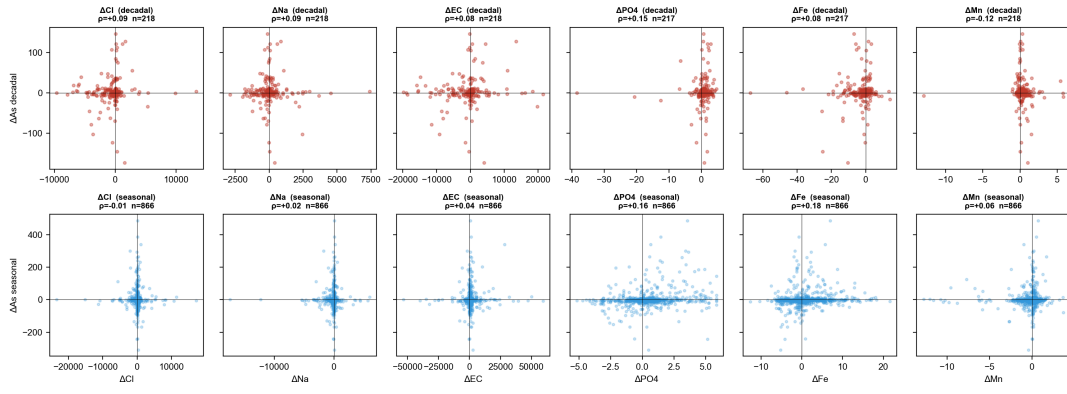


Supplementary Information

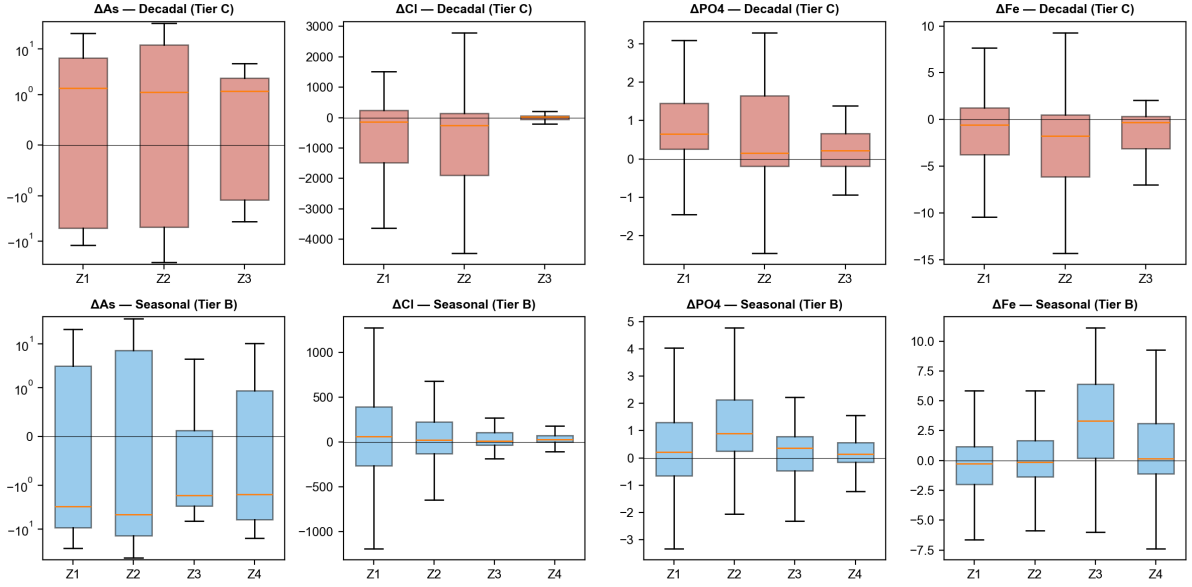
A regime-specific mechanism portfolio for arsenic mobilization in coastal Bangladesh

Md Rakib Hasan, Shoumik Zubayer, Mst Anika Khatun Rupa, Fazla Zawadul Arabi, Anwar Zahid

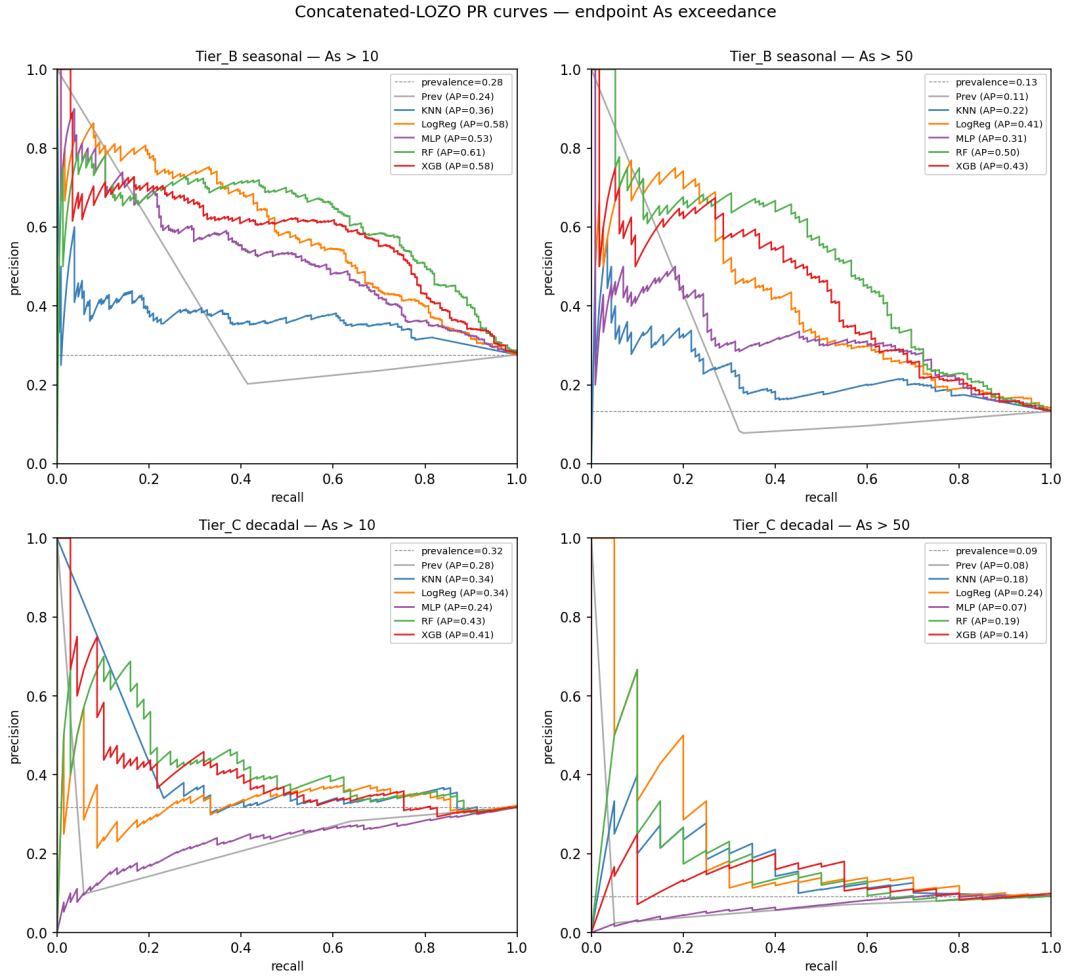
This Supplementary Information collects secondary display items that support but are not essential to the headline claims of the main manuscript: precision-recall companions to the baseline and MAGNET ROC curves (Supplementary Fig. 3, Supplementary Fig. 4), the bulk-change context behind the freshening-plus-loading paradox (Supplementary Fig. 1, Supplementary Fig. 2), the PHREEQC saturation-index multitask negative result (Supplementary Fig. 5), the regime-stratified transfer test on the BRGM French subregions (Supplementary Fig. 6), the method-triangulation summary (Supplementary Table 1), and a pointer to the full released PCMCi edge list (Supplementary Table 2). Cross-references to Methods, Results sections, and Extended Data items refer to the main manuscript.



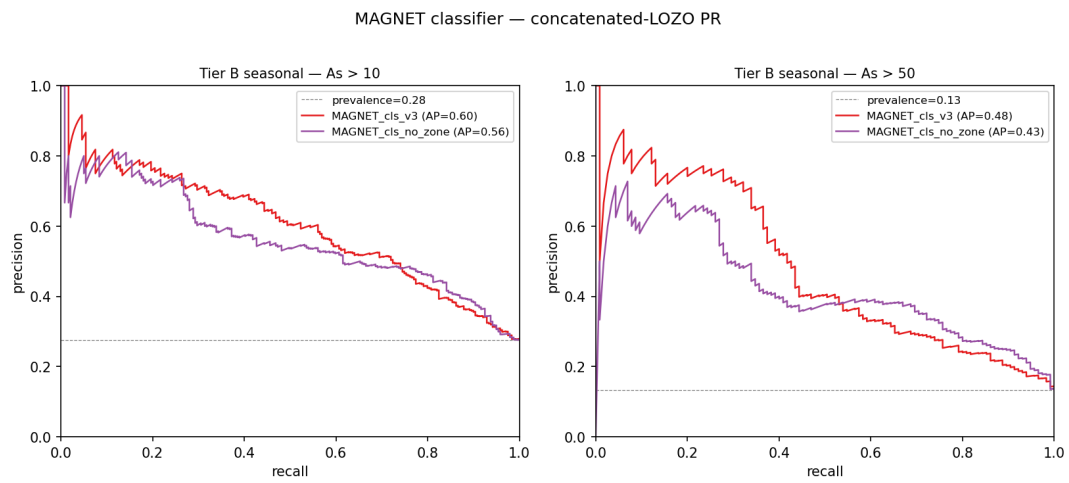
Supplementary Fig. 1: Pairwise salinity-redox covariation across the decadal cohort. Bivariate scatter of ΔCl vs. ΔEh , ΔNa vs. ΔpH and ΔEC vs. ΔFe across the 235 decadal wells, colour-coded by zone. The pairwise correlations motivate the PCMCi conditioning treatment of Section M3: any unconditioned bivariate analysis would over-attribute Δ -As to salinity proxies whose apparent association is mediated through redox covariates.



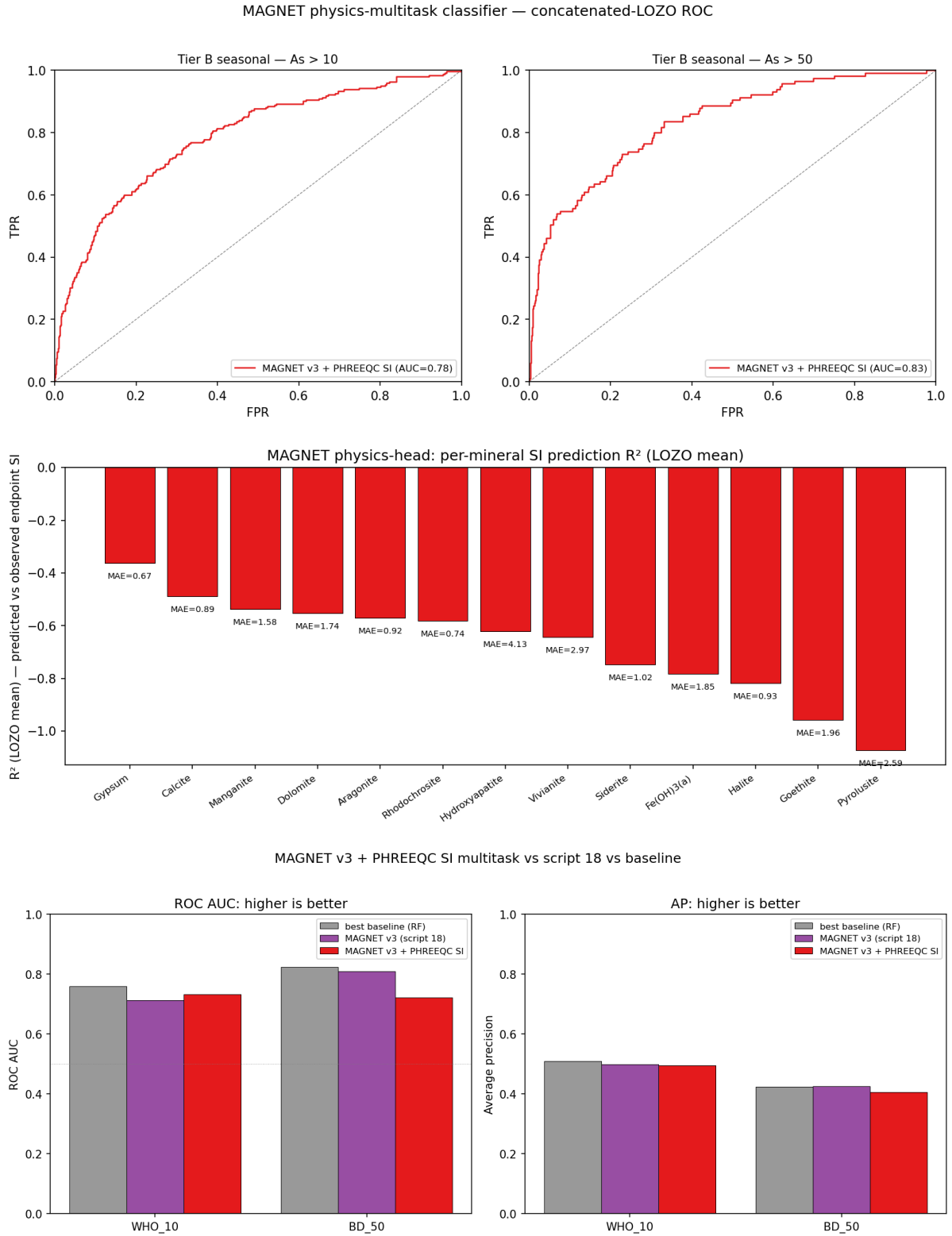
Supplementary Fig. 2: Zone-stratified per-well decadal change distributions for the six headline parameters. Boxplots of ΔAs , ΔFe , ΔPO_4 , ΔHCO_3 , ΔCl , ΔTDS across Z1, Z2, Z3 (Tier C, $n = 212$ paired wells). Boxes show median and IQR; whiskers span $1.5 \times \text{IQR}$; significance is paired Wilcoxon signed-rank vs. a null of zero change with Holm correction. The freshening signal ($\Delta\text{Cl} < 0$) is uniform across coastal zones; the anthropogenic loading signal ($\Delta\text{HCO}_3 > 0$, $\Delta\text{TDS} > 0$) intensifies from Z1 to Z3.



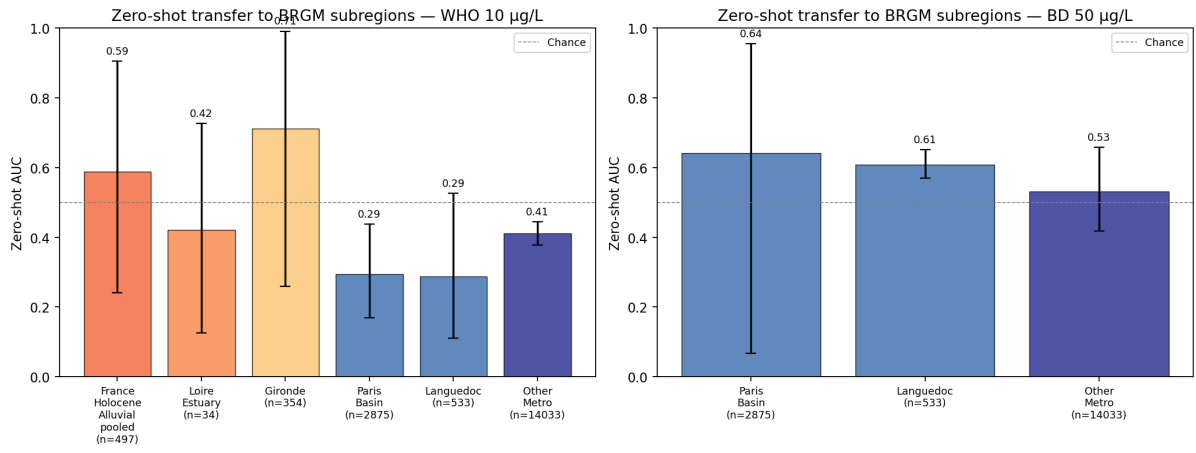
Supplementary Fig. 3: Baseline classifier precision-recall curves. Companion precision-recall view of Extended Data Fig. 4 under the same LOZO protocol. Average precision is reported alongside the ROC AUC in Extended Data Table 1.



Supplementary Fig. 4: MAGNET endpoint classifier precision-recall curves. Companion precision-recall view of Extended Data Fig. 5.



Supplementary Fig. 5: PHREEQC saturation-index multitask experiment (negative result). A MAGNET variant trained jointly on As-exceedance and the 13 PHREEQC SI auxiliary targets (Methods M4) reduced BD-50 LOZO AUC by ~ 0.09 relative to the headline classifier. The result is reported as a negative result and motivates the decision to use SIs only as PCMCi inputs (Layer 2), not as multitask DL targets. (a) ROC of the SI-multitask MAGNET variant. (b) SI prediction quality across the 13 auxiliary heads. (c) Head-to-head AUC of MAGNET-SI-multitask vs. headline MAGNET-classification and RF baseline.



Supplementary Fig. 6: Regime-stratified zero-shot transfer to BRGM French subregions. Bangladesh-trained classifier evaluated zero-shot on six BRGM hydrogeological subregions (Methods M9). The two unambiguous carbonate regimes (Paris Basin, Languedoc) yield confidence-interval-bounded anti-transfer (AUC = 0.29). The Holocene-alluvial subregions have insufficient ambient WHO-10 prevalence ($\sim 1\%$) to discriminate the model.

Supplementary Table 1: Triangulated Δ -As parents. Edges that survive PCMCi $\cap$ NOTEARS $\cap$ bootstrap-stability $\geq 50\%$ at $\alpha = 0.01$, summarised by scale. The seasonal Fe-PO₄ motif is triangulated; the decadal HCO₃ edge survives PCMCi bootstrap but not the underpowered NOTEARS run (Results §3).

Cohort	PCMCi parents	NOTEARS parents	Bootstrap $\geq 50\%$	Triple intersection
Seasonal (Tier B)	Fe, PO ₄	PO ₄	Fe, PO ₄	PO ₄
Decadal (Tier C)	HCO ₃	(none)	HCO ₃	(none)

Supplementary Table 2: Zone-stratified PCMCi Δ -As edge list, both scales. Every candidate Δ -As parent surviving $\alpha = 0.05$ in the zone-stratified PCMCi runs (Methods M3), with partial correlation, p -value, whether the edge also survives the stricter $\alpha = 0.01$ threshold ($\checkmark$), and per-zone bootstrap stability (fraction of zone-stratified bootstrap resamples in which the edge recurs). Parents are ordered by $|\text{partial } r|$ within each zone. Z3 Chittagong returns no parent at $\alpha = 0.05$ in the seasonal cohort ($n = 42$; underpowered) and is therefore absent from the seasonal block. The pooled-cohort runs are shown in Fig. 2b and Extended Data Fig. 1; the full machine-readable edge list, including non-surviving candidates, is released with the source data.

Zone	<i>n</i>	Parent	partial <i>r</i>	<i>p</i>	$\alpha \leq 0.01$	Bootstrap stab.
<i>Seasonal cohort (Tier B)</i>						
Z1 Ganges Tidal	223	Fe	+0.22	< 0.001	✓	0.88
		PO ₄	+0.17	0.011		0.53
Z2 Meghna Estuarine	154	Eh	−0.24	0.002	✓	0.60
		PO ₄	+0.21	0.009	✓	0.59
Z4 Inland	447	pH	+0.21	0.010	✓	0.50
		PO ₄	+0.23	< 0.001	✓	0.92
		pH	+0.16	< 0.001	✓	0.73
		Fe	+0.13	0.004	✓	0.57
<i>Decadal cohort (Tier C)</i>						
Z1 Ganges Tidal	109	Fe	+0.27	0.005	✓	0.55
		pH	−0.25	0.008	✓	0.50
		Eh	+0.23	0.016		0.46
Z2 Meghna Estuarine	64	TDS	+0.35	0.005	✓	0.52
		EC	+0.34	0.006	✓	0.52
		HCO ₃	+0.32	0.010	✓	0.46
		Cl	+0.25	0.047		0.18
Z3 Chittagong	39	HCO ₃	+0.45	0.004	✓	0.57
		PO ₄	+0.44	0.005	✓	0.55