Electronic Supplementary Material (ESI) for Nanoscale.

Highly-accurate solvent identification using dynamic volatilization reflection spectra from an inverse opal sensor combined with a deep learning model

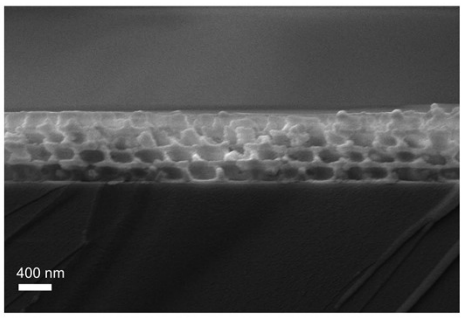

Figure S1. SEM image of the side view of the IO.

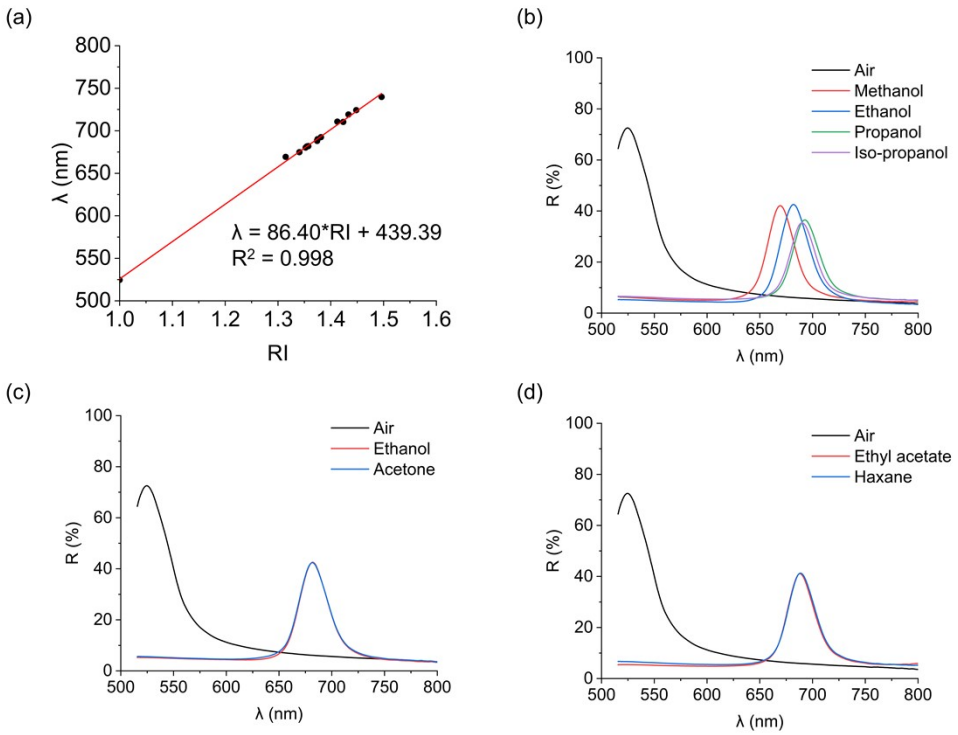

Figure S2. SRS detection of different solvents. (a) The change in reflection wavelength with the solvent RI. The red line represents the least squares fit of the data. (b) SRS detection of solvents with different RIs, including methanol (RI = 1.3145), ethanol (RI = 1.3575), iso-propanol (RI = 1.3750), and propanol (RI = 1.3814). (c) and (d) SRS detection of solvents with similar RIs, such as ethanol (RI = 1.3575) compared with acetone (RI = 1.3547) and ethyl acetate (RI = 1.3743) compared with hexane (RI = 1.3741).

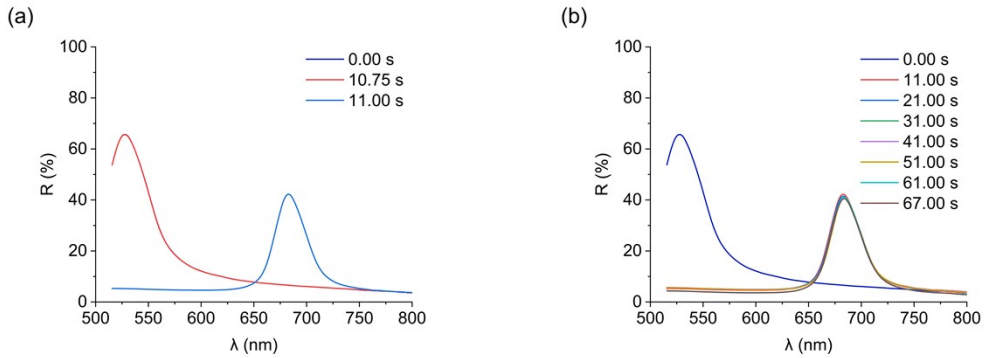

Figure S3 Evolution of the reflection spectrum of the IO during ethanol volatilization. (a) Phase I. The spectrum at 0.00 and 10.75 s are completely overlapping. (b) Phase II. The solvent is added to the IO at the 11th second.

Table S1. Composition information and partitioning of the DERS dataset.

Solvents	Number of Data Set		
	Training Set	Test Set	All Data Set
Dichloromethane	49	21	70
Trichloromethane	49	21	70
Tetrachloromethane	49	21	70
Methanol	49	21	69
Ethanol	49	21	70
Iso-propanol	49	21	70
Propanol	50	21	71
Cyclohexane	49	21	70
Hexane	49	21	70
Ether	49	21	70
Ethyl acetate	50	22	72
Acetonitrile	49	21	70
Acetone	50	22	72
Toluene	50	21	71
Total	**689**	**296**	**985**

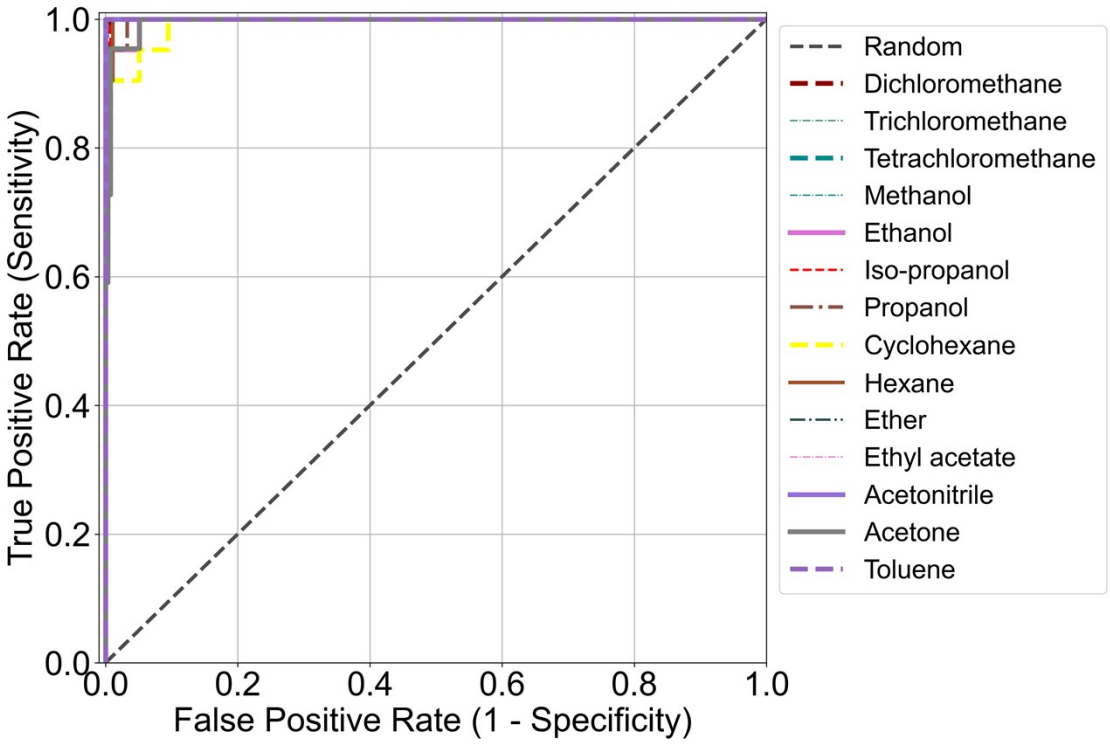

Figure S4. ROC curve of XGBoost on the test set.

Table S2. Classification performance of XGBoost for various solvents in the test set, with precision, recall, F1-Score, Accuracy, and ROC-AUC metrics used to evaluate the model.

Solvents	**Precision**	**Recall**	**F1-Score**	**Accuracy**	**ROC-AUC**	**Support**
Dichloromethane	0.8400	1.0000	0.9130	1.0000	0.9977	21
Trichloromethane	1.0000	0.9524	0.9756	0.9524	1.0000	21
Tetrachloromethane	1.0000	0.9524	0.9756	0.9524	1.0000	21
Methanol	1.0000	0.9524	0.9756	0.9524	1.0000	21
Ethanol	0.9091	0.9524	0.9302	0.9524	0.9974	21
Iso-propanol	0.9130	1.0000	0.9545	1.0000	0.9988	21
Propanol	1.0000	0.9048	0.9500	0.9048	0.9981	21
Cyclohexane	1.0000	0.9048	0.9500	0.9048	0.9931	21
Hexane	0.9048	0.9048	0.9048	0.9048	0.9986	21
Ether	0.9545	1.0000	0.9767	1.0000	0.9998	21
Ethyl acetate	0.8462	1.0000	0.9167	1.0000	0.9998	22
Acetonitrile	0.9545	1.0000	0.9767	1.0000	1.0000	21
Acetone	0.9375	0.6818	0.7895	0.6818	0.9955	22
Toluene	1.0000	1.0000	1.0000	1.0000	1.0000	21
Macro avg	0.9471	0.9433	0.9421	0.9433	0.9985	296
Weighted avg	0.9467	0.9426	0.9415	0.9426	0.9985	296

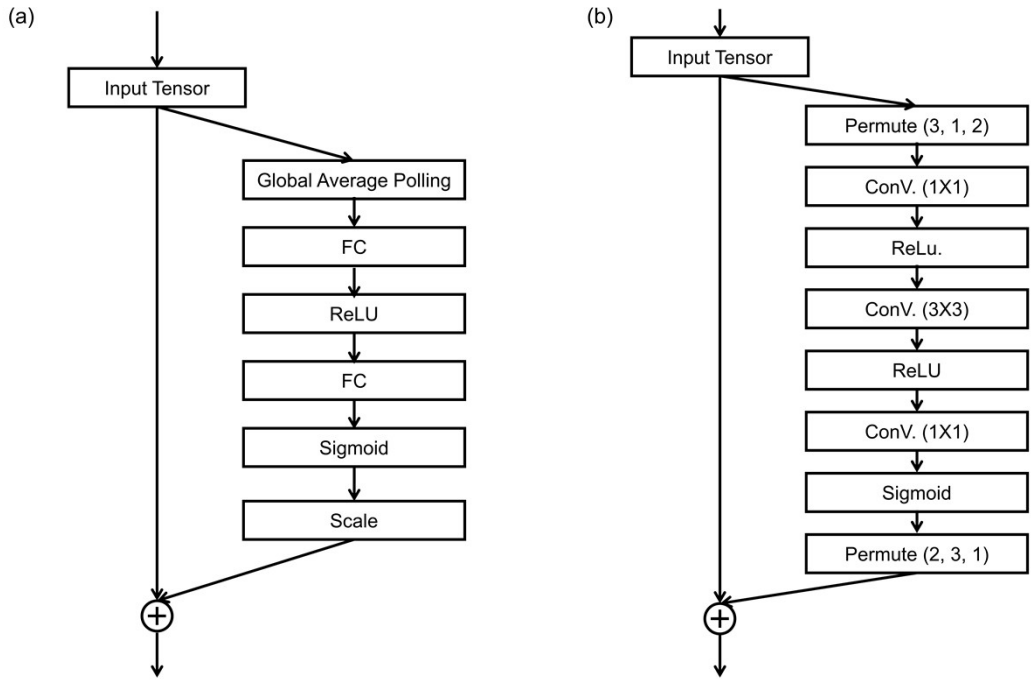

Figure S5. Schematic diagram of the channel attention mechanism module (a) and spatial attention mechanism module (b).

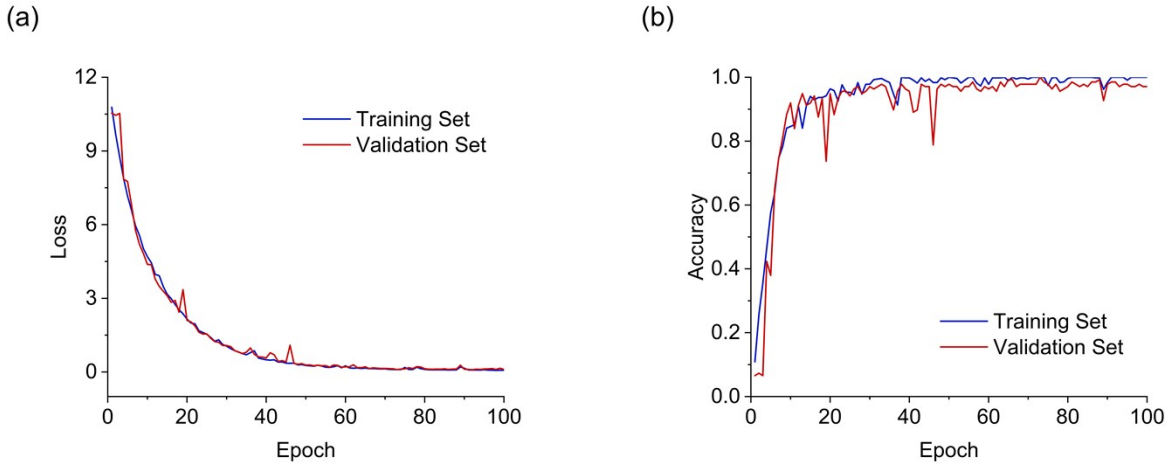

Figure S6. Loss (a) and accuracy (b) during the training process of Resnet18-CBAM.

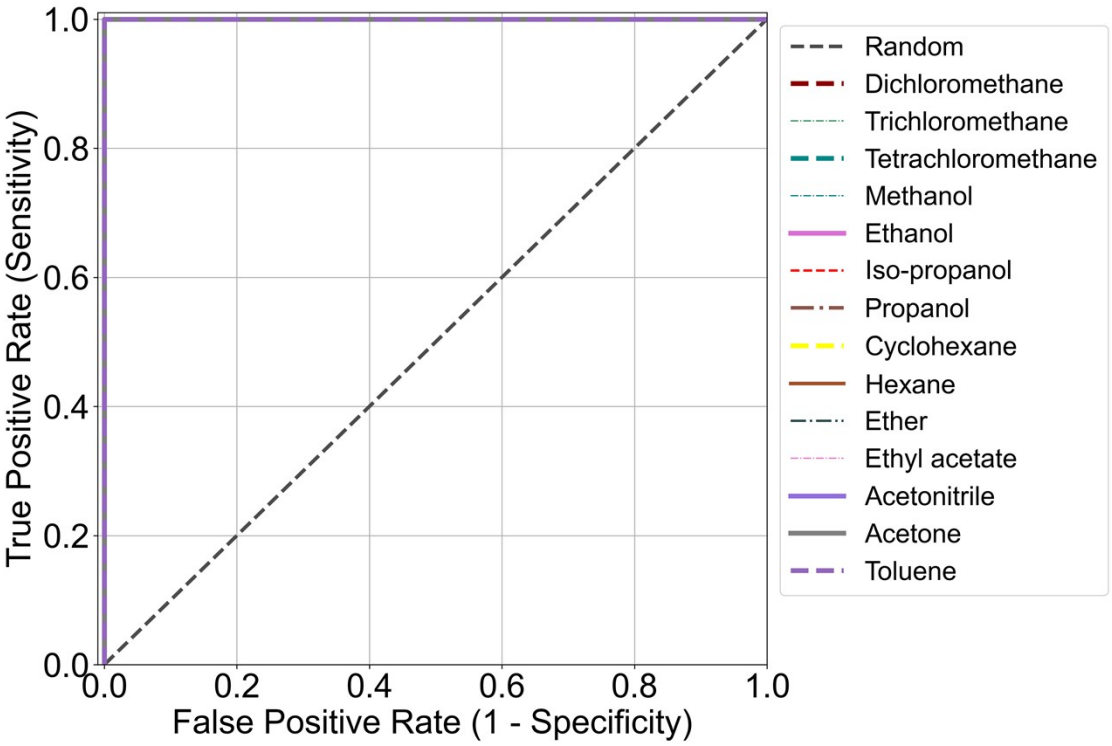

Figure S7. ROC curve of Resnet18-CBAM on the test set.

Table S3. Classification accuracy and F1-Score of various machine learning models and deep learning models on the test set.

Model	ACC	F1-Score
LR	0.706	0.694
DT	0.889	0.889
KNN	0.946	0.945
MLP	0.905	0.902
GaussianNB	0.909	0.908
SVM	0.926	0.926
RF	0.922	0.922
XGBoost	0.943	0.942
7-layer CNN	0.959	0.959
Resnet18	0.980	0.980
Resnet18-CBAM	**1.000**	**1.000**