

Supplementary Information

Artificial Intelligence Modelling to Support the Groundwater Chemistry-Dependent Selection of Groundwater Arsenic Remediation Approaches in Bangladesh

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Supplementary Materials

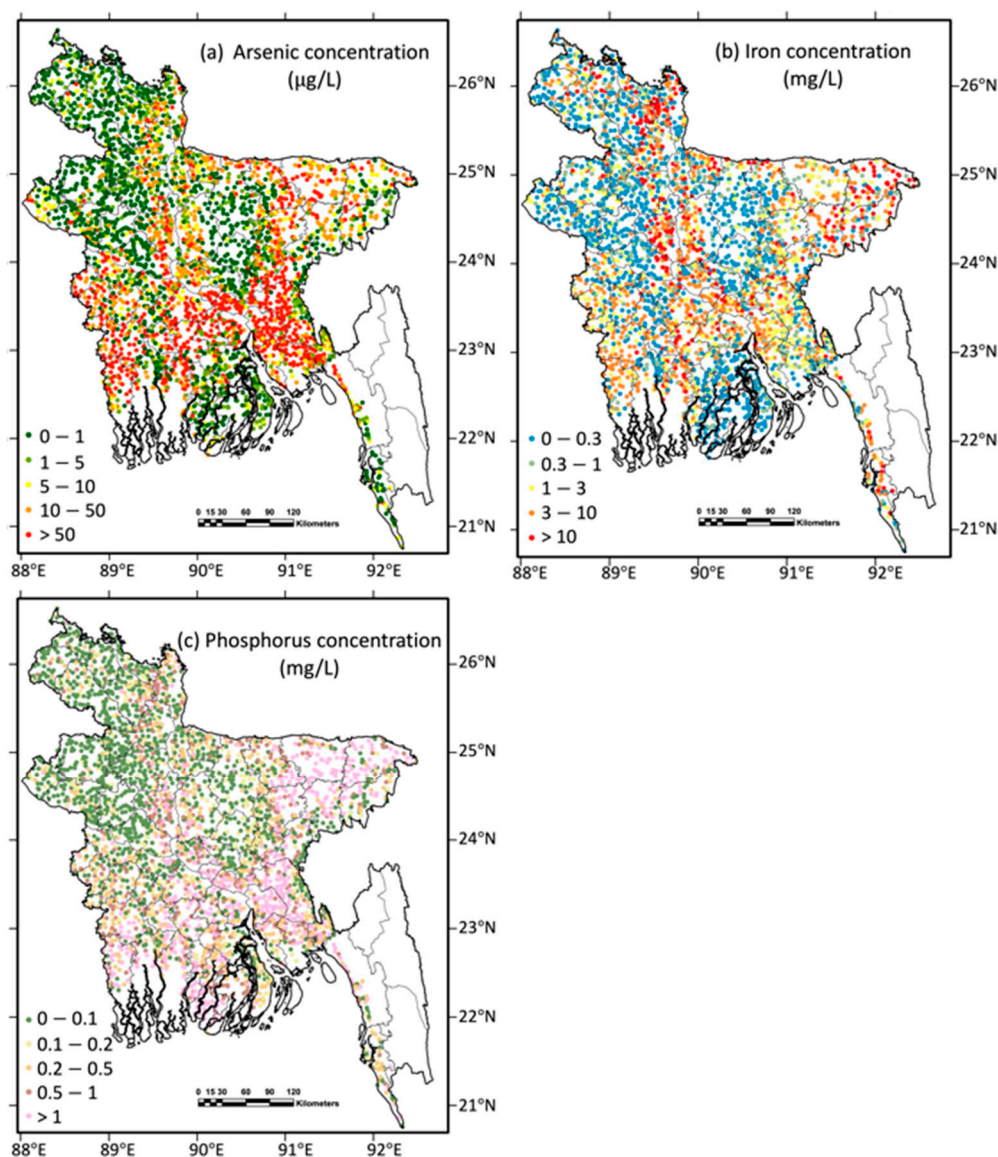


Figure S1. Distribution of secondary groundwater concentration data reported by (DPHE / BGS, 2001) of (a) As, (b) Fe, and (c) P in Bangladesh.

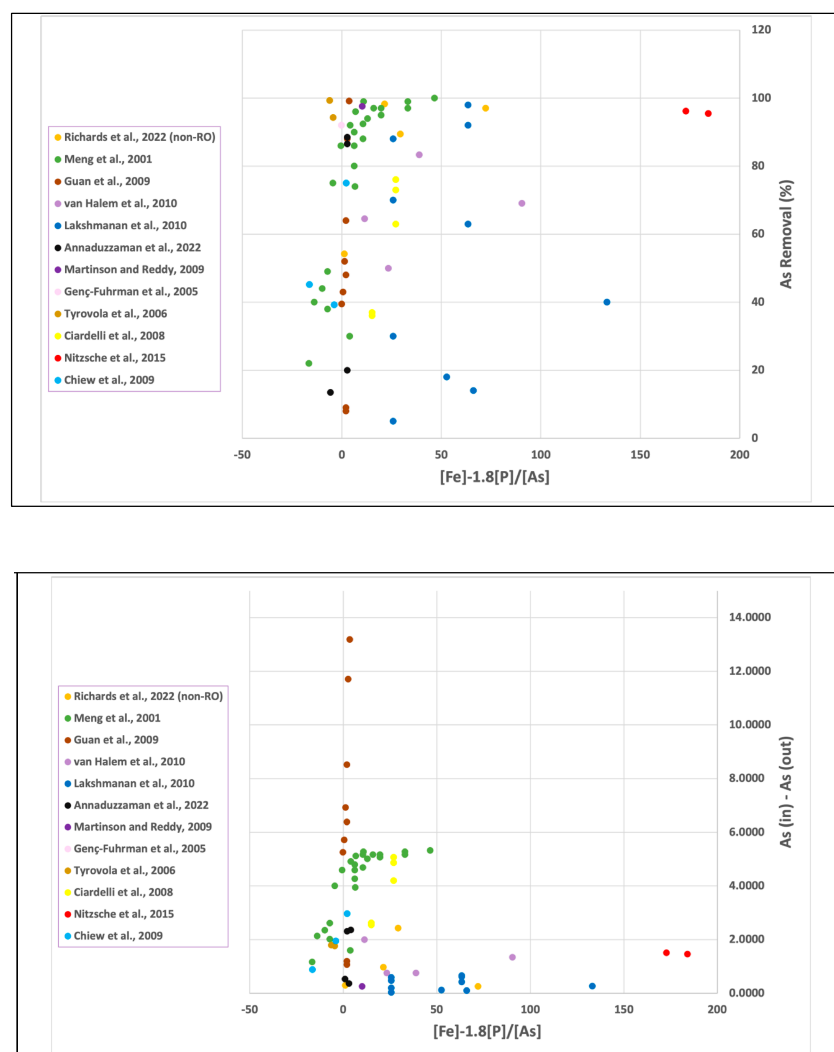


Figure S2. Meta-analysis plot of (top) measured As removal (%) versus molar ratio of $\frac{[Fe] - 1.8[P]}{[As]}$ and (bottom) measured As removal (absolute, expressed as $As (in) - As (out)$, μM) for adsorption or co-precipitation based arsenic removal technologies, in either field or laboratory settings. Data compiled from Meng et al., 2001 (co-precipitation using ferric salts followed by filtration using 0.4 μm membrane filter and co-precipitation using ferric and hypochlorite salts followed by filtration using bucket sand filter), Genç-Fuhrman et al., 2005 (adsorption onto Activated Bauxsol Coated sand), Tyrovola et al., 2006 (removal using columns filled with sand and iron filings in series), Ciardelli et al., 2008 (removal using addition of Fe(II) aided by natural oxidation; removal using addition of Fe(II) aided by natural oxidation and followed by seeding using hydroxylapatite crystals immediately; two-step process that has a gap in between Fe(II) and hydroxylapatite addition), Guan et al., 2009 (KMnO₄-Fe(II) process for As(III) removal), Martinson and Reddy, 2009 (CuO nanoparticles), Chiew et al., 2009 (household BioSand filter amended with iron nails), van Halem et al., 2010 (community-scale facility using subsurface As removal and adsorptive-catalytic oxidation mechanism), Lakshmanan et al., 2010 (FeCl₃ chemical coagulation), Nitzsche et al., 2015 (household sand filter), Annaduzzaman et al., 2022 (adsorption onto hydrous ferric oxides), Richards et al., 2022b (removal by homemade bucket filtration system (non-RO) and multi-stage filtration system in a non-household setting and multi-stage filtration system (non-RO) in a non-household setting are included, and removal by reverse osmosis (RO)-based technology are excluded).

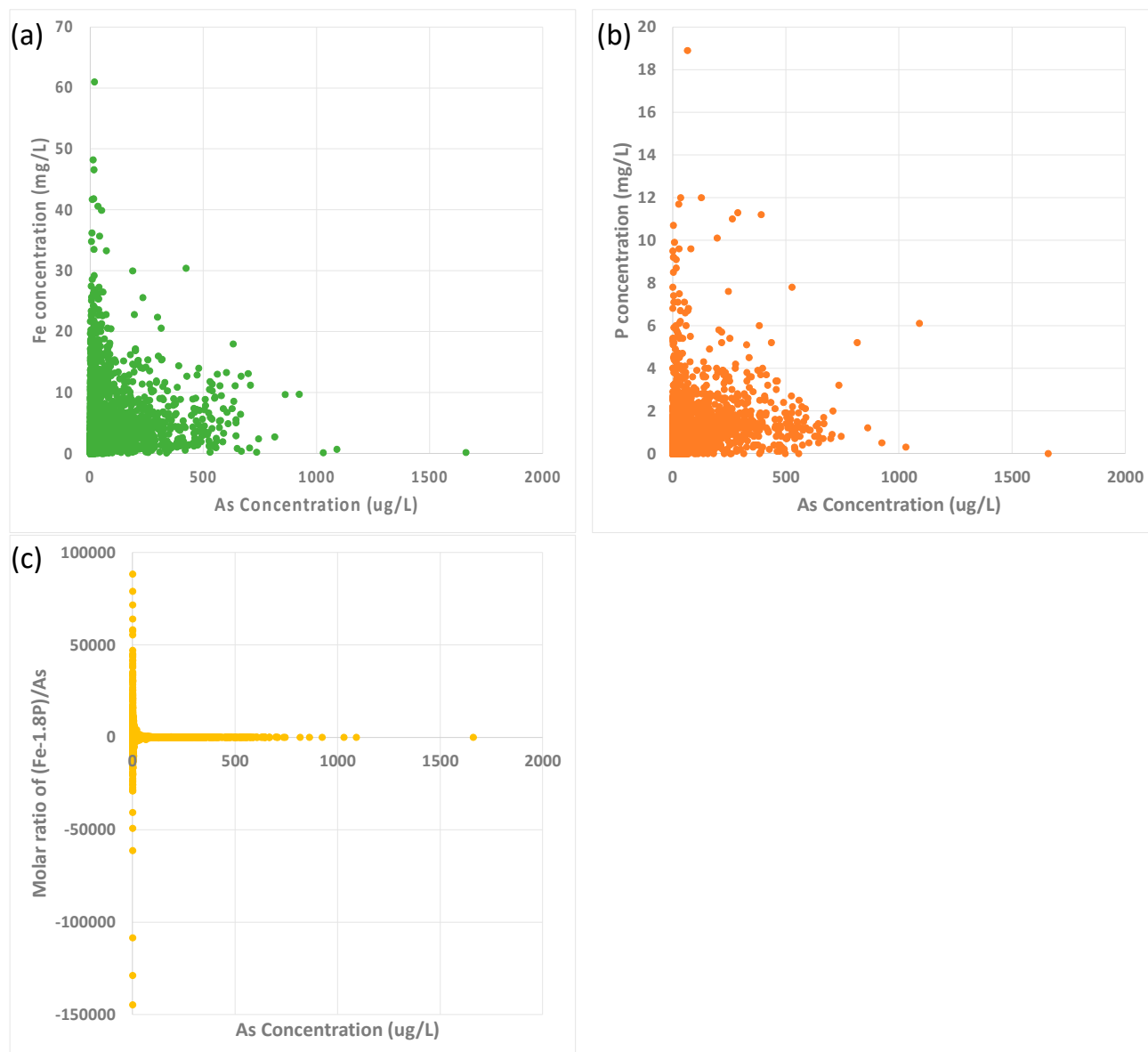


Figure S3. Bivariate plots between groundwater concentrations of (a) Fe and (b) P and (c) molar ratio of $([\text{Fe}] - 1.8[\text{P}]) / [\text{As}]$ versus As (As in (c) is $> 10 \mu\text{g/L}$), Fe, P and As data all from (DPHE / BGS, 2001).

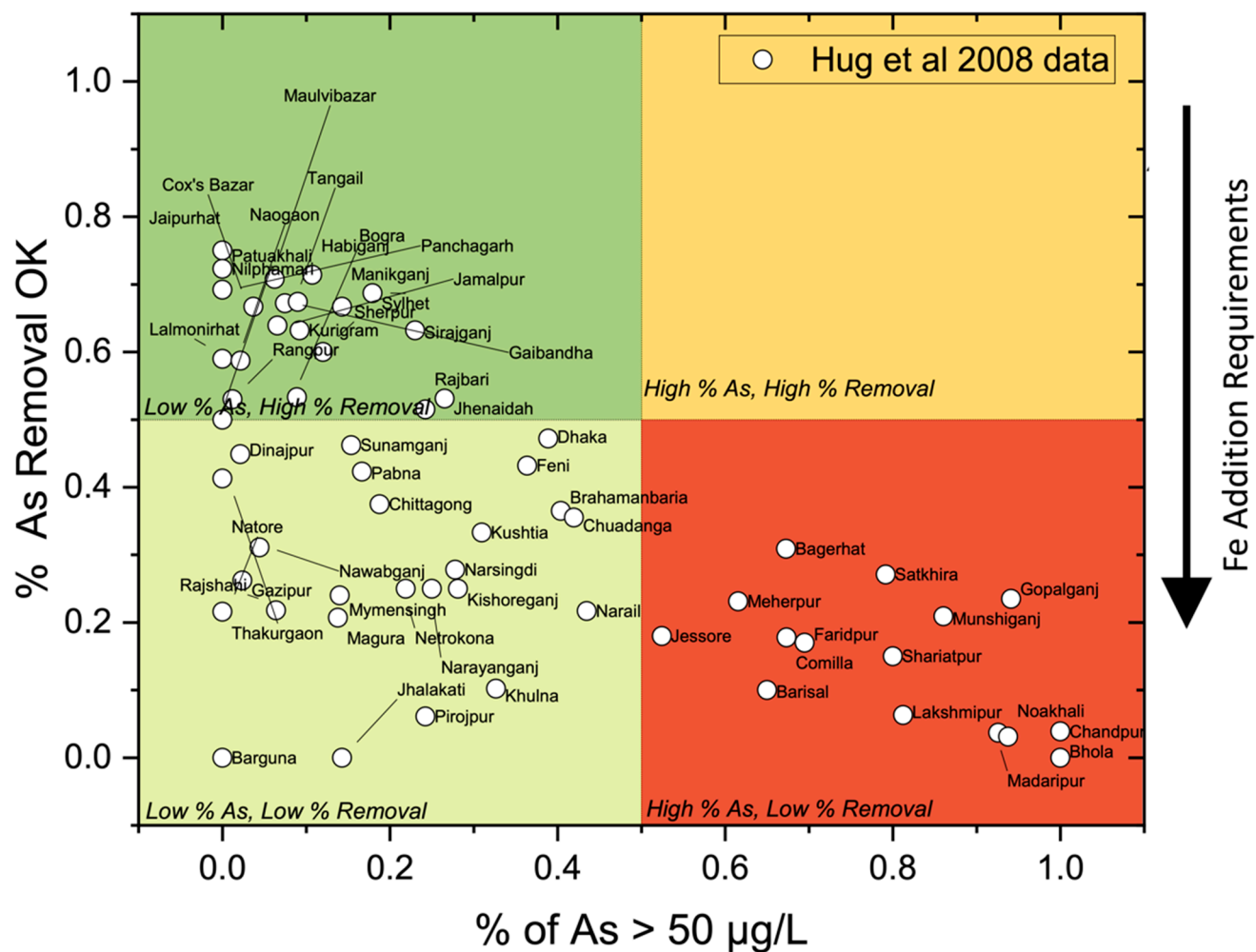


Figure S4. District-level sampled As remediation efficiency (% of samples with As removal OK) versus the percentage of samples with groundwater arsenic exceeding 50 µg/L based on Hug et al (2008) data.

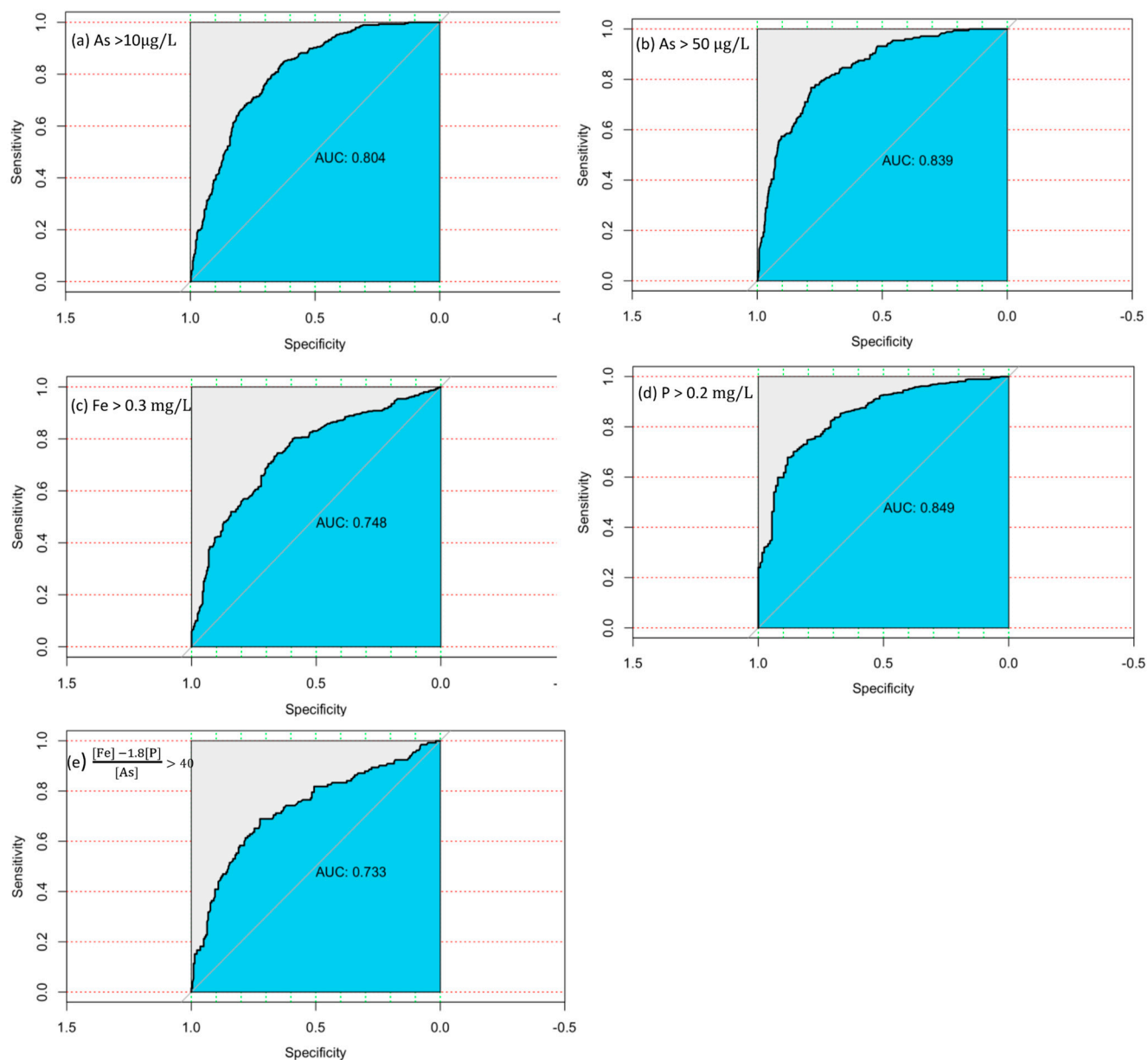


Figure S5. AUC curves of generated random forest models (this study) of distribution of (a) As > 10 $\mu\text{g/L}$, (b) As > 50 $\mu\text{g/L}$, (c) Fe > 0.3 mg/L, (d) P > 0.2 mg/L, and (e) molar ratio of $([\text{Fe}] - 1.8[\text{P}]) / [\text{As}] > 40$.

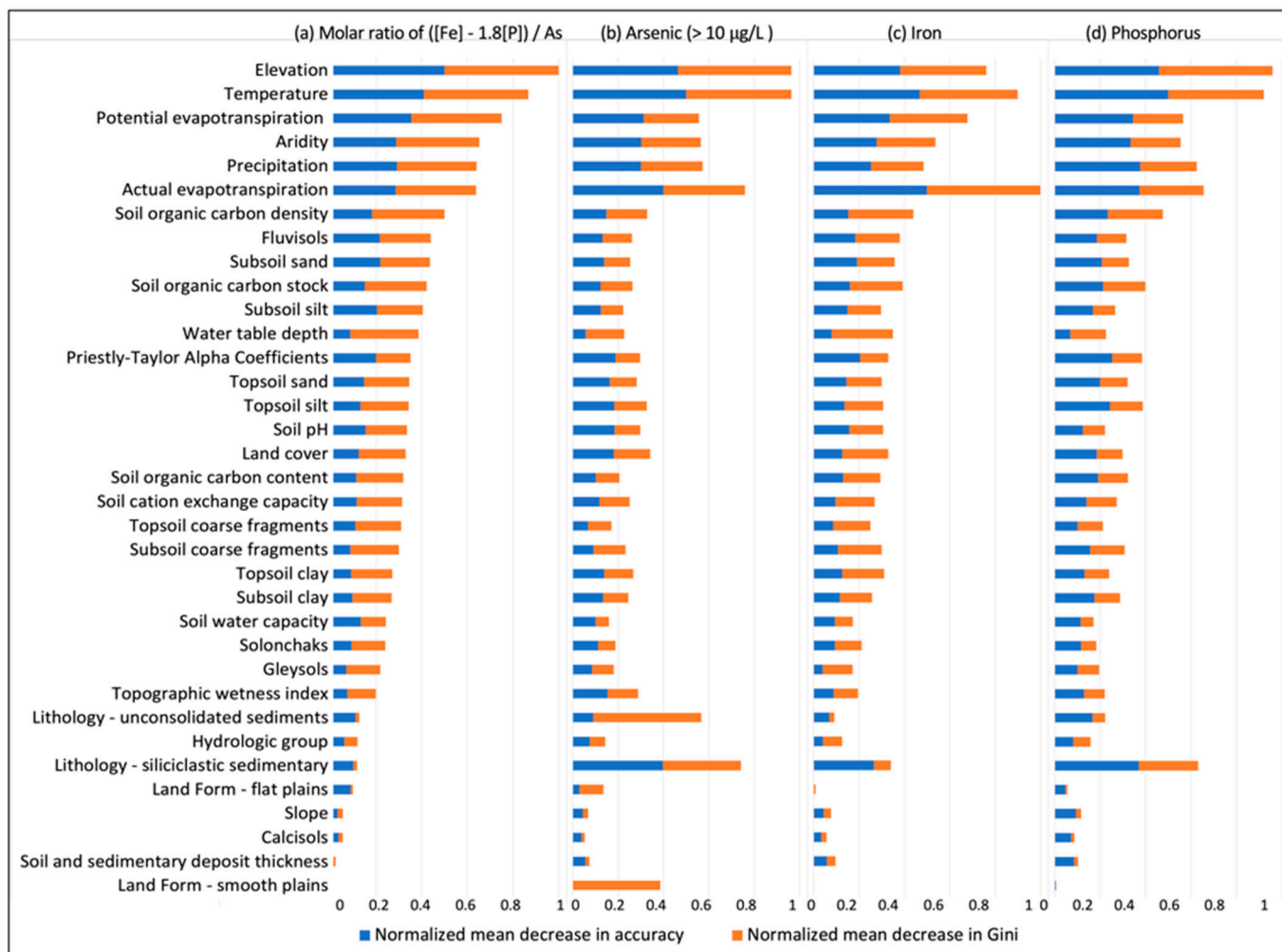


Figure S6. Normalized importance of predictors in terms of mean decrease values in accuracy and in Gini node impurity in the random forest models (this study) of distribution of (a) As ($> 10 \mu\text{g/L}$), (b) Fe, (c) P, and (d) molar ratio of $([Fe] - 1.8[P]) / [As]$. Environmental predictors ($n=35$) for secondary chemical concentration locations were abstracted and a predictor dataset at 1 km^2 resolution for the whole of Bangladesh was generated in ArcGIS (version 10.2) to finalize the entire dataset for the further modelling and prediction. The importance of the predictors in the four random forest models of As $> 10 \mu\text{g/L}$, Fe $> 0.3 \text{ mg/L}$, P $> 0.2 \text{ mg/L}$ and molar ratio of $([Fe] - 1.8[P]) / [As] > 40$ was assessed by the mean decrease in both accuracy and Gini node impurity, normalized by the maximum value calculated among all predictors. The orders of importance of predictors in four random forest models has certain similarities, and this may be due to the same predictor combination used in different random forest models. The selection of environmental predictors in this study was mainly based on the mobility, releasement, and enrichment mechanisms of As in groundwater (Smedley and Kinniburgh 2002; Islam et al. 2004; McArthur et al. 2004; Charlet and Polya 2006; Polya and Charlet 2009; Rodríguez-Lado et al. 2013; Polya and Middleton 2017; Podgorski et al. 2017; Polya et al. 2019a, b). Therefore, updating the environmental predictor dataset based on various chemicals' mobility mechanisms of As, Fe, and P may improve the models as the distribution of the different target values (i.e. for As, Fe, and P) are related to different geochemistry processes.

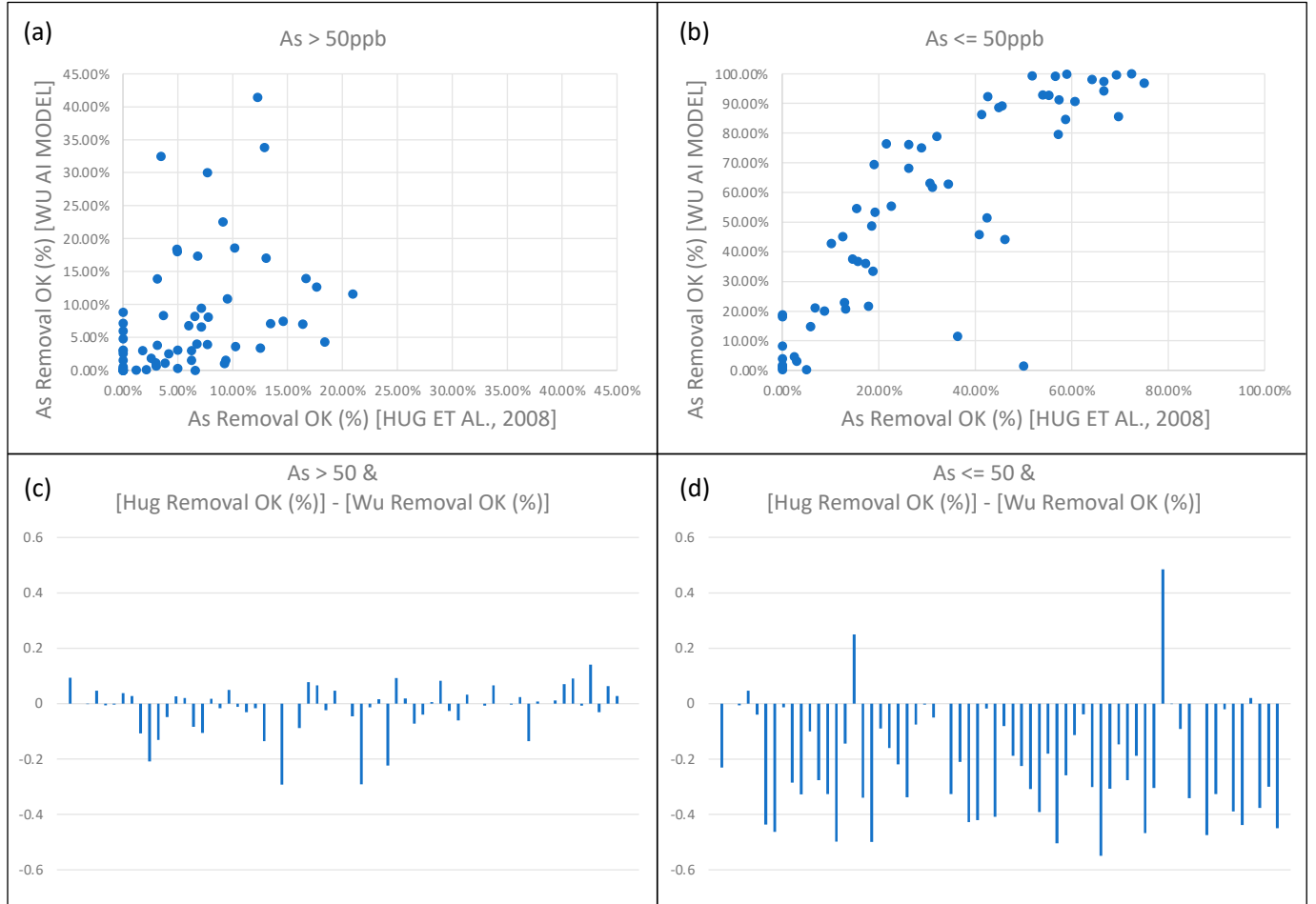


Figure S7. Comparison between model-predicted district-level 1 km² pixel-level proportion (%) of As removal OK (using molar ratio of 40) with district-level measured well proportion of As removal OK calculated by Hug et al (2008) according to DPHE / BGS National Hydrochemical Survey data (DPHE / BGS, 2001) within 10-90m depth in two different As concentration ranges – 0 - 50 µg/L and > 50 µg/L. (a) model-predicted district-level pixel proportion (%) of As removal OK (using molar ratio of 40) vs. district-level measured well proportion of As removal OK calculated by Hug et al (2008) according to DPHE / BGS National Hydrochemical Survey data in As range of 0 - 50 µg/L; (b) model-predicted district-level pixel proportion (%) of As removal OK (using molar ratio of 40) vs. district-level measured well proportion of As removal OK calculated by Hug et al (2008) according to DPHE / BGS National Hydrochemical Survey data in As range of > 50 µg/L; (c) district-level measured well proportion of As removal OK calculated by Hug et al (2008) according to DPHE / BGS National Hydrochemical Survey data - model-predicted district-level pixel proportion (%) of As removal OK (using molar ratio of 40) vs in As range of 0 - 50 µg/L; (d) district-level measured well proportion of As removal OK calculated by Hug et al (2008) according to DPHE / BGS National Hydrochemical Survey data - model-predicted district-level pixel proportion (%) of As removal OK (using molar ratio of 40) vs in As range of > 50 µg/L.

Table S1. Description of predictors used in the random forest models..

Variable	Variables	Descriptions	Data Sources
Climate	Actual evapotranspiration	Average rate of actual evapotranspiration (mm/yr)	[Trabucco et al., 2010]
Climate	Aridity	PET/Precipitation	[Trabucco et al., 2009]
Climate	Potential evapotranspiration	Average rate of potential evapotranspiration (mm/yr)	[Trabucco et al., 2009]
Climate	Precipitation	Average rate of precipitation (mm/yr)	[Trabucco et al., 2010]
Climate	Priestley-Taylor alpha coefficient	AET/PET	[Trabucco et al., 2010]
Climate	Temperature	Average temperature (°C)	[Trabucco et al., 2009]
Soil	Calcisols	Probability of the occurrence of calcisols	[Hengl et al., 2017]
Soil	Fluvisols	Probability of the occurrence of fluvisols	[Hengl et al., 2017]
Soil	Gleysols	Probability of the occurrence of gleysols	[Hengl et al., 2017]
Soil	Subsoil clay	Weight % of clay particles (<0.0002 mm) at 2 m depth	[Hengl et al., 2017]
Soil	Subsoil coarse fragments	Volume % of coarse fragments (>2 mm) at 2 m depth	[Hengl et al., 2017]
Soi	Subsoil sand	Weight % of sand particles (0.05 - 2 mm) at 2 m depth	[Hengl et al., 2017]
Soil	Subsoil silt	Weight % of silt particles (0.0002 - 0.05 mm) at 2 m depth	[Hengl et al., 2017]
Soil	Topsoil clay	Weight % of clay particles (<0.0002 mm) at 0 m depth	[Hengl et al., 2017]
Soil	Topsoil coarse fragments	Volume % of coarse fragments (>2 mm) at 0 m depth	[Hengl et al., 2017]
Soi	Topsoil sand	Weight % of sand particles (0.05 - 2 mm) at 0 m depth	[Hengl et al., 2017]
Soil	Topsoil silt	Weight % of silt particles (0.0002 - 0.05 mm) at 0 m depth	[Hengl et al., 2017]
Soil	Soil cation exchange capacity	Cation exchange capacity (cmolc/kg) at 2 m depth	[Hengl et al., 2017]
Soil	Soil pH	Soil pH measured in water at 2 m depth	[Hengl et al., 2017]
Soil	Soil organic carbon content	Soil organic carbon content (g/kg) at 2 m depth	[Hengl et al., 2017]
Soil	Soil organic carbon density	Soil organic carbon density (kg/m ³) at 2 m depth	[Hengl et al., 2017]
Soil	Soil organic carbon stock	Soil organic carbon stock (t/ha) at 2 m depth	[Hengl et al., 2017]
Soil	Soil and sedimentary deposit thickness	The thickness of soil and sedimentary deposit (m)	[Pelletier et al., 2016]
Soil	Solonchaks ¹	Probability of the occurrence of solonchaks	[Hengl et al., 2017]
Soil	Water wilting point	Volume % of available soil water until wilting point at 2 m	[Hengl et al., 2017]
Topography	Slope	Slope (arc)	[Hengl et al., 2018]
Topography	Elevation	Elevation (m)	[USGS, 1996]
Topography	Landform – flat plains	A kind of landform - flat plains	[Hengl et al., 2018]
Topography	Landform – smooth plains	A kind of landform - smooth plains	[Hengl et al., 2018]
Topography	Topographic wetness index	Combination of upslope contributing area and slope	[Hengl et al., 2018]
Others	Water table depths	Water table depths (m)	[Fan et al., 2013]
Others	Land cover	17 different categories of land cover	[Friedl et al., 2010]
Others	Lithology - siliciclastic sedimentary	A kind of lithology - siliciclastic sedimentary rocks	[Hengl et al., 2018]
Others	Lithology – unconsolidated sediments	A kind of lithology - unconsolidated sediments	[Hengl et al., 2018]
Others	Hydrologic soil group	4 different hydrologic soil group	[Hengl et al., 2017]

Table S2. Bangladesh district-level comparison between this study and Hug et al (2008) of percentage of groundwater for which satisfactory/OK As removal is predicted. Both models utilise the same secondary data, i.e. DPHE / BGS National Hydrochemical Survey data (DPHE / BGS, 2001) within 10 m -90 m depth range. The blank cell in this table is due to there is no data form Hug et al (2008)'s study.

District	Samples included by [HUG ET AL, 2008]	As (mean \pm std) ($\mu\text{g/L}$) [HUG ET AL, 2008]	As ($\mu\text{g/L}$) > 50 [HUG ET AL, 2008]	As removal OK [HUG ET AL, 2008]	As removal OK (%) [HUG ET AL, 2008]	% of As ($\mu\text{g/L}$) \leq 50 & (Fe-1.8P)/As (mol/mol) > 40 [HUG ET AL, 2008]	% of As ($\mu\text{g/L}$) > 50 & (Fe-1.8P)/As (mol/mol) > 40 [HUG ET AL, 2008]	% of As ($\mu\text{g/L}$) > 10 [this study]	% of As removal OK (for all As ranges) [this study]	% of As ($\mu\text{g/L}$) > 50 & As removal OK [this study]	% of As ($\mu\text{g/L}$) \leq 50 & As removal OK [this study]	As removal OK (%) [HUG ET AL, 2008] - % of As removal OK (for all As ranges) [this study]
Bagerhat	55	175 \pm 172	37	17	30.9%	14.6%	16.4%	60.0%	44.6%	7.0%	37.5%	-13.7%
Bandarban								0.0%	100.0%	8.5%	91.5%	
Barguna	3	5 \pm 6	0	0	0.0%	0.0%	0.0%	0.0%	0.7%	0.2%	0.6%	-0.7%
Barisal	40	189 \pm 202	26	4	10.0%	5.0%	5.0%	31.6%	0.6%	0.3%	0.3%	9.4%
Bhola	2	201 \pm 54	2	0	0.0%	0.0%	0.0%	1.0%	4.5%	0.6%	4.0%	-4.5%
Bogra	90	18 \pm 70	8	48	53.3%	45.6%	7.8%	12.4%	97.3%	8.1%	89.2%	-43.9%
Brahmanbaria	52	103 \pm 159	21	19	36.5%	28.9%	7.7%	58.1%	79.0%	3.9%	75.1%	-42.5%
Chandpur	52	410 \pm 178	52	2	3.9%	0.0%	3.9%	96.6%	2.4%	1.1%	1.3%	1.5%
Chittagong	32	39 \pm 80	6	12	37.5%	34.4%	3.1%	14.8%	76.8%	13.8%	62.9%	-39.3%
Chuadanga	31	82 \pm 124	13	11	35.5%	22.6%	12.9%	97.6%	89.2%	33.8%	55.4%	-53.7%
Comilla	101	150 \pm 152	68	18	17.8%	12.9%	5.0%	84.6%	41%	18.0%	22.8%	-23.0%
Cox's Bazar	27	4 \pm 13	1	18	66.7%	66.7%	0.0%	0.0%	99.0%	4.8%	94.3%	-32.4%
Dhaka	36	51 \pm 71	14	17	47.2%	30.5%	16.7%	66.0%	77.0%	13.9%	63.1%	-29.8%
Dinajpur	94	3 \pm 8	2	42	44.9%	42.6%	2.1%	0.0%	92.5%	0.1%	92.3%	-47.8%
Faridpur	59	149 \pm 155	41	10	17.0%	6.8%	10.2%	94.6%	39.7%	18.6%	21.2%	-22.8%

Feni	44	62±87	16	19	43.2%	36.4%	6.8%	79.4%	28.9%	17.4%	11.4%	14.3%
Gaibandha	67	22±87	5	45	67.2%	64.2%	3.0%	7.7%	99.3%	1.2%	98.1%	-32.1%
Gazipur	42	4±24	1	11	26.2%	26.2%	0.0%	8.2%	77.7%	1.6%	76.1%	-51.5%
Gopalganj	34	229±153	32	8	23.5%	5.9%	17.6%	99.4%	27.4%	12.6%	14.8%	-3.9%
Habiganj	56	23±47	6	40	71.4%	69.6%	1.8%	61.9%	88.6%	3.0%	85.6%	-17.2%
Jaipurhat	40	1±2	0	30	75.0%	75.0%	0.0%	0.0%	99.9%	3.0%	96.9%	-24.9%
Jamalpur	61	15±35	4	39	63.9%	57.4%	6.6%	7.3%	99.4%	8.2%	91.2%	-35.4%
Jessore	61	76±81	32	11	18.0%	13.1%	4.9%	90.5%	39.1%	18.4%	20.7%	-21.0%
Jhalakati	14	54±144	2	0	0.0%	0.0%	0.0%	4.5%	0.3%	0.0%	0.3%	-0.3%
Jhenaidah	49	49±91	13	26	53.1%	40.8%	12.2%	75.4%	87.3%	41.4%	45.8%	-34.2%
Khagrachhari								0.3%	100.0%	43.2%	56.9%	
Khulna	49	52±89	16	5	10.2%	10.2%	0.0%	75.4%	51.6%	8.8%	42.8%	-41.4%
Kishoreganj	96	55±96	27	24	25.0%	15.6%	9.4%	68.7%	38.2%	1.5%	36.7%	-13.2%
Kurigram	76	21±57	7	48	63.2%	56.6%	6.6%	14.9%	99.3%	0.0%	99.3%	-36.1%
Kushtia	42	15±311	13	14	33.3%	26.2%	7.1%	25.1%	77.7%	9.4%	68.2%	-44.3%
Lakshmipur	16	323±279	13	1	6.3%	0.0%	6.3%	77.3%	3.3%	1.5%	1.8%	2.9%
Lalmonirhat	39	1±3	0	23	59.0%	59.0%	0.0%	0.0%	99.9%	0.0%	99.9%	-40.9%
Madaripur	27	255±193	25	1	3.7%	0.0%	3.7%	93.6%	16.5%	8.3%	8.1%	-12.8%
Magura	29	25±53	4	6	20.7%	17.2%	3.5%	50.3%	68.5%	32.5%	36.1%	-47.8%
Manikganj	42	23±25	6	28	66.7%	57.1%	9.5%	79.9%	90.4%	10.8%	79.6%	-23.8%
Maulvibazar	48	17±39	3	34	70.8%	66.7%	4.2%	43.8%	100.0%	2.5%	97.5%	-29.2%
Meherpur	13	115±145	8	3	23.1%	15.4%	7.7%	89.3%	84.6%	30.0%	54.5%	-61.5%
Munshiganj	43	198±146	37	9	20.9%	0.0%	21%	91.7%	29.6%	11.6%	18.1%	-8.7%
Mymensingh	100	17±35	14	24	24.0%	19.0%	5.0%	12.5%	72.5%	3.1%	69.4%	-48.5%
Naogaon	92	6±30	2	54	58.7%	58.7%	0.0%	0.1%	91.8%	7.2%	84.6%	-33.1%
Narail	23	92±99	10	5	21.7%	8.7%	13.0%	84.7%	37.1%	17.1%	20.0%	-15.3%
Narayanganj	28	52±97	7	7	25.0%	17.9%	7.1%	66.2%	28.3%	6.6%	21.7%	-3.3%
Narsingdi	54	43±64	15	15	27.8%	18.5%	9.3%	54.7%	49.7%	1.0%	48.7%	-22.0%

Natore	51	1±3	0	11	21.6%	21.6%	0.0%	0.5%	79.1%	2.6%	76.5%	-57.5%
Nawabganj	45	7±14	2	14	31.1%	31.1%	0.0%	6.3%	67.7%	6.0%	61.7%	-36.6%
Netrokona	64	30±43	14	16	25.0%	18.8%	6.3%	66.7%	36.4%	3.0%	33.4%	-11.4%
Nilphamari	47	2±5	0	34	72.3%	72.3%	0.0%	0.0%	100.0%	0.0%	100.0%	-27.7%
Noakhali	32	231±167	30	1	3.1%	0.0%	3.1%	65.4%	22.6%	3.8%	18.8%	-19.4%
Pabna	78	32±90	13	33	42.3%	32.1%	10.3%	11.0%	82.5%	3.7%	78.8%	-40.2%
Panchagarh	39	3±6	0	27	69.2%	69.2%	0.0%	0.0%	99.6%	0.0%	99.6%	-30.4%
Patuakhali	2	7±6	0	1	50.0%	50.0%	0.0%	0.4%	1.8%	0.3%	1.5%	48.2%
Pirojpur	33	42±74	8	2	6.1%	3.0%	3.0%	31.8%	3.8%	0.7%	3.1%	2.3%
Rajbari	33	50±91	8	17	51.5%	42.4%	9.1%	41.0%	74.0%	22.5%	51.5%	-22.5%
Rajshahi	78	8±18	5	17	21.8%	19.2%	2.6%	5.9%	55.2%	1.8%	53.4%	-33.4%
Rangamati								4.4%	99.4%	32.3%	67.1%	
Rangpur	83	8±33	1	44	53.0%	51.8%	1.2%	3.8%	99.3%	0.0%	99.3%	-46.3%
Satkhira	48	156±130	38	13	27.1%	12.5%	14.6%	93.2%	52.5%	7.5%	45.1%	-25.5%
Shariatpur	40	184±166	32	6	15.0%	2.5%	12.5%	91.1%	8.0%	3.4%	4.6%	7.0%
Sherpur	50	23±36	6	30	60.0%	54.0%	6.0%	24.4%	99.7%	6.8%	92.9%	-39.7%
Sirajganj	87	31±53	20	55	63.2%	44.8%	18.4%	53.9%	92.9%	4.3%	88.6%	-29.7%
Sunamganj	13	41±62	2	6	46.2%	46.2%	0.0%	87.9%	47.2%	3.1%	44.1%	-1.1%
Sylhet	67	19±28	12	46	68.7%	55.2%	13.4%	41.8%	99.8%	7.1%	92.8%	-31.2%
Tangail	89	20±33	8	60	67.4%	60.7%	6.7%	35.7%	94.6%	4.0%	90.6%	-27.2%
Thakurgaon	46	1±1	0	19	41.3%	41.3%	0.0%	0.0%	86.3%	0.0%	86.3%	-45.0%

Supplementary Information References

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