Multi-Component Metabolite Electrochemical Detection and Analysis Based on Machine Learning

Jianing Shen[a], Bo Zhang[a], Tianhao Xue[a], Yao Zhang[a], Guixian Zhu[a*]

a School of Instrument Science and Optoelectronic Engineering, Beijing Information Science and Technology University, Beijing, 100192, China

To characterize the apparent electron transfer rate constant (ks) of the electrode, 100 μl of 50 mM potassium ferricyanide solution was dropped onto the working area of the bare electrode and the cyclic voltammetry curves were tested under different scan rate conditions.

When $n \cdot \triangle Ep \geq 200$mV, we use the Nicholson method to estimate the apparent electron transfer rate constant ks of the system, and the formula is as follows:

$$\Psi = ks[\pi DnvF/(RT)]^{\frac{-1}{2}}$$

$$\Psi = 2.18[\beta/\pi]^{\frac{1}{2}} exp\left[-(\beta^2 F/RT)n\Delta E_p\right]$$

Ψ is the kinetic parameter, D is the diffusion coefficient, n is the number of electrons transferred in the reaction (n=1), F is Faraday's constant (F=96485C/mol), v is the scan rate, R is the gas constant (R=8.314), and T is the Kelvin temperature (T=293K). Figure S3 shows the linear relationship between the logarithm of the scan rate and the peak potential, and Figure S4 shows the asymptote of Ks using Ψ.

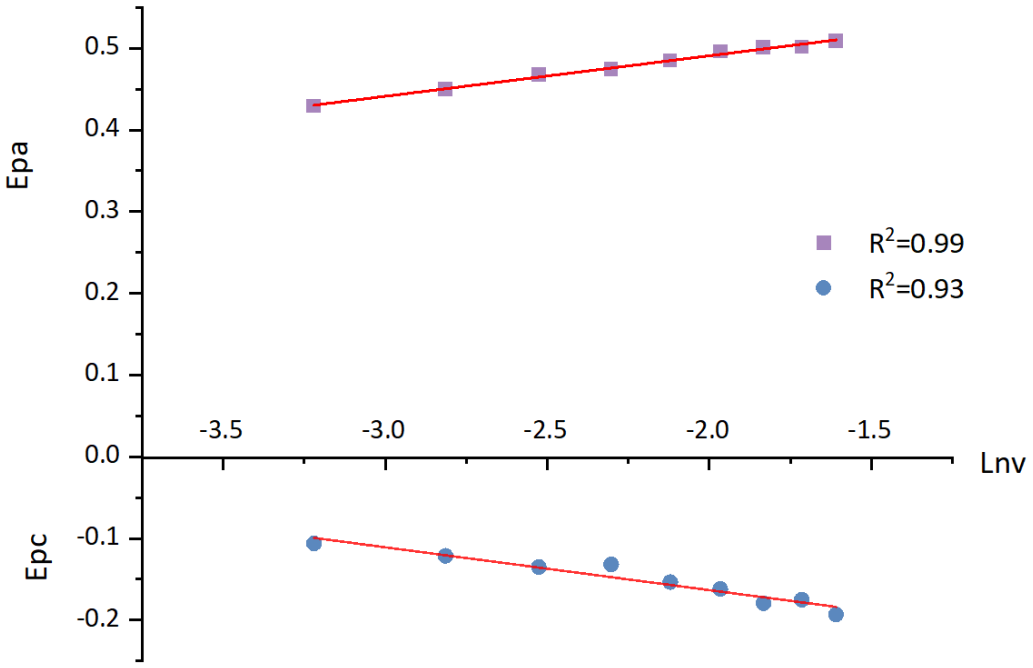

Figure S1 Linear relationship between the logarithm of the scan rate and the peak potential

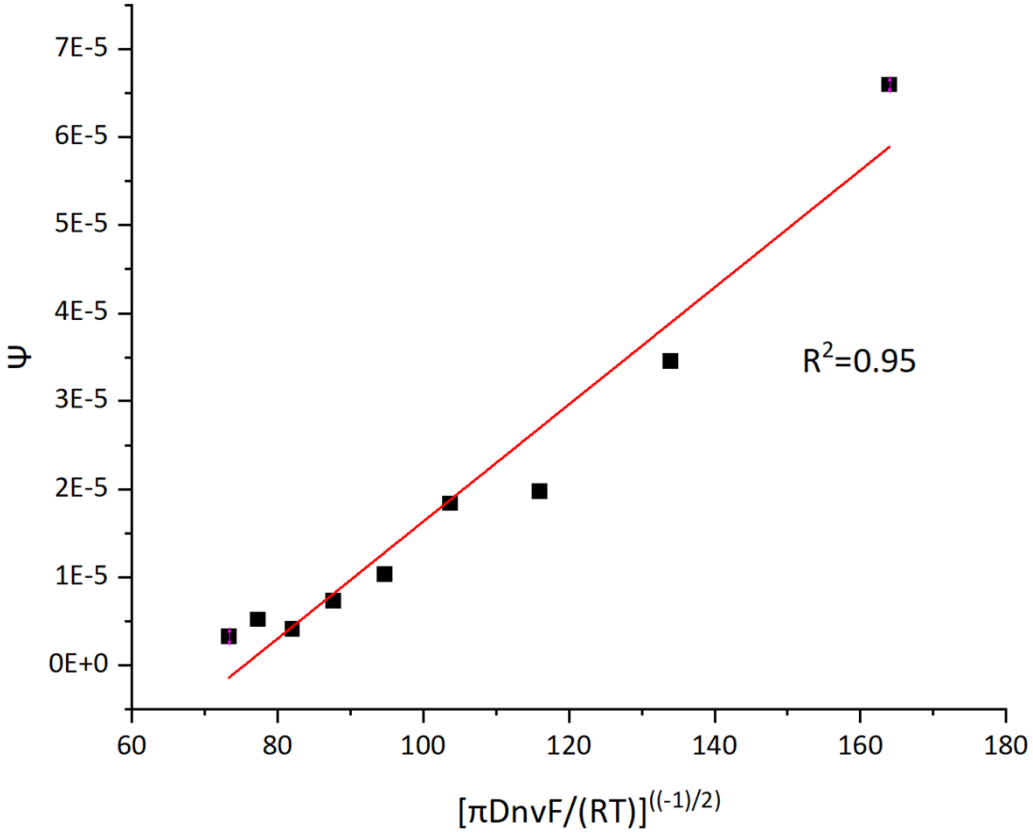

Figure S2 Nickelson's picture: Asymptotic line of ks.

Table S1 Classification Model Hyperparameters

Model	Hyperparameters	Parameter value
ANN	hidden_layer_sizes	(100,50)
	activation	relu
	max_iter	200
	alpha	0.01
SVM	kernel	rbf
	random_state	42
	tol	0.001
	gamma	scale
KNN	n_neighbors	5
	leaf_size	30
	p	1.6
	metric	minkowski
RF	n_estimators	150
	max_depth	4
	min_samples_split	2

Table S2 Regression Model Hyperparameters

Model	Hyperparameters	Parameter value
XGBoost	Learning_rate	0.3
	max_depth	3
	n_estimators	400
	subsample	0.8
RF	random_state	40
	n_estimators	200
	max_features	auto
	min_samples_split	2

Table S3 Regression Model Evaluation Index

Analyte and Models		Evaluation Indicators			
		MAE/(μmol/L)	RMSE/(μmol/L)	R-Squared	Average R-Squared
XGBoost	AA	26.862	58.511	0.939	0.962
	DA	22.124	30.276	0.963	
	UA	12.255	22.018	0.984	
RF	AA	44.958	74.750	0.933	0.959
	DA	26.672	41.336	0.952	
	UA	16.776	30.530	0.973	