Supplementary Information (SI) for Analyst.

A Practical Framework for Super-resolution of Mass Spectrometry Images via Adaptation of Deep Learning Models

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Table S1. The six quality metrics across all pre-trained model for the mouse brain images.

Model	Quality metrics	mean	s.e.m
MOSR	PSNR	16.758	0.181
MOSR	SSIM	0.279	0.01
MOSR	VIF	0.042	0.002
MOSR	SD	1.008	0.006
MOSR	NQM	4.0	0.233
MOSR	DISTS	0.227	0.003
SwinIR_L	PSNR	16.881	0.209
SwinIR_L	SSIM	0.307	0.009
SwinIR_L	VIF	0.054	0.003
SwinIR_L	SD	0.993	0.006
SwinIR_L	NQM	3.793	0.247
SwinIR_L	DISTS	0.278	0.002
MambaIR_L	PSNR	16.863	0.21
MambaIR_L	SSIM	0.307	0.009
MambaIR_L	VIF	0.054	0.003
MambaIR_L	SD	0.993	0.006
MambaIR_L	NQM	3.765	0.248
MambaIR_L	DISTS	0.277	0.002
ResShift_B	PSNR	16.444	0.189
ResShift_B	SSIM	0.271	0.009
ResShift_B	VIF	0.041	0.002
ResShift_B	SD	1.013	0.006
ResShift_B	NQM	3.526	0.227
ResShift_B	DISTS	0.243	0.003
ResShift_R	PSNR	17.418	0.198
ResShift_R	SSIM	0.326	0.009
ResShift_R	VIF	0.064	0.003
ResShift_R	SD	0.971	0.007

ResShift_R	NQM	4.493	0.23
ResShift_R	DISTS	0.281	0.003

Table S2. The testing dataset of horizontal section of mouse brain in this study.

ID	***m/z***	**tissue**	**The weighed score**		
			Fine-tuned	**Pre-trained**	**Fine-tuned/Pre-trained**
1	258.774	mouse brain	0.657115	0.631265	1.040949
2	303.083	mouse brain	0.799053	0.431532	1.851665
3	174.017	mouse brain	0.692114	0.697901	0.991708
4	239.115	mouse brain	0.849319	0.671986	1.263893
5	124.007	mouse brain	0.827092	0.561886	1.471994
6	130.889	mouse brain	0.654322	0.188548	3.470323
7	463.283	mouse brain	0.475803	0.489067	0.97288
8	502.294	mouse brain	0.583704	0.552531	1.056418
9	265.065	mouse brain	0.613409	0.219339	2.796621
10	186.041	mouse brain	0.653642	0.447425	1.460897
11	173.009	mouse brain	0.558316	0.436168	1.280048
12	225.099	mouse brain	0.70208	0.462693	1.517377
13	298.07	mouse brain	0.892641	0.723965	1.232989
14	283.243	mouse brain	0.705692	0.169385	4.166209
15	183.963	mouse brain	0.697114	0.506162	1.377254
16	300.067	mouse brain	0.702204	0.215795	3.254028
17	147.049	mouse brain	0.764328	0.35523	2.151644
18	234.882	mouse brain	0.450455	0.168317	2.676231
19	347.04	mouse brain	0.541399	0.299328	1.808713
20	211.001	mouse brain	0.652398	0.327297	1.993289
21	197.94	mouse brain	0.854886	0.231192	3.697732
22	360.971	mouse brain	0.472525	0.141212	3.346206
23	197.808	mouse brain	0.772828	0.660668	1.169769
24	315.051	mouse brain	0.55175	0.226073	2.44058
25	316.059	mouse brain	0.521067	0.273189	1.907352
26	327.233	mouse brain	0.714751	0.562779	1.270038
27	160.842	mouse brain	0.791096	0.294351	2.687592
28	162.839	mouse brain	0.779247	0.466776	1.669422
29	184.986	mouse brain	0.591414	0.532164	1.111338

30	146.065	mouse brain	0.611046	0.176714	3.457826
31	172.882	mouse brain	0.530542	0.206159	2.57346
32	216.036	mouse brain	0.638372	0.193381	3.301106
33	176.045	mouse brain	0.587917	0.320049	1.836959
34	192.023	mouse brain	0.604678	0.240254	2.516824
35	243.966	mouse brain	0.530509	0.24251	2.187575
36	315.135	mouse brain	0.662779	0.580533	1.141674
37	140.051	mouse brain	0.648024	0.367707	1.762338
38	359.125	mouse brain	0.619939	0.520779	1.190408
39	159.03	mouse brain	0.641287	0.27875	2.300581
40	181.966	mouse brain	0.831149	0.591313	1.4056
41	243.027	mouse brain	0.516131	0.280486	1.840131
42	195.811	mouse brain	0.760752	0.442386	1.719656
43	292.104	mouse brain	0.561764	0.247763	2.267346
44	508.341	mouse brain	0.348942	0.362547	0.962474
45	133.034	mouse brain	0.574789	0.232359	2.47371

Table S3. The testing dataset of mouse kidney in this study.

ID	***m/z***	**tissue**	**The weighed score**		
			Fine-tuned	**Pre-trained**	**Fine-tuned/Pre-trained**
1	176.996	mouse kidney	0.388625	0.242296	1.603928
2	179.056	mouse kidney	0.750062	0.574006	1.306714
3	181.966	mouse kidney	0.63486	0.437875	1.449867
4	69.751	mouse kidney	0.494882	0.365987	1.352185
5	197.94	mouse kidney	0.621291	0.470059	1.321731
6	242.882	mouse kidney	0.460703	0.281018	1.639405
7	228.84	mouse kidney	0.499616	0.290666	1.718865
8	281.249	mouse kidney	0.596402	0.386066	1.544817
9	197.022	mouse kidney	0.88716	0.700801	1.265922
10	176.936	mouse kidney	0.421156	0.355637	1.18423
11	206.877	mouse kidney	0.501505	0.355864	1.409262
12	125.036	mouse kidney	0.435746	0.328531	1.326344
13	185.963	mouse kidney	0.626476	0.42346	1.479422
14	249.08	mouse kidney	0.671179	0.519064	1.293058
15	186.904	mouse kidney	0.760776	0.64897	1.172282
16	162.839	mouse kidney	0.756282	0.657884	1.149568
17	160.842	mouse kidney	0.74682	0.656748	1.137148
18	209.858	mouse kidney	0.591434	0.442743	1.335841
19	256.962	mouse kidney	0.354537	0.235823	1.503405
20	180.043	mouse kidney	0.568222	0.379836	1.495965
21	133.014	mouse kidney	0.624793	0.562303	1.111133
22	209.876	mouse kidney	0.568454	0.434018	1.309747
23	158.925	mouse kidney	0.50851	0.370078	1.374063
24	132.03	mouse kidney	0.722198	0.574189	1.257772
25	234.838	mouse kidney	0.532822	0.343729	1.550121
26	171.006	mouse kidney	0.718358	0.571513	1.256941
27	210.874	mouse kidney	0.552659	0.377471	1.464111
28	185.022	mouse kidney	0.784274	0.523035	1.499468

29	174.879	mouse kidney	0.594473	0.452859	1.312711
30	218.848	mouse kidney	0.550132	0.479402	1.147538
31	199.937	mouse kidney	0.575048	0.458155	1.255136
32	308.099	mouse kidney	0.301626	0.189874	1.58856

Supporting Figures

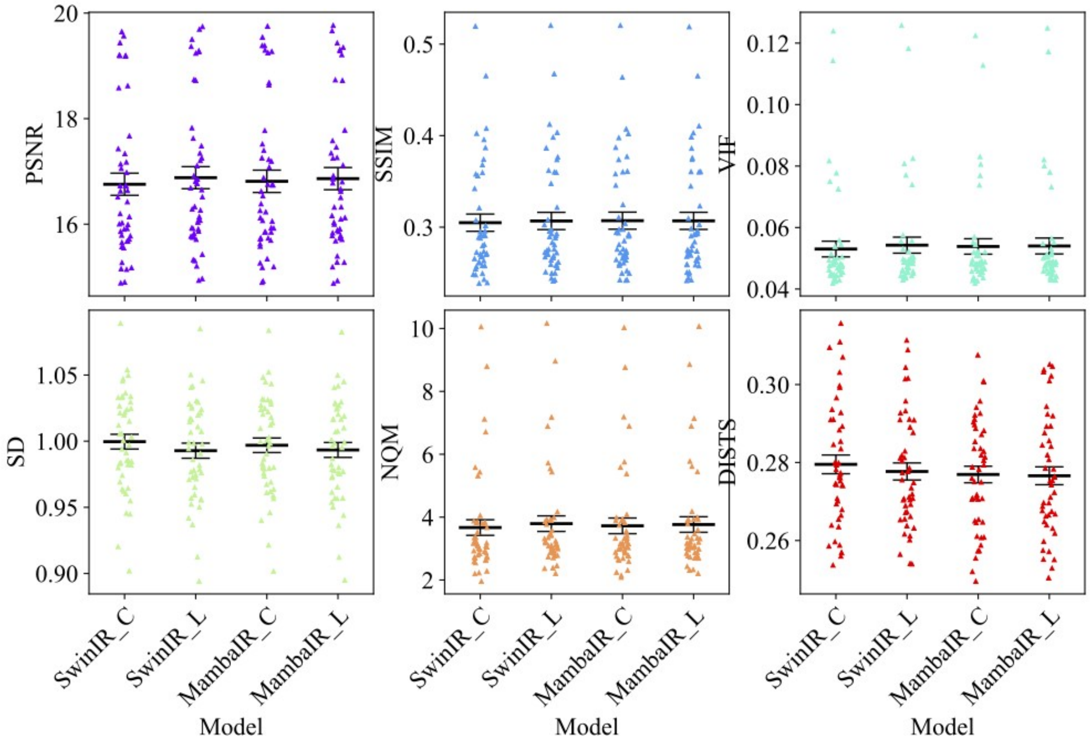

Fig S1. Six image quality metrics were obtained for SwinIR and MambaIR models, by calculating the predicted images versus corresponding ground-truth HR images from mouse brain images.

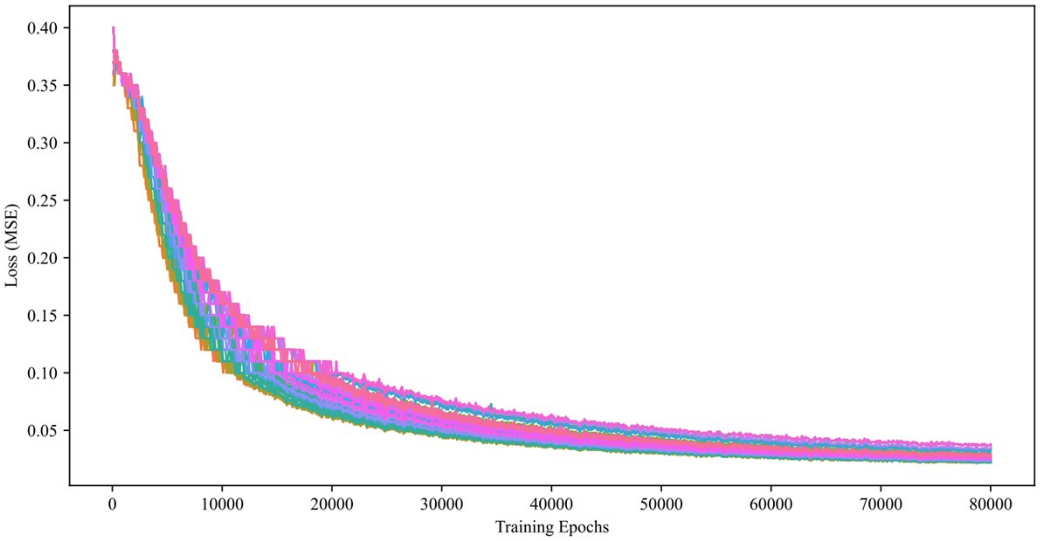

Fig S2: Comparison of training loss curves for those 64 fine-tuned models. All models were optimized using Adam and trained for 80k epochs.

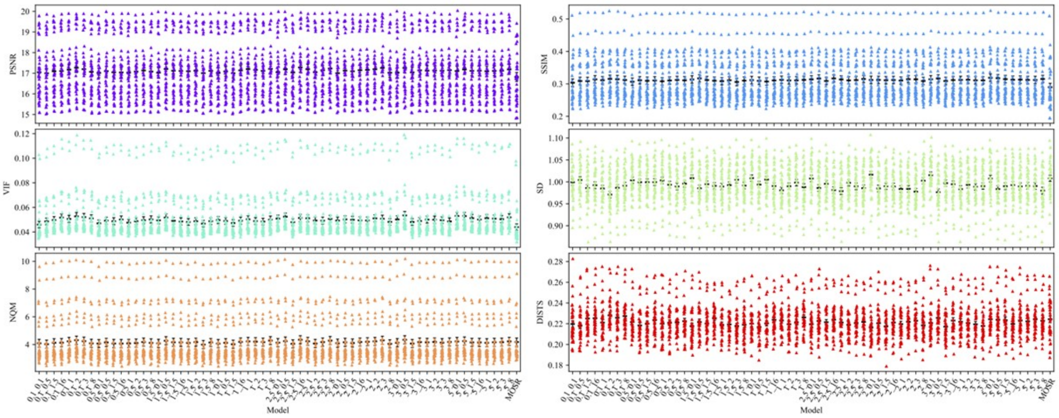

Fig S3. Six image quality metrics were obtained for those 64 fine-tuned models, by calculating the predicted images versus corresponding ground-truth HR images from mouse brain images.

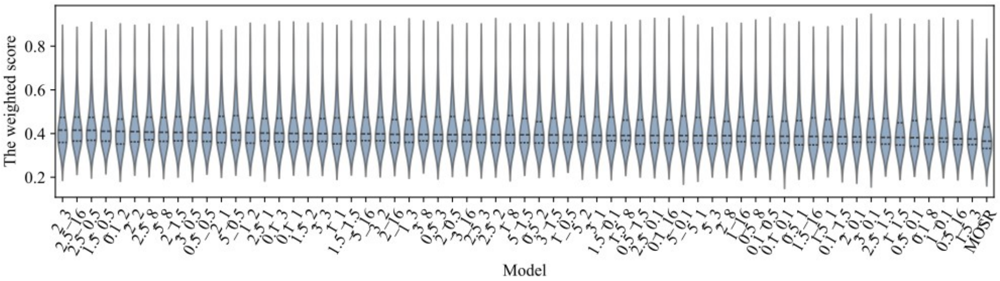

Fig S4. The weighted score of 64 fine-tuned models.

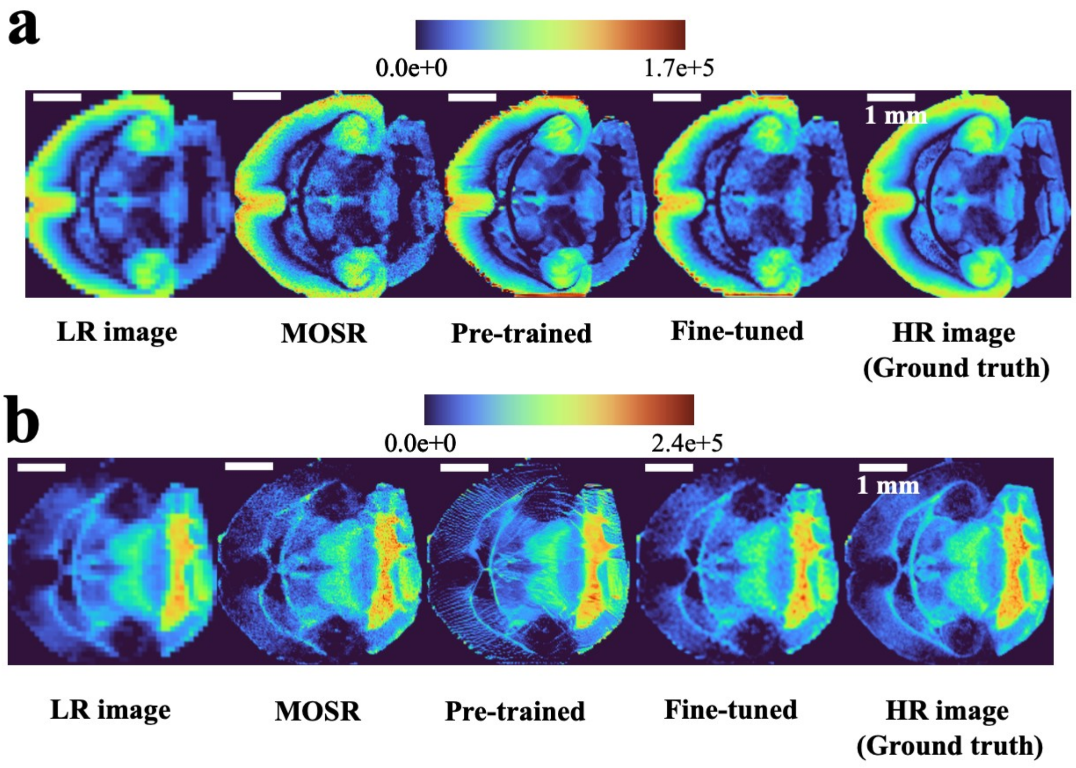

Figure S5. Evaluation of fine-tuned SR models on mouse brain images. a ($C_6H_7O_6$, *m/z*=4.017), b ($C_9H_{18}NO_8P$, *m/z*=298.07) in negative ionization mode, *m/z* ppm tolerance < 1. Colorbar represents the scale of ion intensity.

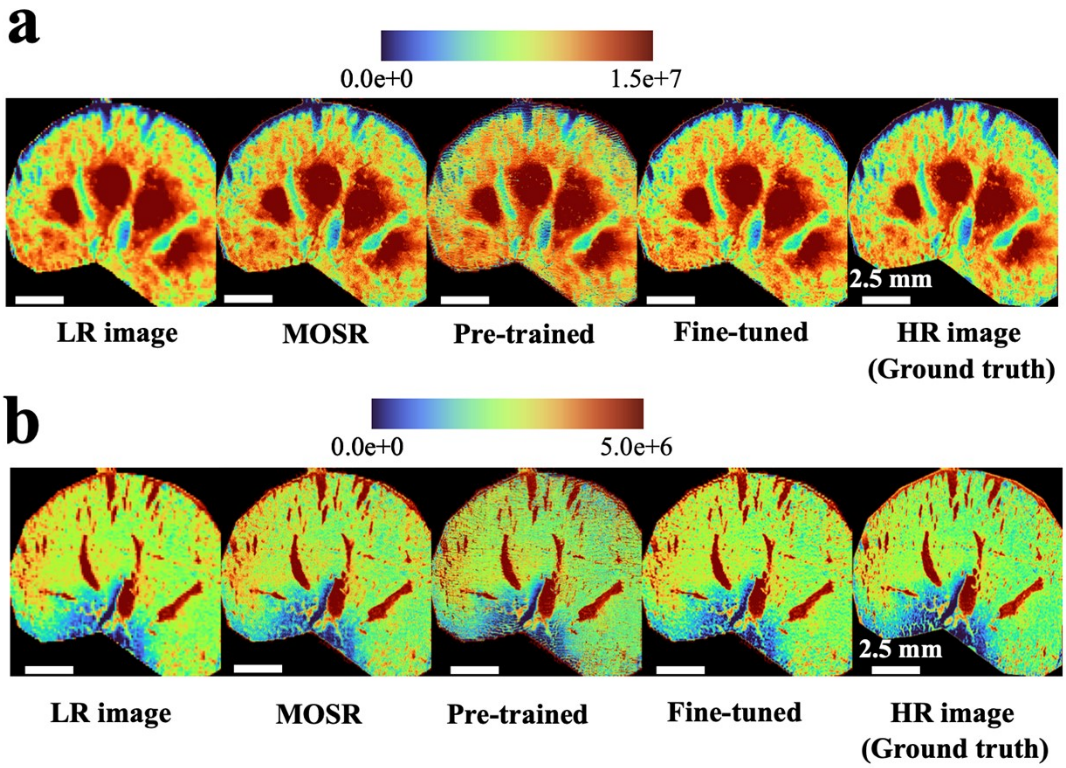

Figure S6. Evaluation of fine-tuned SR models on mouse kidney images. a ($C_6H_{12}O_6$, *m/z*=179.056), b ($C_{12}H_{15}N_2O_2P$, *m/z*=249.08) in negative ionization mode, *m/z* ppm tolerance < 1. Colorbar represents the scale of ion intensity.

Equations of six quality metrics.

1. PSNR (Peak Signal-to-Noise Ratio):

$$PSNR = 10log_{10}\left(\frac{MAX_I^2}{MSE}\right)$$

where MAX_I is the maximum possible pixel value and MSE is the mean squared error between the super-resolved (SR) and high-resolution (HR) images.

2. SSIM (Structural Similarity Index Measure):

$$SSIM(x,y) = \frac{(2\mu_x\mu_y + C_1)(2\sigma_{xy} + C_2)}{(\mu_x^2 + \mu_y^2 + C_1)(\sigma_x^2 + \sigma_y^2 + C_2)}$$

where μ_x, μ_y are the means, σ_x, σ_y are the standards deviations, and σ_{xy} is the covariance of images x and y. C_1 , C_2 are constants to stabilize division.

3. VIF (Visual Information Fidelity):

$$VIF = \frac{\sum_{j \in subbands} \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{M} log_2(1 + \frac{S_i^2\lambda_k}{\sigma_n^2})}{\sum_{j \in subbands} \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{M} log_2(1 + \frac{g_i^2S_i^2\lambda_k}{\sigma_v^2 + \sigma_n^2})}$$

The final VIF value is obtained by summing over all subbands, and its overall framework is a ratio : Numerator represents the total information extracted from the distorted image. Denominator represents the total information extracted from the reference image.The parameters in these formulas are defined as:

S_i^2: The variance of the reference signal, derived from the Gaussian Scale Mixture (GSM) model .

λ_k: The eigenvalues of the covariance matrix of the image blocks .

σ_n^2: The variance of the visual noise in the Human Visual System (HVS) model .

g_i: The gain/attenuation factor applied to the original signal by the distortion process .

σ_v^2: The variance of the additive noise introduced by the distortion process .

4. SD (Standard Deviation):

$$SD_{norm} = \frac{\sigma_{SR}}{\sigma_{HR}}$$

where σ_{SR} and σ_{SR} are the standard deviations of the SR and HR images, respectively. Values closer to 1.0 indicate better preservation of intensity variation.

5. NQM (Noise Quality Measure):

$$NQM = 10log_{10}\left(\frac{\sum_x\sum_y O_s^2(x,y)}{\sum_x\sum_y (O_s(x,y) - I_s(x,y)^2}\right)$$

where $O_s(x,y)$ represents the simulated version of the model restored image (reference). It is obtained by processing the original (uncorrupted) image through a nonlinear model of the human visual system (HVS) based on Peli's contrast pyramid (E. Peli, “Contrast in complex images,” *J. Opt. Soc. Amer. A*, vol. 7, pp.2032–2039, Oct. 1990). $I_s(x,y)$ represents the simulated version of the restored image (test). It is obtained by applying the same HVS model to the distorted (or restored) image whose quality is being evaluated. x,y are the spatial pixel coordinates over the entire image.

6. DISTS (Deep Image Structure and Texture Similarity):

$$DISTS(X,Y) = 1 - \sum_{i=0}^{m}\sum_{j=0}^{n}(\alpha_{ij} \cdot L_c(\tilde{X}_{ij},\tilde{Y}_{ij}) + \beta_{ij} \cdot L_s(\tilde{X}_{ij},\tilde{Y}_{ij}))$$

where X,Y represent the reference image and the distorted (test) image, respectively.

i: Index over the scales (stages) of a pre-trained VGG network, where m is the total number of scales.

j: Index over the channels within each scale, where n is the number of channels in that scale.

$L_c(\tilde{X}_{ij},\tilde{Y}_{ij})$ is the structural similarity term, computed as the correlation between the mean values of the feature maps. It is defined as:

$$L_c(\tilde{X}_{ij},\tilde{Y}_{ij}) = \frac{2\mu_x\mu_y + C_1}{\mu_x^2 + \mu_y^2 + C_1}$$

where μ_x and μ_y are the spatial means of $\tilde{X}_{ij}$ and $\tilde{Y}_{ij}$, and C_1 is a small constant for numerical stability.

$L_s(\tilde{X}_{ij},\tilde{Y}_{ij})$ is the textural similarity term, computed as the similarity between the standard deviations (contrasts) of the feature maps. It is defined as:

$$L_s(\tilde{X}_{ij},\tilde{Y}_{ij}) = \frac{2\sigma_x\sigma_y + C_2}{\sigma_x^2 + \sigma_y^2 + C_2}$$

where σ_x and σ_y are the spatial means of $\tilde{X}_{ij}$ and $\tilde{Y}_{ij}$, and C_2 is a small constant. α_{ij} and β_{ij} represent the learnable weights that balance the contribution of each channel and scale.