Supplementary materials

Riverine Organic Matter Dynamics in the Headwaters of the China's Yellow River under Climate Change

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Table S1 Definitions of riverine indicators sensitive to organic matter concentrations, following Yan et al. (2025).

Indicators	Equation
NDCI	NDCI = $(SR_{red} - SR_{green}) / (SR_{red} + SR_{green})$
OC_Index	OC_Index = $(SR_{red} + SR_{nir}) / (SR_{blue} + SR_{swir1})$
Hue Angel	$X = 11.053 \times SR_{ultrablue} + 6.950 \times SR_{blue} + 51.135 \times SR_{green} + 34.475 \times SR_{red}$ $Y = 1.320 \times SR_{ultrablue} + 21.053 \times SR_{blue} + 66.023 \times SR_{green} + 18.034 \times SR_{red}$ $Z = 58.083 \times SR_{ultrablue} + 34.931 \times SR_{blue} + 2.606 \times SR_{green} + 0.016 \times SR_{red}$ $x = X / (X + Y + Z)$ $y = Y / (X + Y + Z)$ $\alpha = [\arctan((y - 1/3) / (x - 1/3)) \bmod 2\pi] \times 180 / \pi$

Table S2 Test and validation scores of different models for COD prediction using satellite data.

No.	Model	Test score	Validation score
1	LightGBMLarge_BAG_L1	-0.22325	-0.66913
2	RandomForestMSE_BAG_L1	-0.2425	-0.661322
3	ExtraTreesMSE_BAG_L1	-0.24681	-0.672584
4	XGBoost_BAG_L1	-0.31248	-0.674913
5	CatBoost_BAG_L1	-0.34349	-0.649774
6	CatBoost_r177_BAG_L1	-0.34857	-0.652313
7	RandomForestMSE_BAG_L2	-0.36146	-0.636188
8	ExtraTreesMSE_BAG_L2	-0.36618	-0.621578
9	NeuralNetTorch_BAG_L2	-0.36816	-0.610234
10	WeightedEnsemble_L3	-0.37258	-0.602517
11	CatBoost_r177_BAG_L2	-0.38146	-0.625719
12	WeightedEnsemble_L2	-0.38381	-0.630267
13	CatBoost_BAG_L2	-0.38433	-0.623588
14	XGBoost_BAG_L2	-0.38697	-0.6598
15	LightGBM_r131_BAG_L1	-0.38935	-0.651746
16	NeuralNetFastAI_BAG_L2	-0.39335	-0.619413
17	LightGBMXT_BAG_L1	-0.39513	-0.673662
18	LightGBMXT_BAG_L2	-0.39965	-0.629565
19	LightGBMLarge_BAG_L2	-0.40136	-0.667139
20	LightGBM_BAG_L2	-0.42184	-0.637511
21	LightGBM_BAG_L1	-0.44421	-0.655706
22	NeuralNetTorch_BAG_L1	-0.51521	-0.722361
23	NeuralNetTorch_r79_BAG_L1	-0.6058	-0.68912
24	NeuralNetFastAI_BAG_L1	-0.68089	-0.773005

Table S3 Test and validation scores of different models for COD prediction based on geographical features.

No.	Model	Test score	Validation score	No.	Model	Test score	Validation score
1	LightGBMLarge_BAG_L1	-0.081138	-0.2644	**19**	CatBoost_r69_BAG_L1	-0.167949	-0.23341
2	XGBoost_r194_BAG_L1	-0.089043	-0.2592	**20**	LightGBM_r131_BAG_L1	-0.168802	-0.23719
3	ExtraTreesMSE_BAG_L1	-0.090097	-0.24898	**21**	LightGBM_BAG_L1	-0.176396	-0.26183
4	ExtraTrees_r42_BAG_L1	-0.092587	-0.25519	**22**	WeightedEnsemble_L2	-0.177354	-0.20715
5	RandomForest_r195_BAG_L1	-0.0953	-0.25655	**23**	NeuralNetTorch_r86_BAG_L1	-0.193151	-0.22308
6	XGBoost_r33_BAG_L1	-0.097439	-0.25877	**24**	NeuralNetTorch_r79_BAG_L1	-0.201559	-0.22065
7	RandomForestMSE_BAG_L1	-0.100664	-0.2697	**25**	NeuralNetTorch_BAG_L1	-0.20326	-0.25054
8	XGBoost_r89_BAG_L1	-0.112642	-0.2575	**26**	NeuralNetTorch_r14_BAG_L1	-0.204362	-0.2446
9	CatBoost_r9_BAG_L1	-0.116537	-0.24187	**27**	NeuralNetTorch_r30_BAG_L1	-0.212912	-0.2288
10	XGBoost_BAG_L1	-0.117449	-0.26967	**28**	NeuralNetFastAI_BAG_L1	-0.213711	-0.26241
11	CatBoost_r13_BAG_L1	-0.13718	-0.23871	**29**	NeuralNetFastAI_r191_BAG_L1	-0.214983	-0.2659
12	LightGBM_r188_BAG_L1	-0.148257	-0.24493	**30**	ExtraTrees_r172_BAG_L1	-0.217508	-0.26801
13	CatBoost_r177_BAG_L1	-0.153872	-0.23387	**31**	NeuralNetFastAI_r103_BAG_L1	-0.224872	-0.23766
14	CatBoost_r50_BAG_L1	-0.156083	-0.23575	**32**	NeuralNetFastAI_r102_BAG_L1	-0.229039	-0.26453
15	CatBoost_BAG_L1	-0.156563	-0.23661	**33**	NeuralNetTorch_r22_BAG_L1	-0.23428	-0.26398
16	LightGBMXT_BAG_L1	-0.15731	-0.24073	**34**	NeuralNetFastAI_r145_BAG_L1	-0.235515	-0.27573
17	LightGBM_r161_BAG_L1	-0.15873	-0.2379	**35**	NeuralNetFastAI_r11_BAG_L1	-0.374389	-0.45661
18	CatBoost_r137_BAG_L1	-0.160723	-0.23589	**36**	LightGBM_r96_BAG_L1	-0.428637	-0.47816

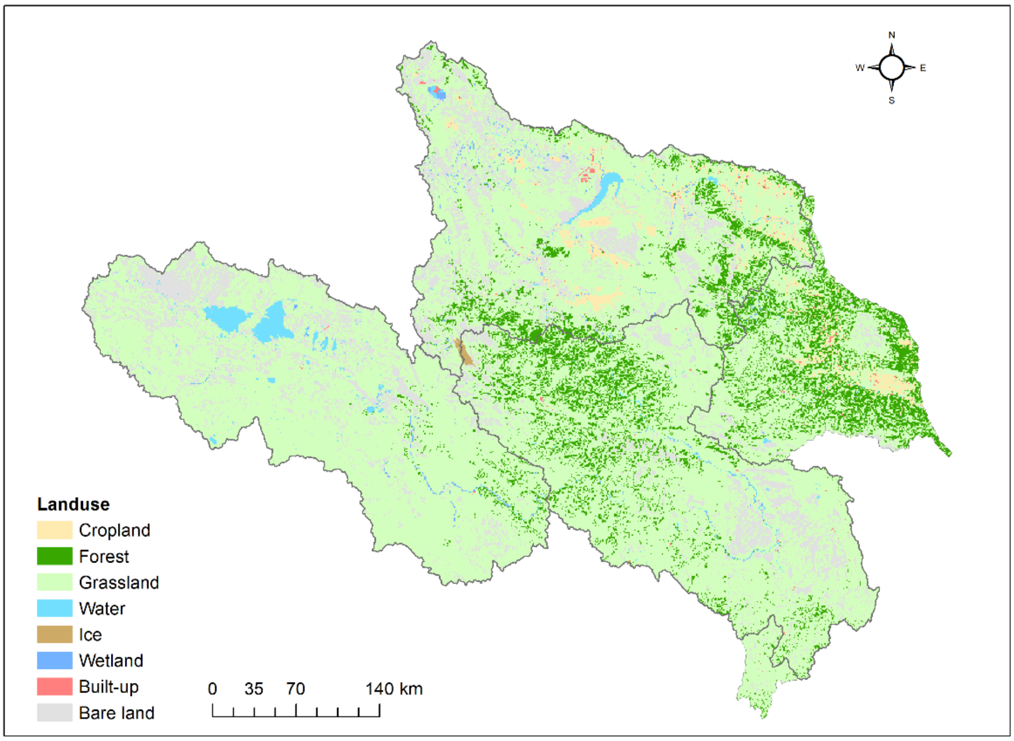

Fig.S1 Land use distribution across the three sub-basins (B1–B3) within the Yellow River source region.

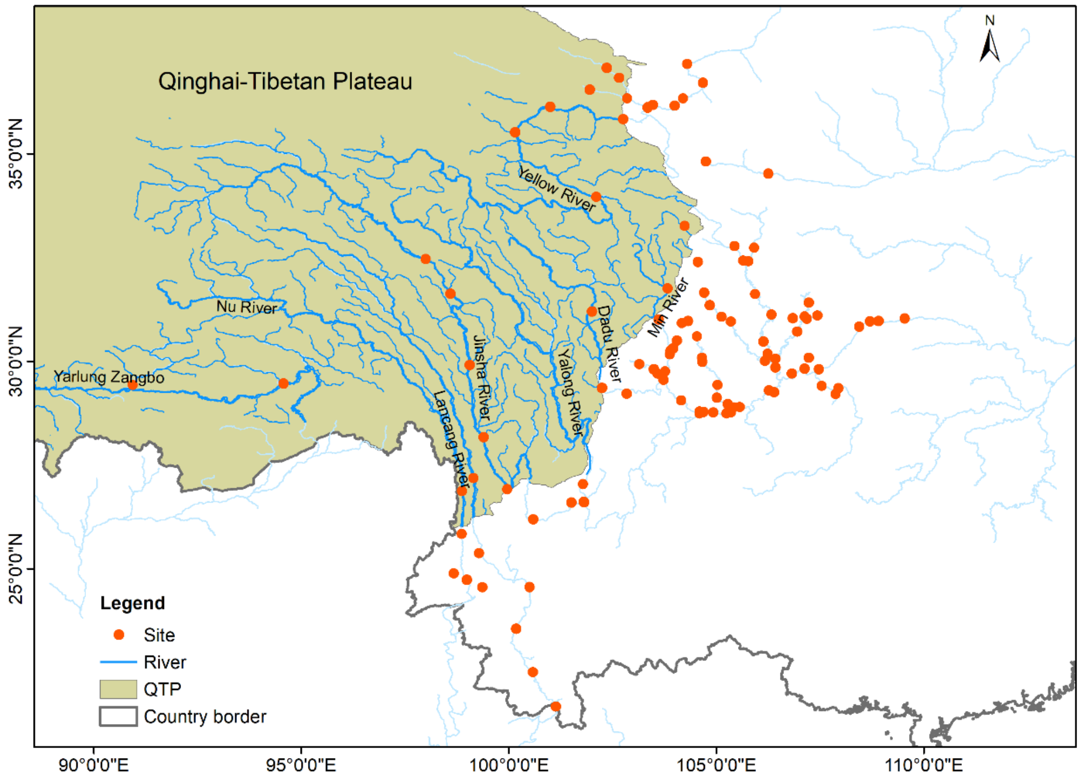

Fig.S2 Locations of data collection sites for model training across the Qinghai–Tibetan Plateau and adjacent areas.

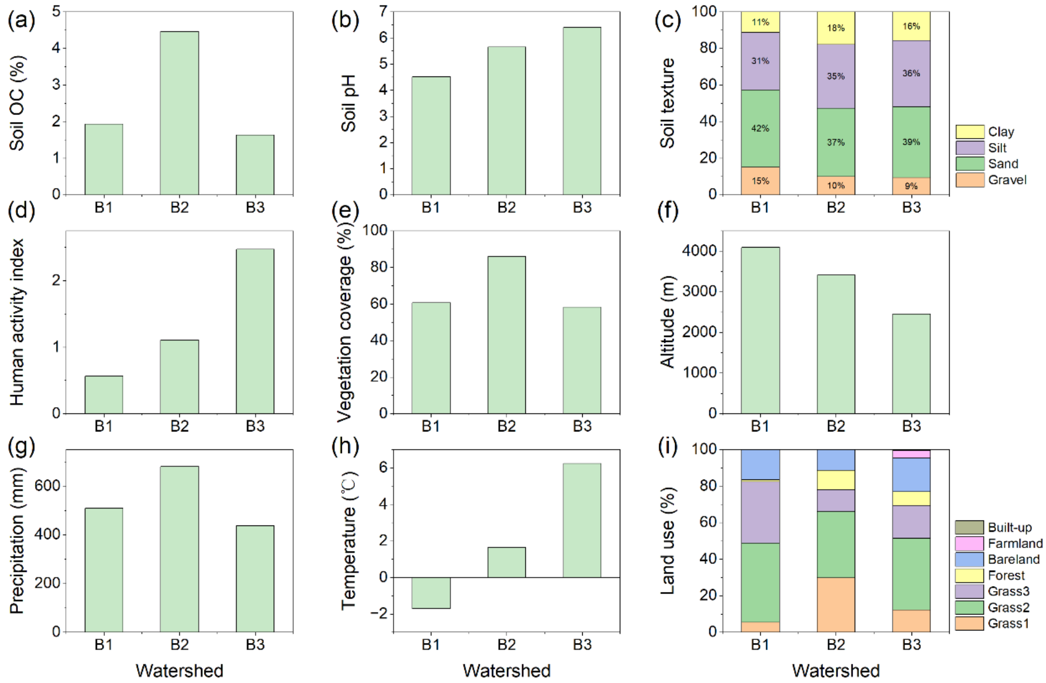

Fig.S3 Geographical characteristics of the sub-basins in the Yellow River source region. (a–c) Soil organic matter, pH, and texture; (d–f) human activity index, vegetation coverage, and altitude; (g–i) average precipitation and temperature over the last ten years, and land use in 2015.

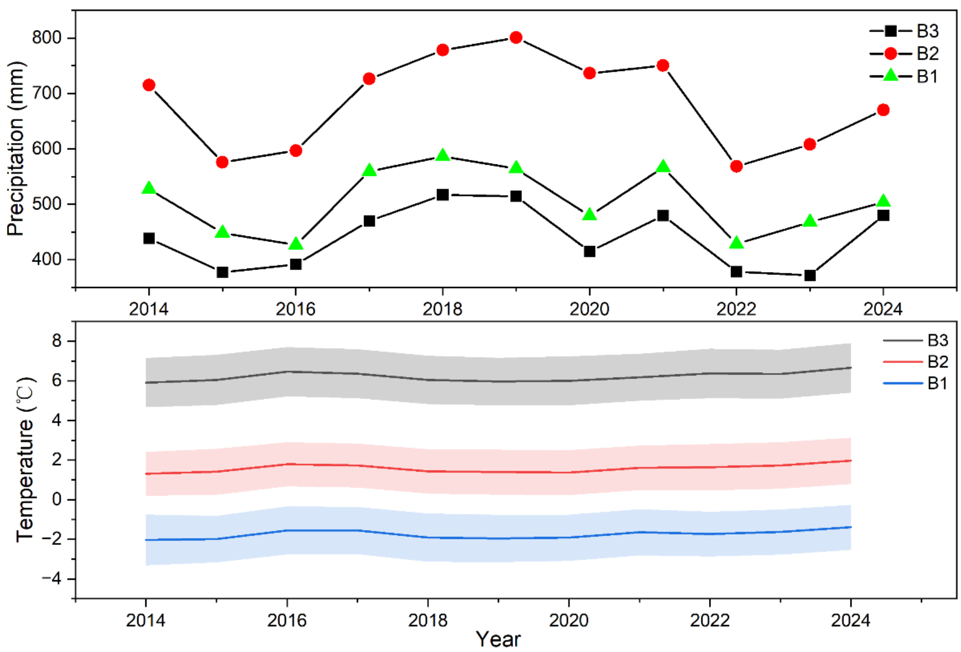

Fig.S4 Variations in precipitation and temperature averaged across different sub-basins of the Yellow River source region during 2014–2024.