Supplementary Information

Monitoring the effects of salt background, alkalinity and temperature on MS2 bacteriophage behaviour *via* solvatochromism, metachromasia and chemical kinetics

Anna Laguta[1,2]

[1] University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic
[2] V. N. Karazin Kharkiv National University, Svoboda Square 4, 61022 Kharkiv, Ukraine
*laguta@karazin.ua

Table S1. Some characterization of the 129 residues protein of the MS2 capsid

Residues	Number per protein [1]	Character at pH = 7–9 [2]	Hydropathy index [3]
V Valine	14	Aliphatic, Nonpolar, Neutral	4.2
A Alanine	14	Aliphatic, Nonpolar, Neutral	1.8
S Serine	13	Hydroxylic, Polar, Neutral	–0.8
N Asparagine	10	Amide, Polar, Neutral	–3.5
G Glycine	9	Aliphatic, Nonpolar, Neutral	–0.4
T Threonine	9	Hydroxylic, Polar, Neutral	–0.7
I Isoleucine	8	Aliphatic, Nonpolar, Neutral	4.5
L Leucine	7	Aliphatic, Nonpolar, Neutral	3.8
K Lysine	6	Cation, Brønsted acid, Positive	–3.9
P Proline	6	Cyclic, Nonpolar, Neutral	–1.6
Q Glutamine	6	Amide, Polar, Neutral	–3.5
E Glutamate	5	Anion Brønsted base, Negative	–3.5
R Arginine	4	Fixed cation, Basic polar, Positive	–4.5
D Aspartate	4	Anion, Brønsted base, Negative	–3.5
F Phenylalanine	4	Aromatic, Nonpolar, Neutral	2.8
Y Tyrosine	4	Aromatic, Brønsted acid	–1.3
C Cysteine	2	Thiol, Brønsted acid	2.5
M Methionine	2	Thioether, Nonpolar, Neutral	1.9
W Tryptophan	2	Aromatic, Nonpolar, Neutral	−0.9

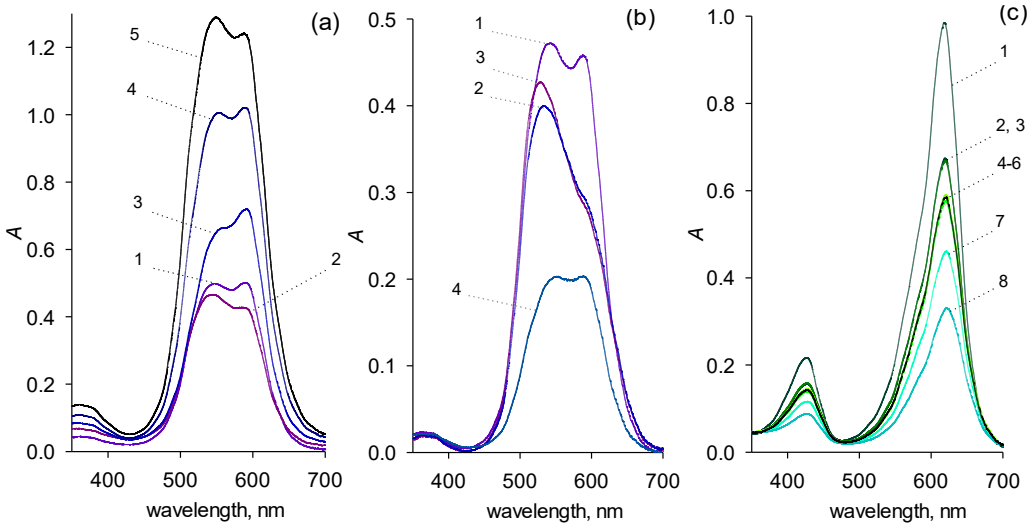

Fig. S1. Absorption spectra of CV (a and b) and MG (c) in a solution of 4×10^{15} PFU/mL MS2 at 25 °C and:

(a) l = 1 cm; c_{CV} = 1×10^{-5} mol/L and without added alkali (1); c_{CV} = 1×10^{-5} mol/L and c_{NaOH} = 2 mM (2); c_{CV} = 2×10^{-5} mol/L and c_{NaOH} = 2 mM (3); c_{CV} = 3×10^{-5} mol/L and c_{NaOH} = 2 mmol/L (4); c_{CV} = 4×10^{-5} mol/L and c_{NaOH} = 2 mmol/L (5);

(b) c_{CV} = 1×10^{-4} mol/L; l = 0.1 cm; without added alkali (1); c_{NaOH} = 2 mmol/L (2); c_{NaOH} = 4 mmol/L (3); c_{NaOH} = 7.5 mmol/L (4);

(c) l = 1 cm; without added alkali (1); c_{NaOH} = 0.6 mmol/L (2); c_{NaOH} = 0.9 mM (3); c_{NaOH} = 1.3 mmol/L (4); c_{NaOH} = 1.8 mmol/L (5); c_{NaOH} = 2.7 mmol/L (6); c_{NaOH} = 3.5 mM (7); c_{NaOH} = 4.4 mmol/L (8). The decrease in absorption is associated with alkaline fading.

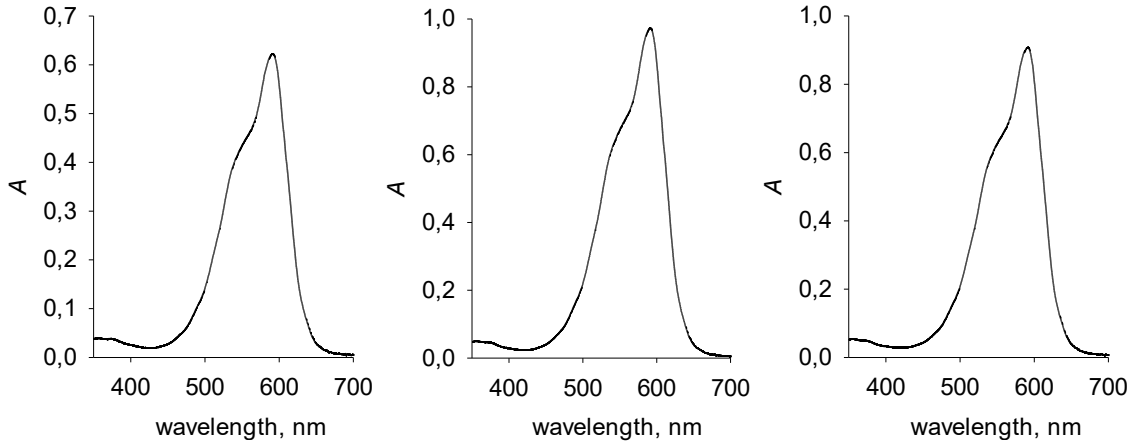

Fig. S2. Absorption spectra of CV^+ in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mM; 10 mmol/L; and 50 mmol/L $CaCl_2$; without added alkali.

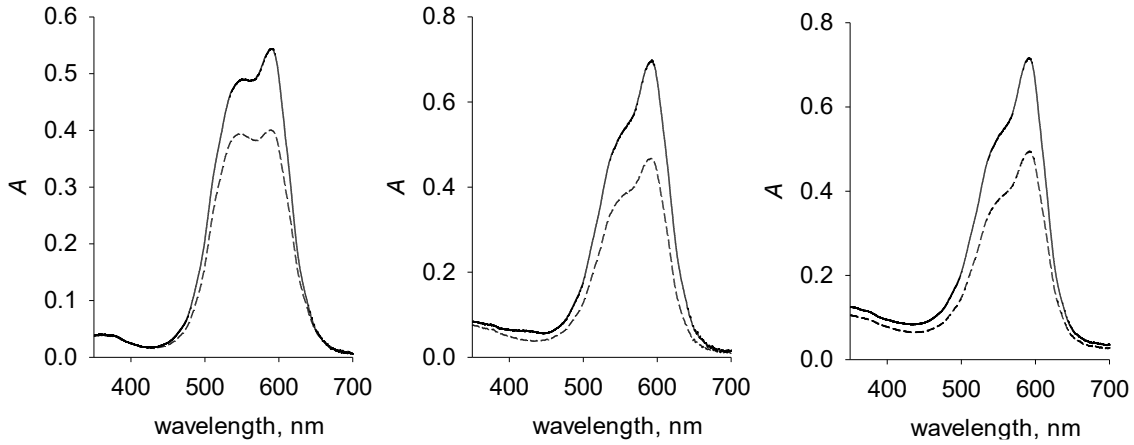

Fig. S3. Absorption spectra of CV^+ in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L RbCl; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

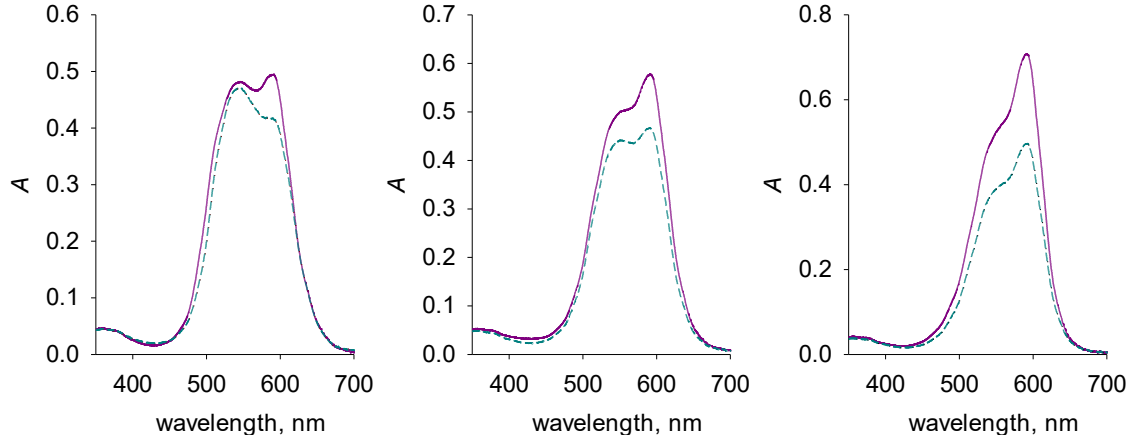

Fig. S4. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L KCl; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

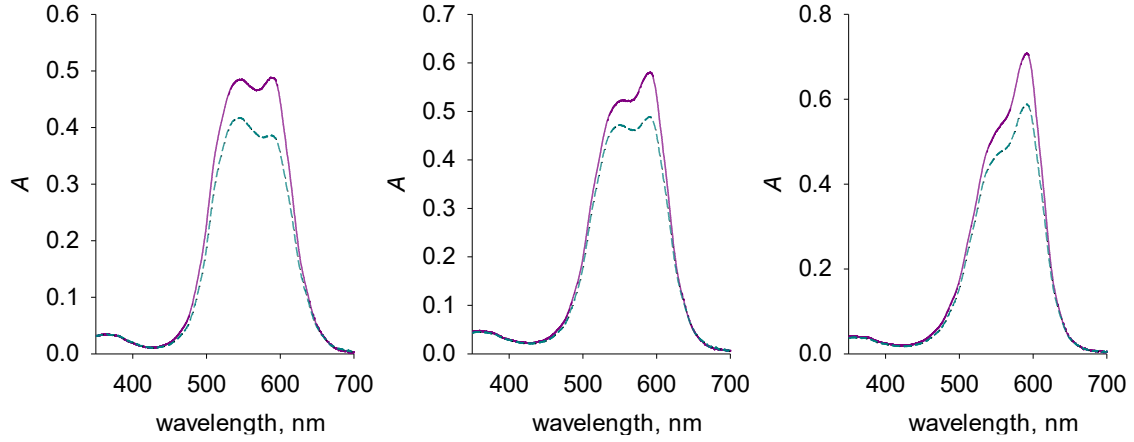

Fig. S5. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaCl; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

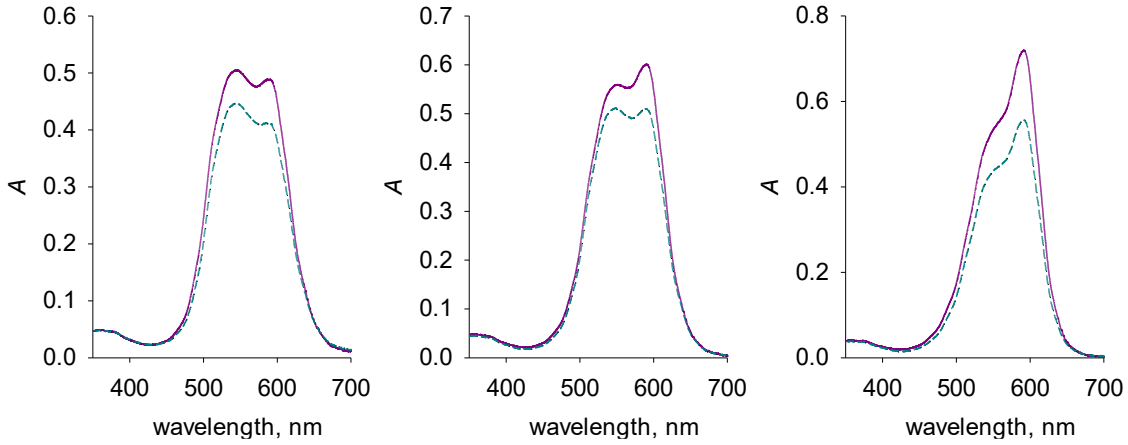

Fig. S6. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaI; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

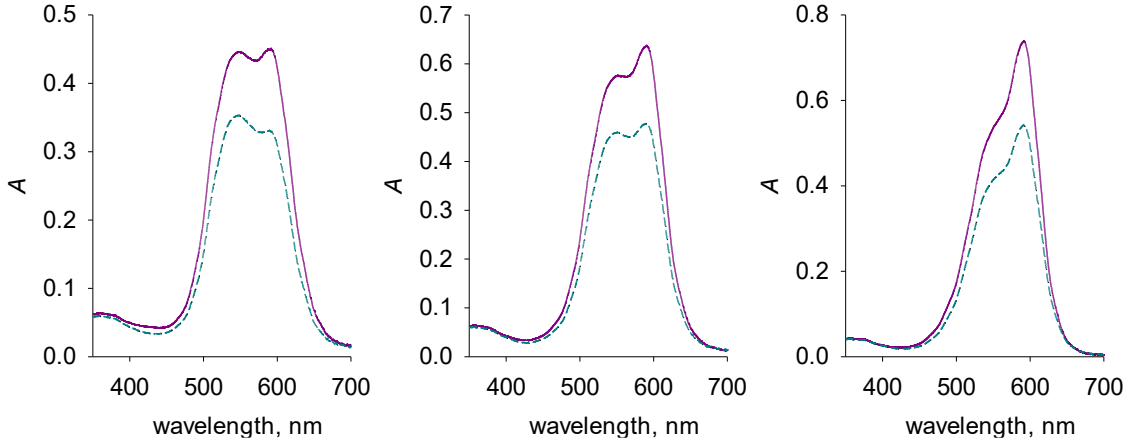

Fig. S7. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L RbCl; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

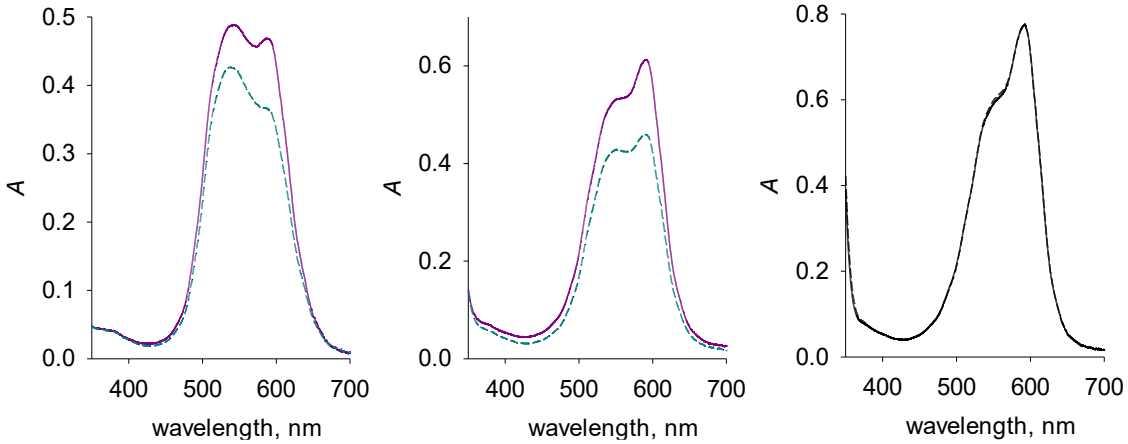

Fig. S8. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaSal; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

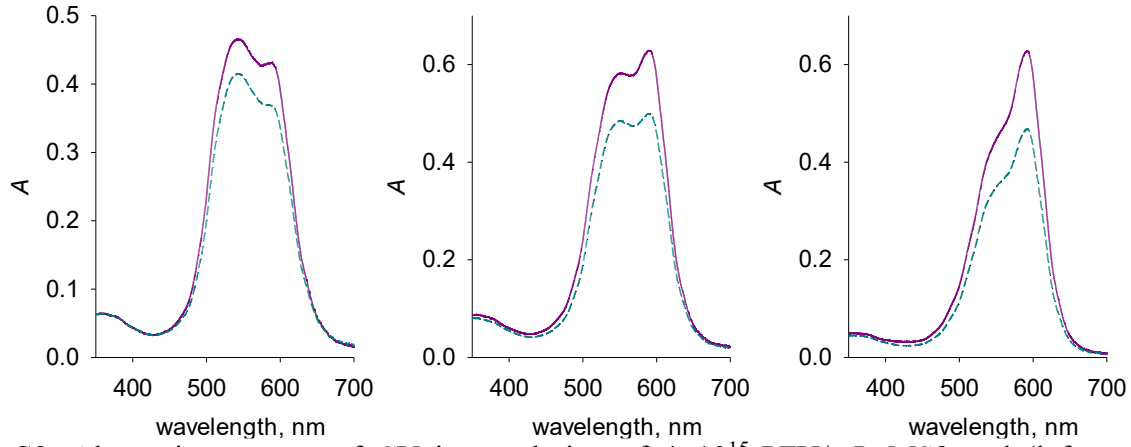

Fig. S9. Absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaBut; solid line: without added alkali; dashed line: at c_{NaOH} = 1 mmol/L.

Table S2. Absorption maxima of MG in solutions of 4×10^{15} PFU/mL MS2 and salts without added alkali and at c_{NaOH} = 0.2 mmol/L. The shape of the spectrum does not change. Cation of MG has λ_{max} at 614 nm in water [4] and 619 nm in salt-free MS2 system.

Salts	without alkali	with alkali	Salts	without alkali	with alkali
	λ_{max}, nm			λ_{max}, nm	
0.001 mol/L $CaCl_2$	617	–	0.0005 mol/L $NaNO_3$	619	619
0.01 mol/L $CaCl_2$	617	–	0.001 mol/L $NaNO_3$	619	619
0.05 mol/L $CaCl_2$	618	618	0.01 mol/L $NaNO_3$	618	619
0.001 mol/L RbCl	617	617	0.05 mol/L $NaNO_3$	618	619
0.01 mol/L RbCl	617	618	0.1 mol/L $NaNO_3$	619	618
0.05 mol/L RbCl	619	618	0.001 mol/L NaAc	619	617
0.001 mol/L KCl	621	621	0.01 mol/L NaAc	618	618
0.01 mol/L KCl	617	618	0.05 mol/L NaAc	618	618
0.05 mol/L KCl	620	619	0.001 mol/L NaSal	618	618
0.001 mol/L NaCl	620	620	0.01 mol/L NaSal	618	618
0.01 mol/L NaCl	620	619	0.05 mol/L NaSal	617	618
0.05 mol/L NaCl	618	618	0.001 mol/L NaBut	618	618
0.1 mol/L NaCl	616	616	0.01 mol/L NaBut	618	617
0.001 mol/L NaI	620	620	0.05 mol/L NaBut	616	617
0.01 mol/L NaI	619	619	0.001 mol/L NaGly	618	617
0.05 mol/L NaI	618	618	0.01 mol/L NaGly	618	618
–	–	–	0.05 mol/L NaGly	618	618

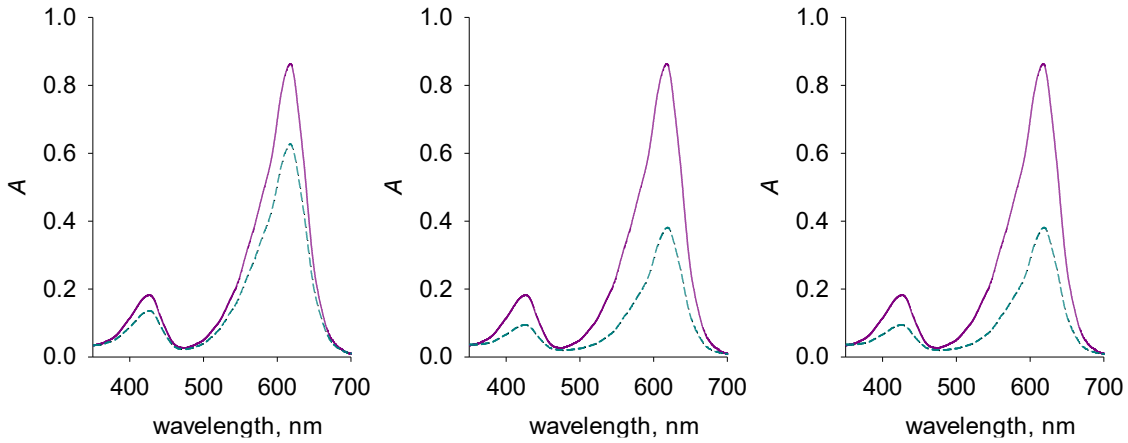

Fig. S10. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L RbCl; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

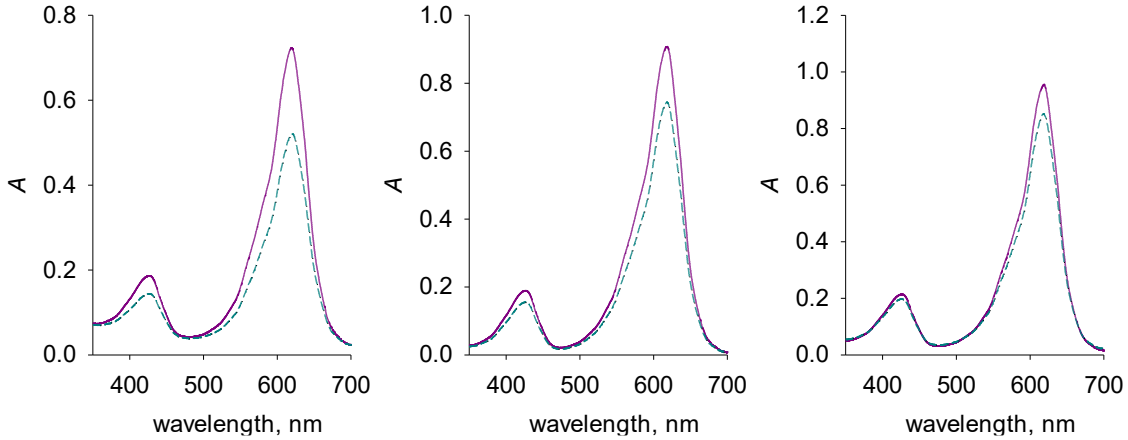

Fig. S11. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L KCl; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

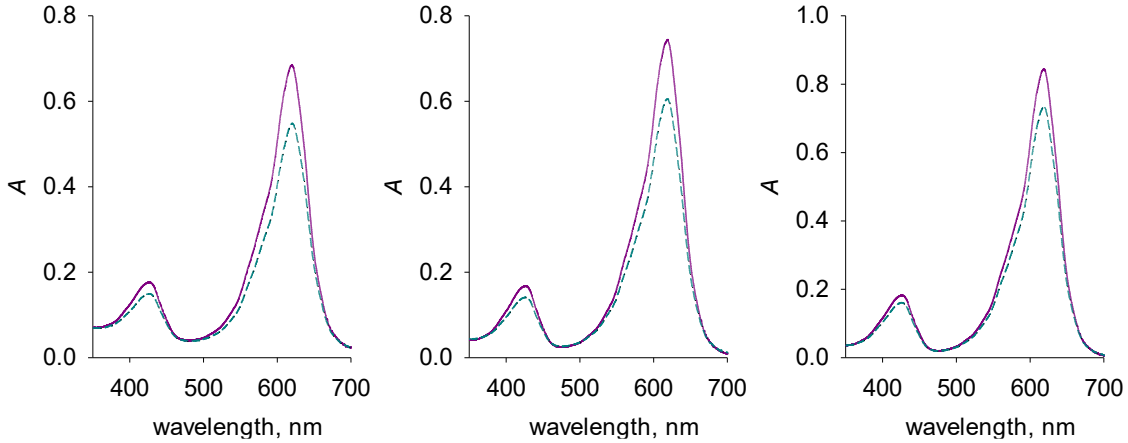

Fig. S12. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaCl; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

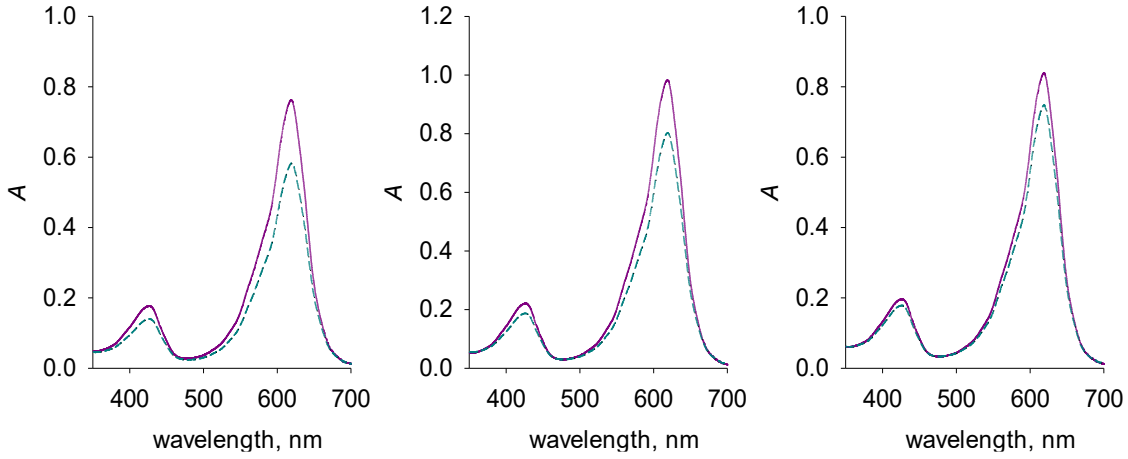

Fig. S13. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L $NaNO_3$; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

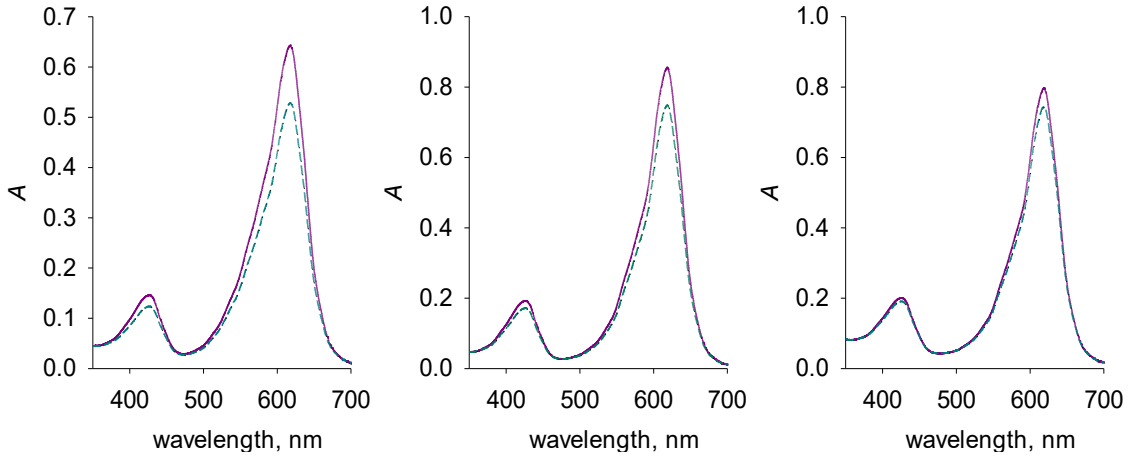

Fig. S14. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaAc; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

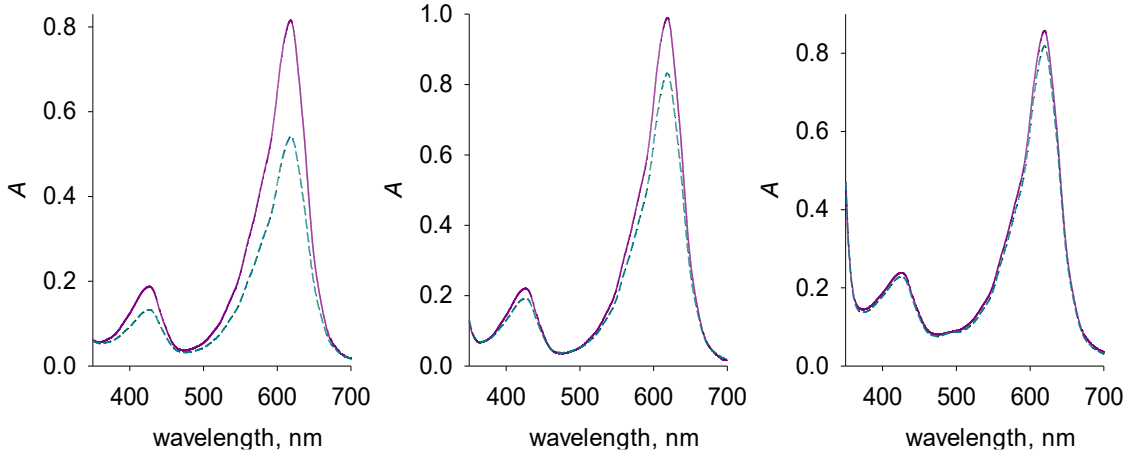

Fig. S15. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaSal; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

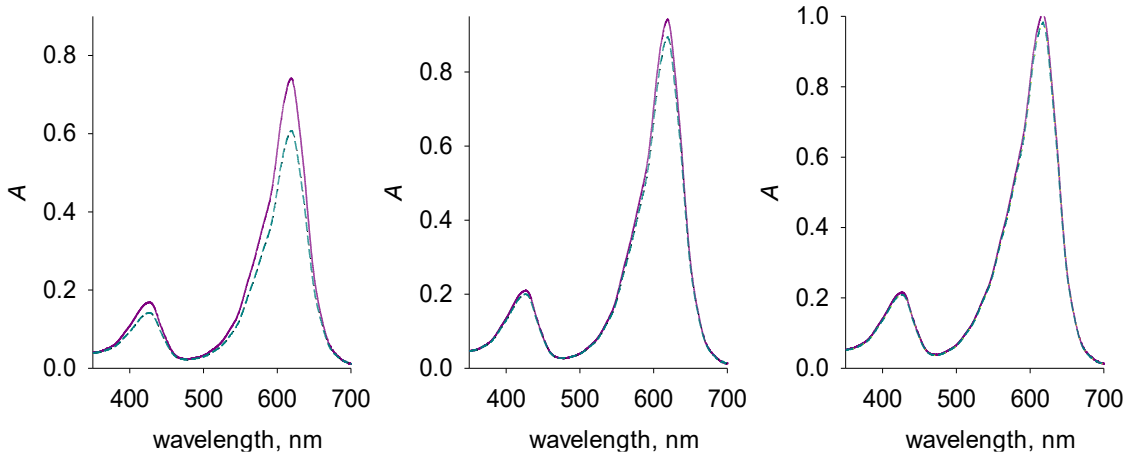

Fig. S16. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaBut; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

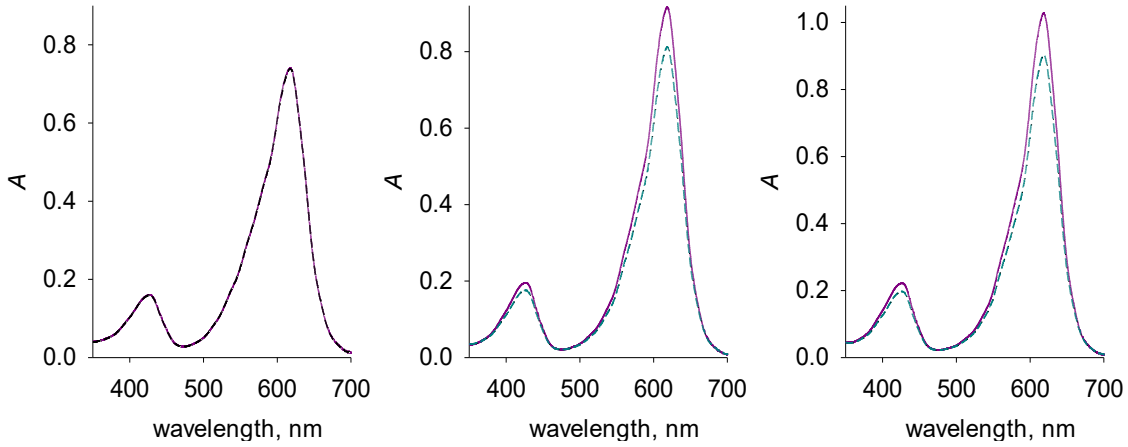

Fig. S17. Absorption spectra of MG in a solution of 4×10^{15} PFU/mL MS2 and (left-to-right) 1 mmol/L; 10 mmol/L; and 50 mmol/L NaGly; solid line: without added alkali; dashed line: at c_{NaOH} = 0.2 mmol/L.

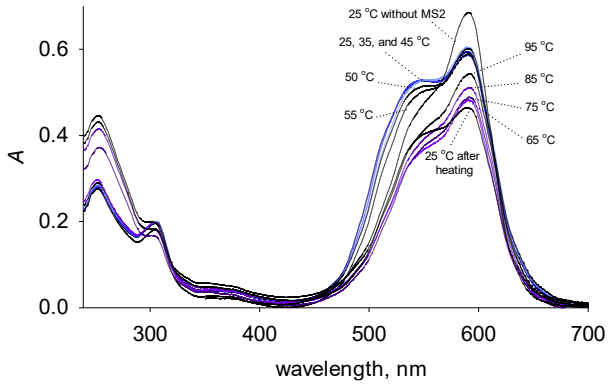

Fig. S18. Temperature influence on absorption spectra of CV in a solution of 4×10^{15} PFU/mL MS2 at 0.01 mol/L NaCl.

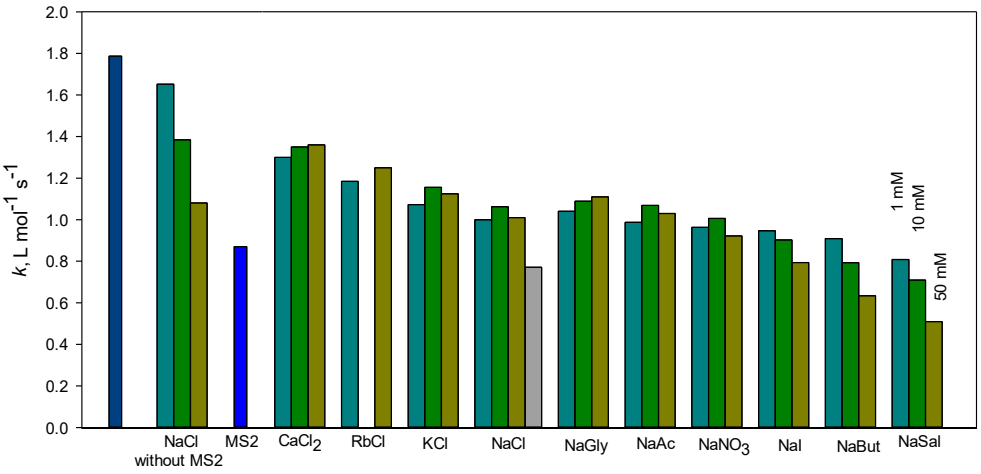

Fig. S19. Rate constant values of $MG^+ + HO^-$ reaction in 1, 10, 50, and 100 mmol/L salts solutions of 4×10^{15} PFU/mL MS2 at 25 °C and c_{NaOH} = 0.2 mmol/L as well as without MS2 for comparison.

References

(1) Ni, C. Z.; White, C. A.; Mitchell, R. S.; Wickersham, J.; Kodandapani, R.; Peabody, D. S.; Ely, K. R. Crystal structure of the coat protein from the GA bacteriophage: model of the unassembled dimer. *Protein science* **1996**, *5* (12), 2485–2493.
(2) Cooper, G. M.; Hausman, R. E. *The cell: a molecular approach*; Artmed Editora, 2016.
(3) Kyte, J.; Doolittle, R. F. A simple method for displaying the hydropathic character of a protein. *Journal of molecular biology* **1982**, *157* (1), 105–132.
(4) Sabnis, R. W. *Handbook of biological dyes and stains: synthesis and industrial applications*; John Wiley & Sons, 2010.