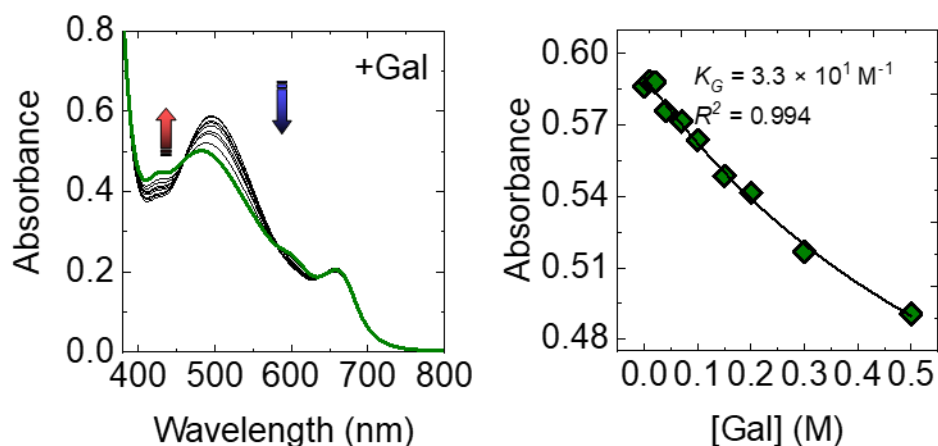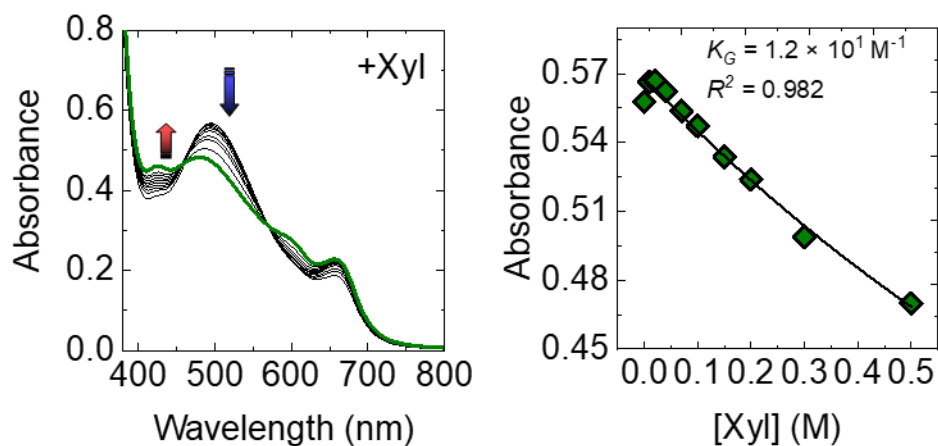

Supplementary Figure 12. UV－vis spectra of the PV (40 μM)－3-NPBA (6 mM) complex upon the addition of xylose in a phosphate buffer solution (100 mM) at a pH of 7.4 at 25 °C.

2 FAB MS Analysis
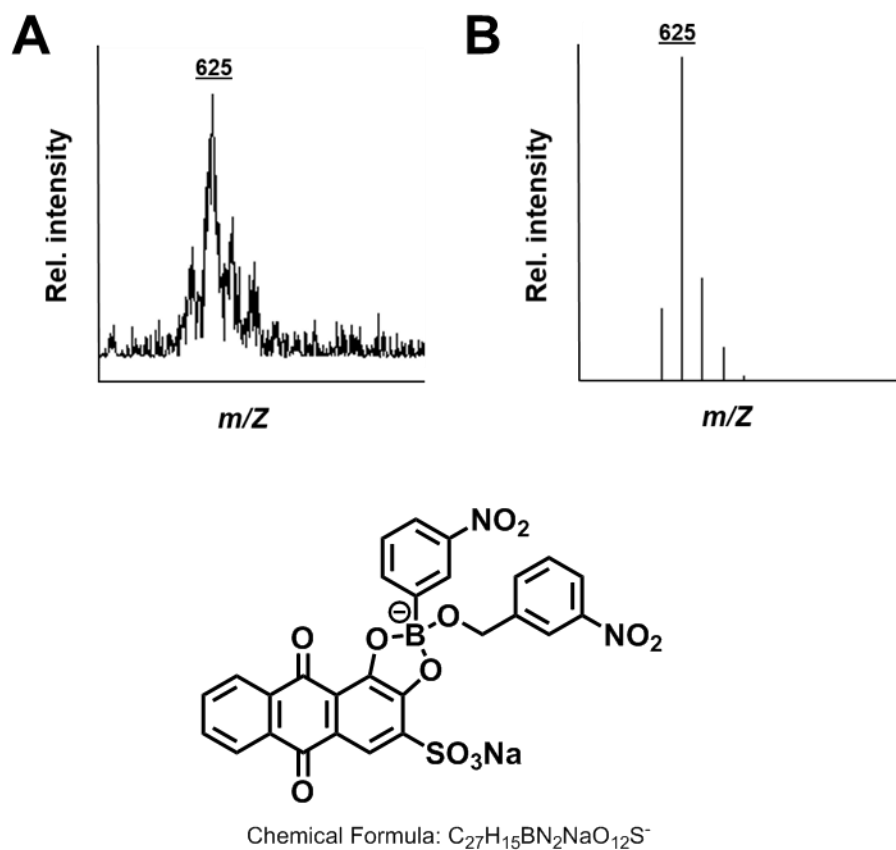

Chemical Formula: $C_{27}H_{15}BN_2NaO_{12}S^-$

Supplementary Figure 13. (A) FAB MS (negative) spectra of the ARS–3-NBPA complex. (B) Calculated isotope pattern for [ARS-2H₂O+3-NPBA+3-NBA-H]⁻. Matrix: 3-nitrobenzylalcohol.

Chemical Formula: $C_{32}H_{20}BN_2O_{13}S^-$
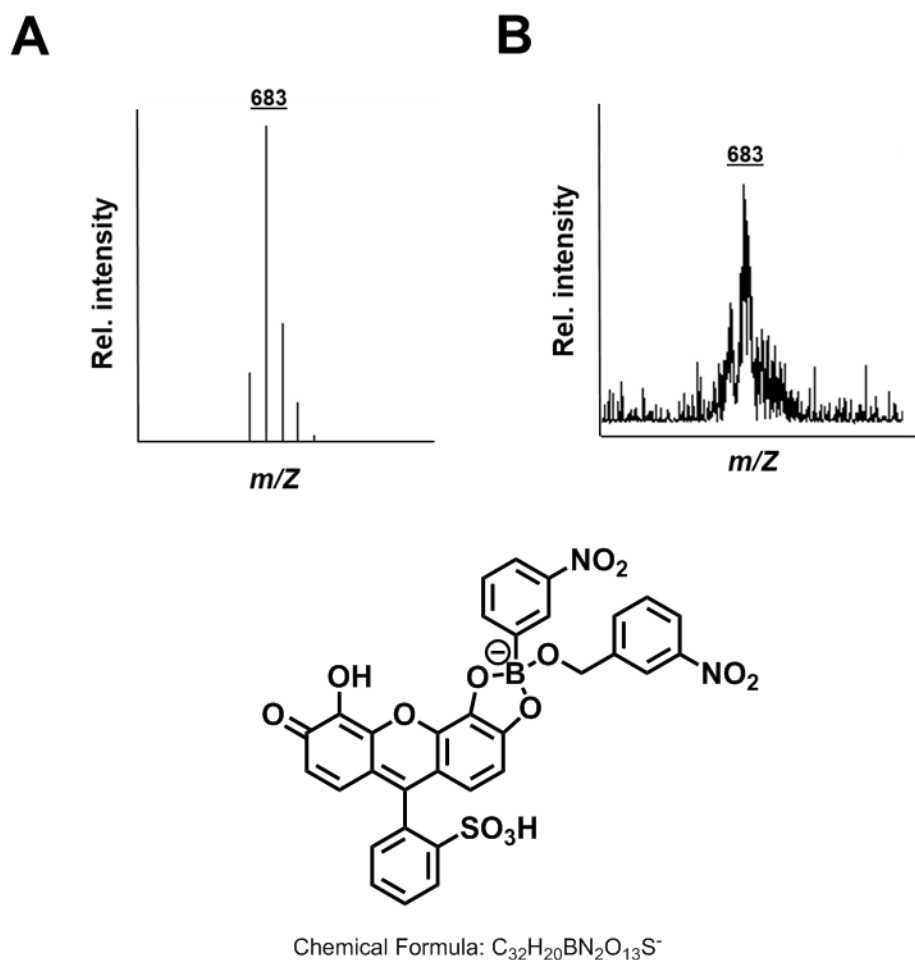
Supplementary Figure 14. (A) FAB MS (negative) spectra of the PR–3-NBPA complex. (B) Calculated isotope pattern for [PR-2H$_2$O+3-NPBA+3-NBA-H]$^-$. Matrix: 3-nitrobenzylalcohol.

3 Analysis-of-Variance (ANOVA)
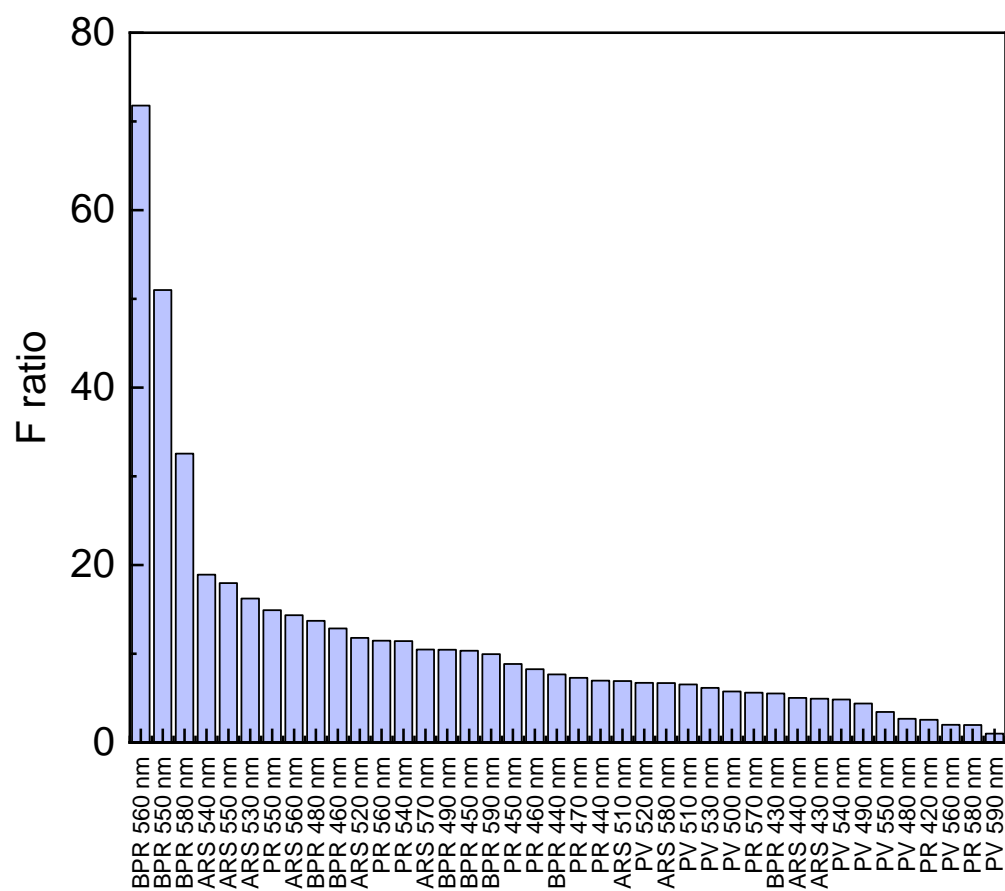
Supplementary Figure 15. One-way ANOVA result of the qualitative analysis.

4   Linear Discriminant Analysis (LDA)
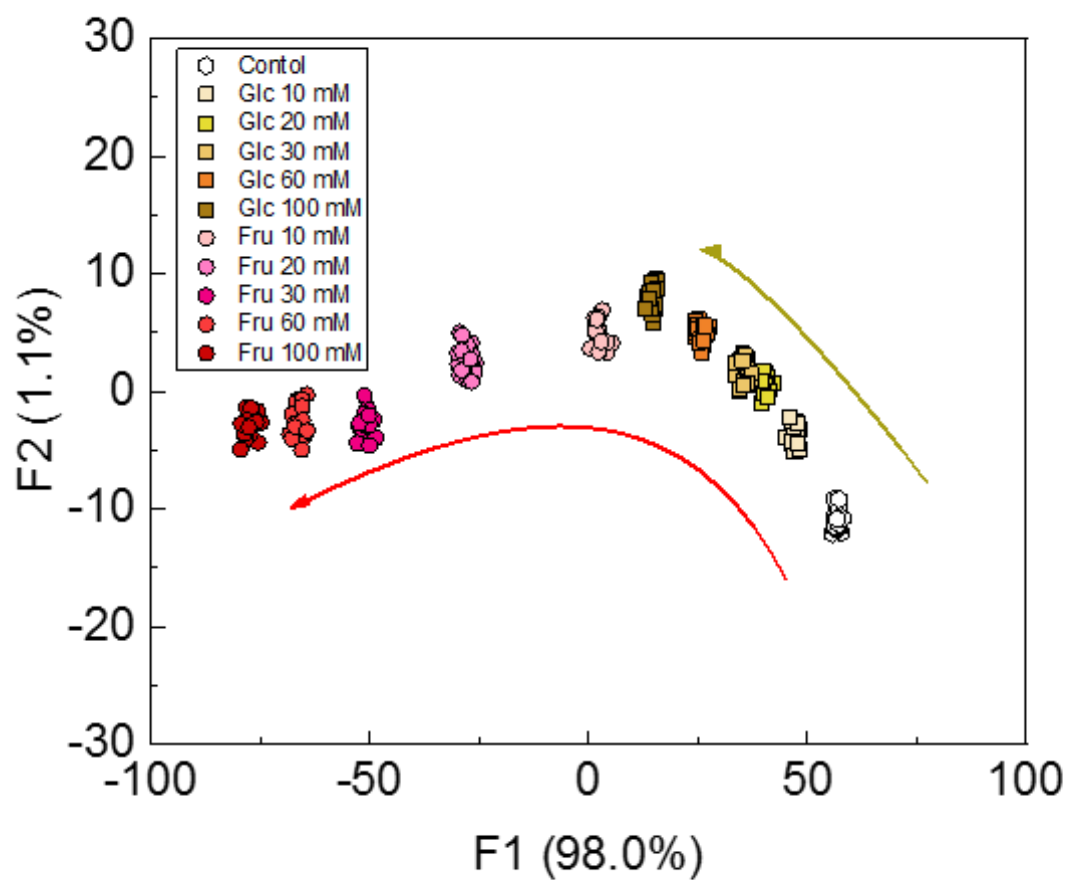
Supplementary Figure 16. LDA plots for the semi-quantitative assay for Fru (○) and Glc (□) at the concentration range of $0-100$ mM. Twenty repetitions were measured for each concentration.

Supplementary Table 1 Jackknifed classification matrix of the qualitative assay for Fru and Glc

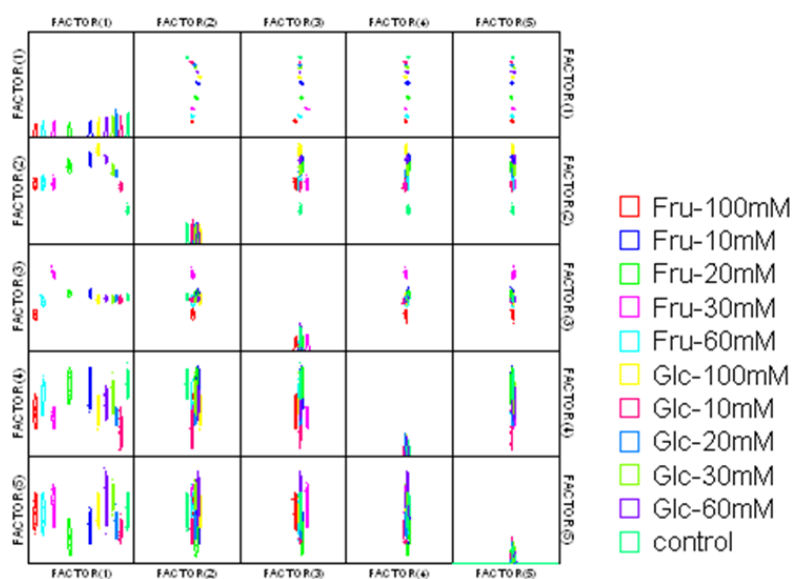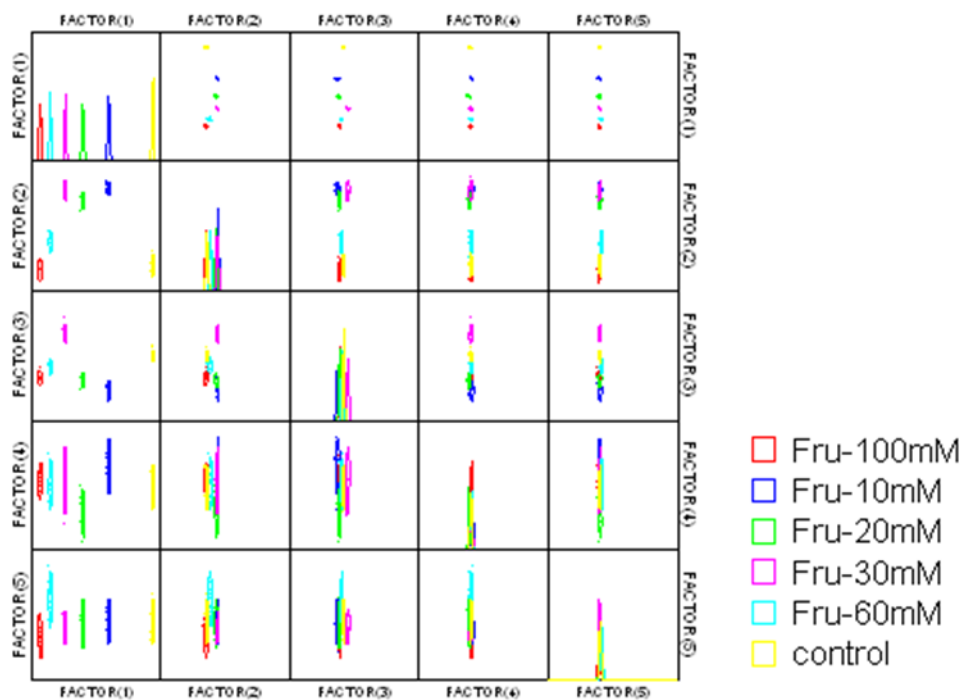| Jackknifed Classification Matrix	Fru-100mM	Fru-10mM	Fru-20mM	Fru-30mM	Fru-60mM	Glc-100mM	Glc-10mM	Glc-20mM	Glc-30mM	Glc-60mM	control	%correct
Fru-100mM	20	0	0	0	0	0	0	0	0	0	0	100
Fru-10mM	0	20	0	0	0	0	0	0	0	0	0	100
Fru-20mM	0	0	20	0	0	0	0	0	0	0	0	100
Fru-30mM	0	0	0	20	0	0	0	0	0	0	0	100
Fru-60mM	0	0	0	0	20	0	0	0	0	0	0	100
Glc-100mM	0	0	0	0	0	20	0	0	0	0	0	100
Glc-10mM	0	0	0	0	0	0	20	0	0	0	0	100
Glc-20mM	0	0	0	0	0	0	0	20	0	0	0	100
Glc-30mM	0	0	0	0	0	0	0	0	20	0	0	100
Glc-60mM	0	0	0	0	0	0	0	0	0	20	0	100
control	0	0	0	0	0	0	0	0	0	0	20	100
Total	20	20	20	20	20	20	20	20	20	20	20	100

Canonical Scores Plot

Supplementary Figure 17. Canonical score plot of the qualitative assay for Fru and Glc.

Supplementary Table 2 Jackknifed classification matrix of the qualitative assay for Fru

| Jackknifed Classification Matrix							
	Fru-100mM	Fru-10mM	Fru-20mM	Fru-30mM	Fru-60mM	control	%correct
Fru-100mM	20	0	0	0	0	0	100
Fru-10mM	0	20	0	0	0	0	100
Fru-20mM	0	0	20	0	0	0	100
Fru-30mM	0	0	0	20	0	0	100
Fru-60mM	0	0	0	0	20	0	100
control	0	0	0	0	0	20	100
Total	20	20	20	20	20	20	100

Supplementary Figure 18. Canonical score plot of the qualitative assay for Fru.

Supplementary Table 3 Jackknifed classification matrix of the qualitative assay for Glc

Jackknifed Classification Matrix							
	Glc-100mM	Glc-10mM	Glc-20mM	Glc-30mM	Glc-60mM	control	%correct
Glc-100mM	20	0	0	0	0	0	100
Glc-10mM	0	20	0	0	0	0	100
Glc-20mM	0	0	20	0	0	0	100
Glc-30mM	0	0	0	20	0	0	100
Glc-60mM	0	0	0	0	20	0	100
control	0	0	0	0	0	20	100
Total	20	20	20	20	20	20	100

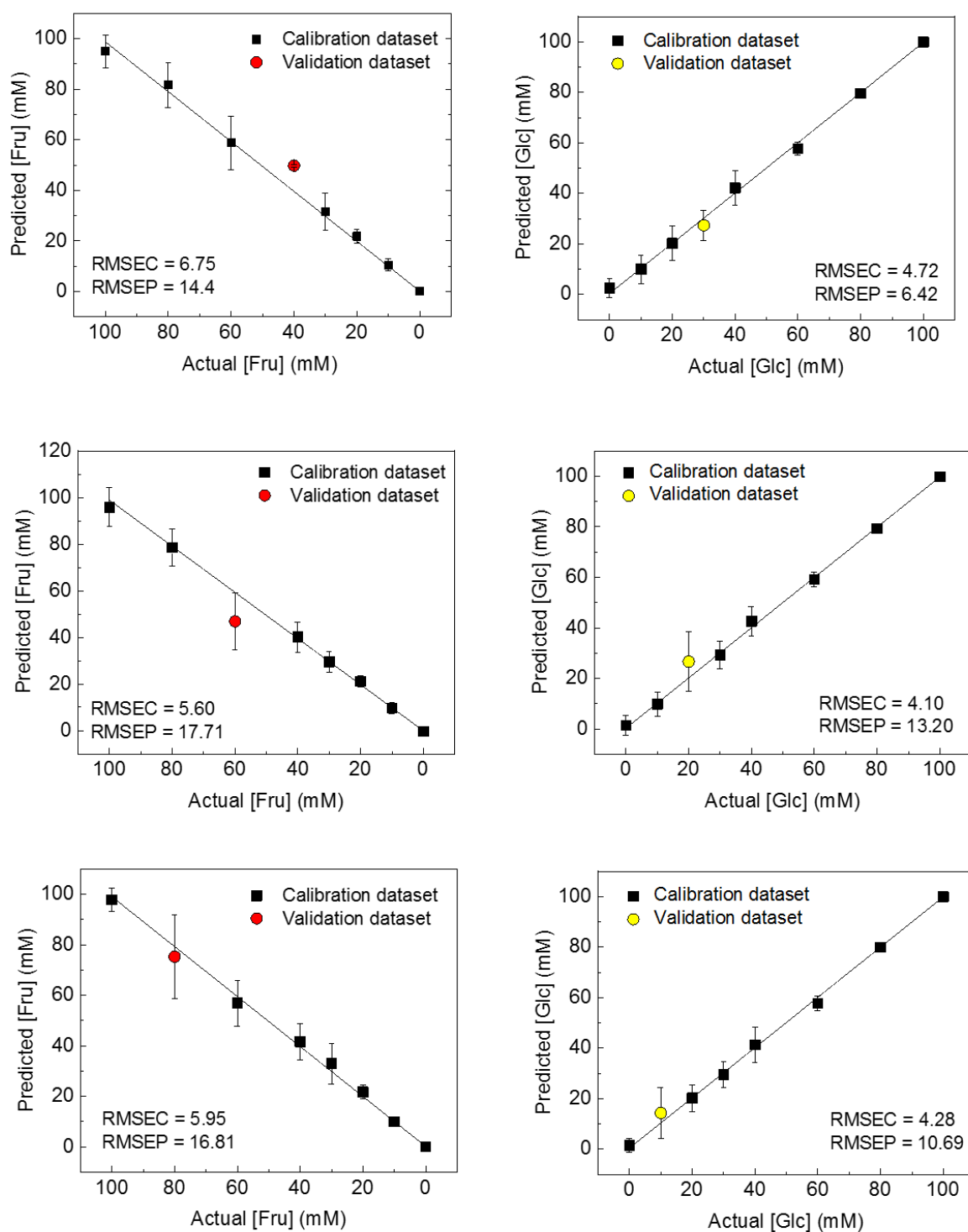**Supplementary Figure 19**. Canonical score plot of the qualitative assay for Glc.

5   Results of Quantitative Analysis
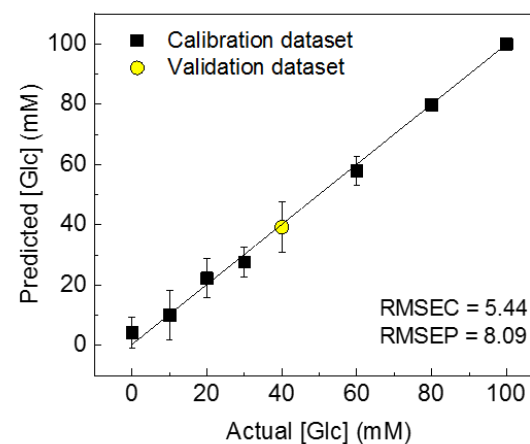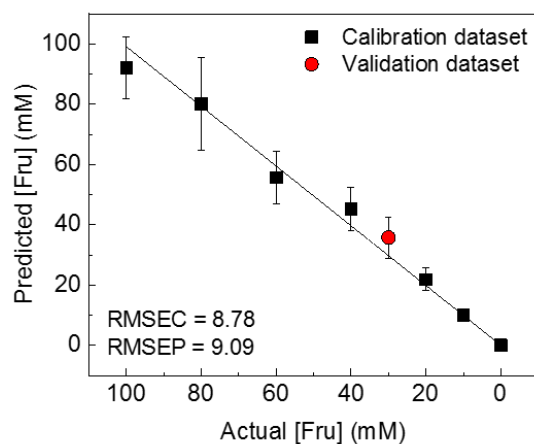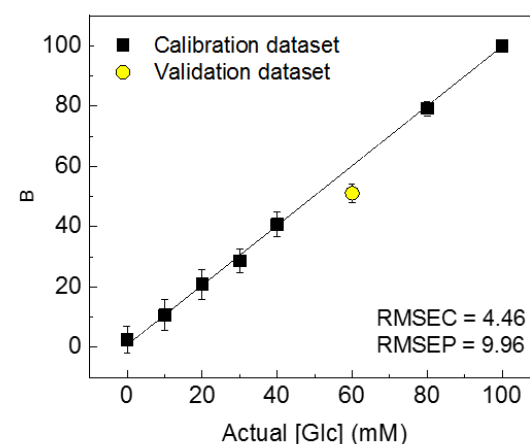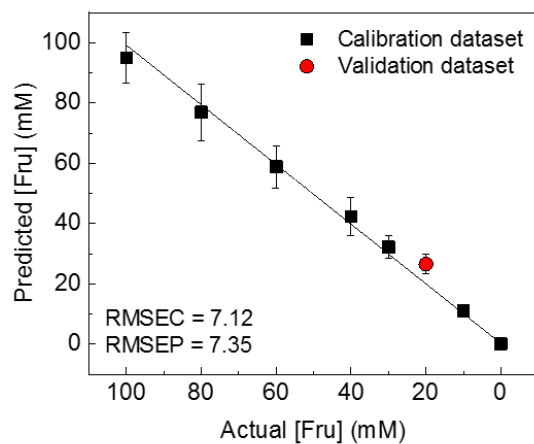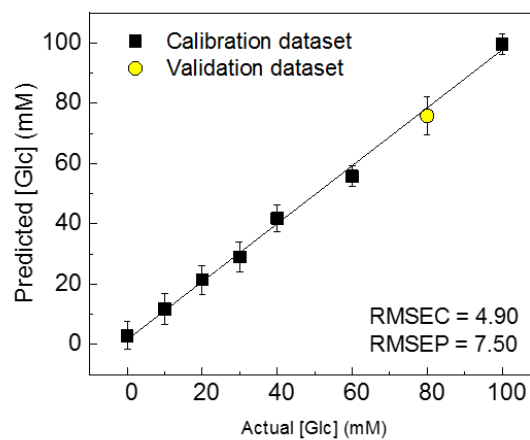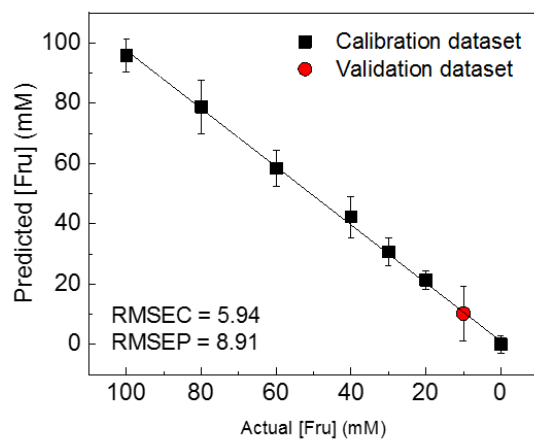
Supplementary Figure 20 SVM regression results used for quantitative analyses of Fru and Glc mixtures. The values of the root-mean-square errors of calibration (RMSEC) and prediction (RMSEP) (shown as insets) attest to the high accuracies of the model and its predictive capacity.