

Supplementary Information

Potentiometric detection of biogenic amines utilizing affinity on a 4-mercaptobenzoic acid monolayer

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General

All reagents and solvents were used without purifications. Methanol (CAS: 67-56-1), hydrochloric acid (CAS: 7647-01-0), sodium hydroxide (CAS: 1310-73-2), and sodium chloride (CAS: 7647-14-5) were purchased from FUJIFILM Wako Pure Chemical Corp. A glass substrate (model: Eagle XG) was purchased from Corning, Inc. Histamine dihydrochloride (CAS: 56-92-8), L-histidine hydrochloride monohydrate (CAS: 5934-29-2), 1,5-diaminopentane dihydrochloride (cadaverine) (CAS: 1476-39-7), L-lysine dihydrochloride (CAS: 657-26-1), and 4-mercaptobenzoic acid (BA) (CAS: 1074-36-8) were purchased from Tokyo Chemical Industry Co., Ltd. 2-Morpholinoethanesulfonic acid monohydrate (MES) (CAS: 145224-94-8) was purchased from Dojindo Laboratories. The analyte solutions were prepared using Milli-Q water (18 M Ω cm at 25 °C).

Gold (Au) metal electrodes were prepared by using a multi-source resistance-heating evaporation system (model: KIS3) from Biemtron Co., Ltd. UV ozone treatment was performed on an UV/ozone processing unit (model: SSP16-110) from SEN LIGHTS Corp. The pH values of solution were measured by a pH meter (model: HM-30G) from DKK-TOA Corp. Potentiometric measurements were carried out using a potentiostat equipment (model: 1200C) from ALS Co., Ltd. The Ag/AgCl electrode (model: RE-1B) as the reference electrode was purchased from BAS, Inc. X-ray photoelectron spectroscopy (XPS) measurements were performed using an AXIS Nova surface analysis spectrometer with AlK α radiation from KRATOS Analytical Ltd. Contact angle goniometry (CAG) measurements were carried out using a droplet contact angle meter (model: DMO-501) from Kyowa Interface Science Co., Ltd.

Estimation of the limit of detection (LOD) and the limit of quantitation (LOQ)

For the determination of the limit of detection (LOD) and the limit of quantitation (LOQ) to histamine (Fig. 3), the intersection of the minimum signal ($=Y$) and the regression line obtained from the value of V in the dynamic range of the titration curve allowed us to estimate the values of the LOD and the LOQ. The value of Y is estimated by the following Equation (1):

$$Y = V + k\sigma \quad (1)$$

V and σ are the average value and the standard deviation of the electrode potential in the absence of histamine, respectively. LOD: $k = 3$, LOQ: $k = 10$.

Potentiometric titrations under different pH conditions

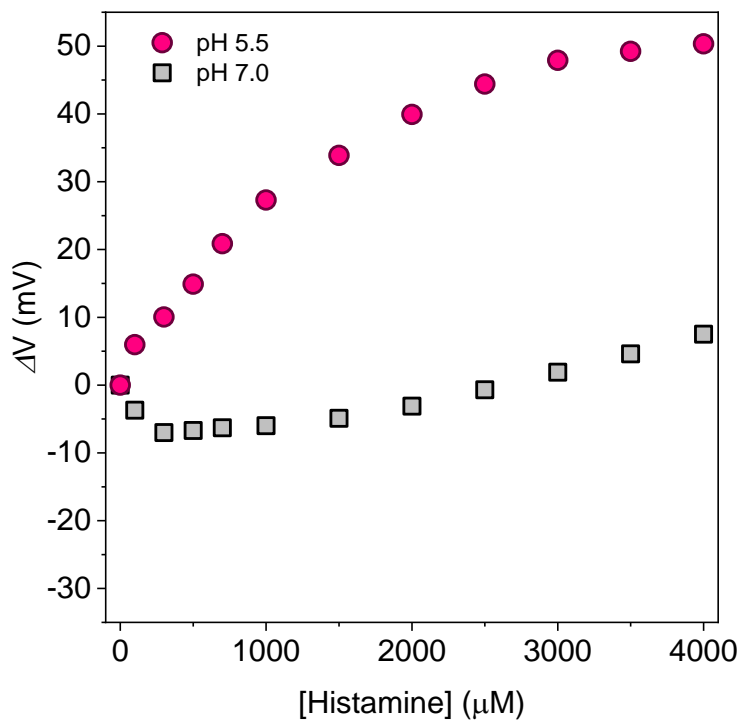


Fig. S1 Potentiometric responses of the BA-SAM modified electrode upon addition of histamine in a MES buffer solution (100 mM) with NaCl (100 mM) with pH 5.5 or pH 7.0, at 27°C.

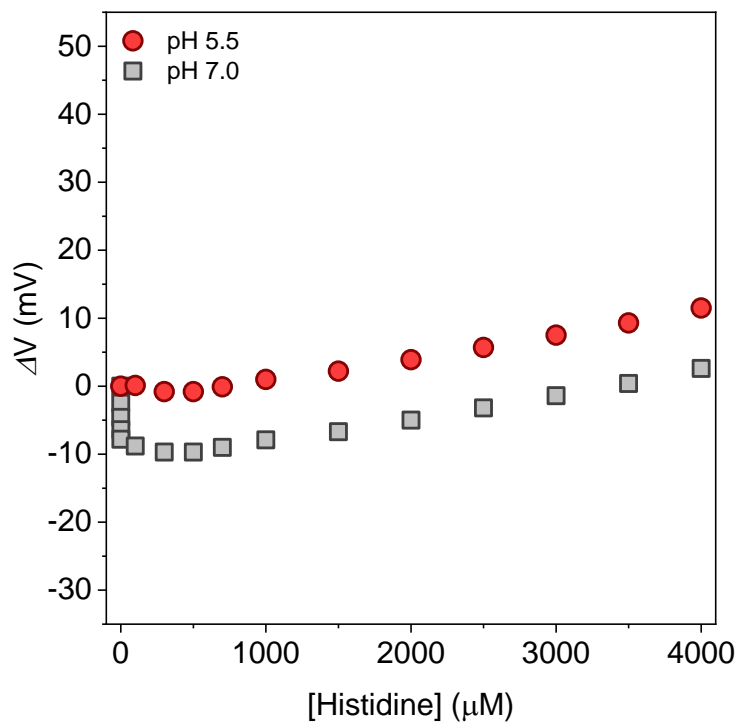


Fig. S2 Potentiometric responses of the BA-SAM modified electrode upon addition of histidine in a MES buffer solution (100 mM) with NaCl (100 mM) with pH 5.5 or pH 7.0, at 27°C.

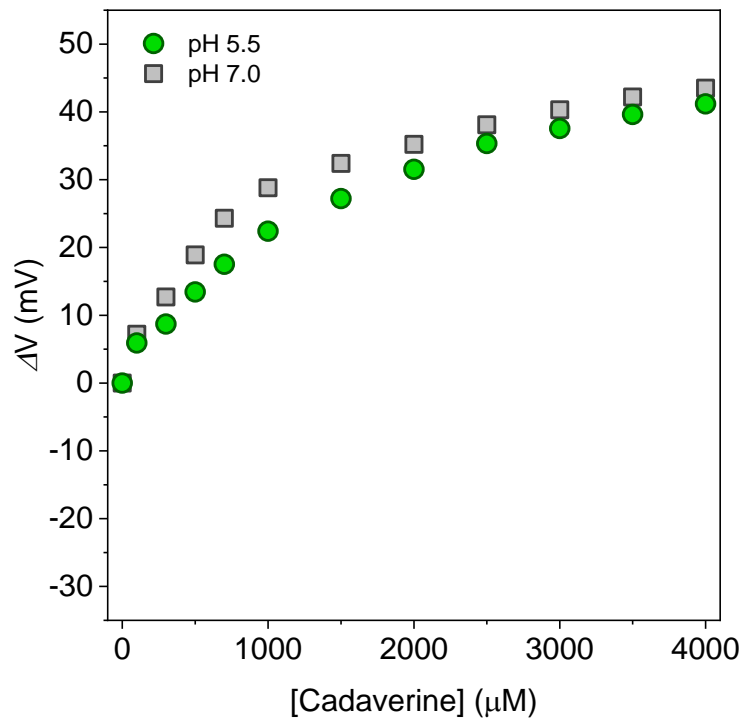


Fig. S3 Potentiometric responses of the BA-SAM modified electrode upon addition of cadaverine in a MES buffer solution (100 mM) with NaCl (100 mM) with pH 5.5 or pH 7.0, at 27°C.

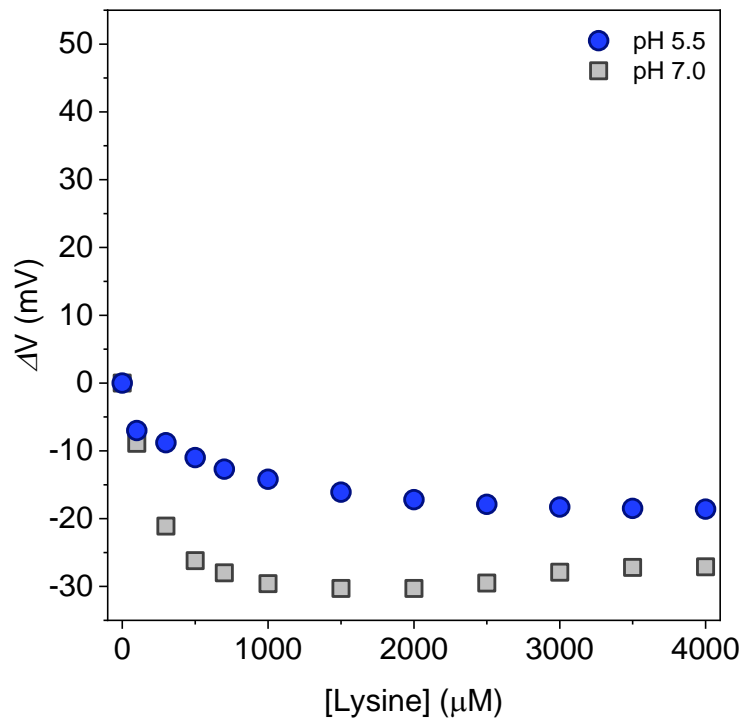


Fig. S4 Potentiometric responses of the BA-SAM modified electrode upon addition of lysine in a MES buffer solution (100 mM) with NaCl (100 mM) with pH 5.5 or pH 7.0, at 27°C.

Reference

- 1 J. N. Miller and J. C. Miller, *Statistics and Chemometrics for Analytical Chemistry*, Pearson, Harlow, UK, 6th edn, 2010.