

Online Measurement of Sodium Nitrite Based on Near-Infrared Spectroscopy

Xianzhe Xu [†], Yongshen Zhang [†], Mingmin Zhang, Dingming Li and Chen Zuo ^{*}

Institute of Radiochemistry, China Institute of Atomic Energy, Beijing 102413, China;

xianzhxu_21@163.com (X.X.); m15110185336@163.com (Y.Z.);

15689736095@163.com (M.Z.);

dingminglee@cnnmail.cn (D.L.)

^{*} Correspondence: zchen_2008@126.com

[†] These authors contributed equally to this work.

Table S1 Predictions and assessment results of the sodium nitrite model

Number	Reference value (mol/L)	Predicted value (mol/L)	Absolute error (mol/L)	Relative error (%)
1	0.529	0.572	0.044	8.23
2		0.561	0.033	6.15
3		0.559	0.031	5.77
4		1.194	0.198	19.86
5	0.996	1.193	0.197	19.76
6		1.196	0.200	20.06
7		1.300	0.041	3.22
8		1.293	0.033	2.66
9	1.260	1.282	0.023	1.79
10		3.296	0.041	1.25
11		3.308	0.053	1.62
12		3.304	0.049	1.50
13	0.949	0.956	0.007	0.79
14		0.949	0.000	0.05
15		0.947	-0.002	-0.16
16		1.688	0.023	1.41
17	1.665	1.687	0.022	1.35
18		1.688	0.023	1.41
19		1.957	0.047	2.44
20		1.949	0.039	2.03
21	1.910	1.948	0.038	1.97
22		2.268	0.064	2.93
23		2.261	0.058	2.61
24		2.266	0.063	2.84
25	2.204	2.992	-0.008	-0.27
26		2.994	-0.006	-0.20
27		3.000	0.000	0.00
28		3.995	-0.005	-0.12

29	4.002	0.002	0.05
30	3.997	-0.003	-0.08

Table S2 Results of different spectral preprocessing methods selected for the calibrated model

Number	Preprocessing method	Wave number (cm ⁻¹)	R ²	RMSECV
1	No spectral pretreatment	5400-7500	0.9985	0.0679
2	eliminating constant offset	5400-7500	0.9989	0.0532
3	subtracting a straight line	5400-7500	0.9988	0.0577
4	vector normalization	5400-7500	0.9999	0.0192
5	max-min normalization	5400-7500	0.9997	0.0317
6	multiple scattering correction(MSC)	5400-7500	0.9999	0.0185
7	First-order derivative	5400-7500	0.9991	0.0495
8	Second-order derivative	5400-7500	0.9963	0.106
9	First-order derivative + subtracting a straight line	5400-7500	0.9991	0.0493
10	First-order derivative+ vector normalization	5400-7500	0.9997	0.0311
11	First-order derivative +MSC	5400-7500	0.9998	0.0255

Table S3 Results of the calibrated model selecting different spectral bands

Number	Wave number (cm ⁻¹)	RMSECV
1	5450-9400	0.0224
2	4250-4600, 6100-7500	0.0269
3	4250-4600, 5400-9400	0.0326
4	4250-4600, 5450-7500	0.0288
5	4250-4600, 6100-9400	0.0344
6	5450-7426	0.0182
7	5450-7500	0.0186
8	6100-7500	0.0404
9	4250-4600, 5450-6100, 7500-9400	0.0341
10	5450-6100	0.0197
11	5450-6100, 7500-9400	0.0863
12	7424-9400	0.0224

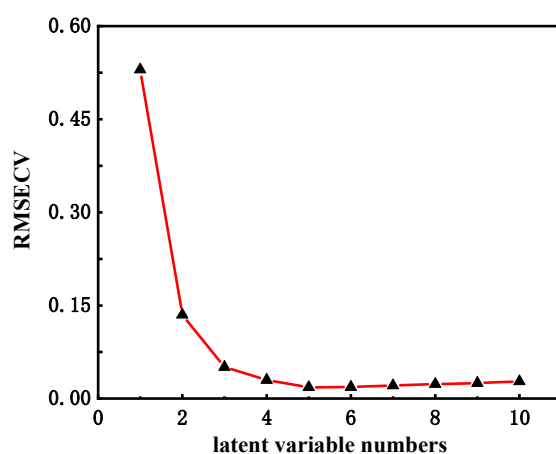


Figure S1 Results of the calibrated model selecting different number of factors

Table S4 Predictions and assessment results of the modified model

Number	Reference value (mol/L)	Predicted value (mol/L)	Absolute error (mol/L)	Relative error (%)
1	0.529	0.532	0.004	0.66
2		0.518	-0.011	-1.99
3		0.518	-0.011	-1.99
4		1.071	0.075	7.51
5		1.064	0.068	6.81
6	0.996	1.071	0.075	7.51
7		1.260	0.000	0.04
8		1.253	-0.007	-0.52
9		1.237	-0.023	-1.79
10		3.248	-0.007	-0.22
11	3.255	3.263	0.008	0.24
12		3.255	0.000	-0.01
13		0.924	-0.025	-2.58
14		0.915	-0.034	-3.53
15		0.916	-0.033	-3.43
16	1.665	1.656	-0.009	-0.52
17		1.662	-0.003	-0.16
18		1.659	-0.006	-0.34
19		1.928	0.018	0.93
20		1.914	0.004	0.19
21	1.910	1.918	0.008	0.40
22		2.232	0.029	1.29
23		2.228	0.025	1.11
24		2.235	0.031	1.43
25		2.966	-0.034	-1.13
26	3.000	2.954	-0.046	-1.53

27		2.941	-0.059	-1.97
28		3.957	-0.043	-1.08
29	4.000	3.961	-0.039	-0.98
30		3.956	-0.044	-1.10

Table S5 Reference values for samples used for calibration and prediction

Reference values of calibration samples (mol/L)	Reference values of prediction samples (mol/L)
0.300	0.529
0.496	0.996
0.707	1.260
0.797	3.255
0.902	0.949
0.398	1.665
0.993	1.910
1.098	2.204
1.203	3.000
1.294	4.000
1.399	
1.504	
1.805	
2.106	
2.407	
2.707	
3.008	
3.204	
3.505	
3.805	
4.000	
4.211	
4.512	
4.798	
4.994	
5.204	
5.505	
5.806	
6.016	
0.404	
1.603	
3.001	
4.397	