Supplementary Information for:
A Decade of Machine Learning for Adsorption of Emerging Contaminants: A Systematic Review of Algorithms, Performance, and Methodological Transparency

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Summary:

Number of Tables: 15 (Tables S1–S15)

Number of Sections: 12 (Sections S1–S12)

Table of Contents

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Abbreviations

AdaBoost	Adaptive Boosting	**MOF**	Metal–Organic Framework
ANFIS	Adaptive Neuro-Fuzzy Inference System	**MLP**	Multilayer Perceptron
ANN	Artificial Neural Network	**MSE**	Mean Squared Error
ARG	Antibiotic Resistance Gene	**PCA**	Principal Component Analysis
BPA	Bisphenol A	**PCP**	Personal Care Product
CatBoost	Categorical Boosting	**PFAS**	Per-/Polyfluoroalkyl Substances
CNN	Convolutional Neural Network	**PFOA**	Perfluorooctanoic Acid
DNN	Deep Neural Network	**PFOS**	Perfluorooctane Sulfonate
DT	Decision Tree	**PRISMA**	Preferred Reporting Items for Systematic Reviews and Meta-Analyses
EC	Emerging Contaminant		
EDC	Endocrine-Disrupting Compound	$q_{\mathbf{max}}$	Maximum Adsorption Capacity
GBM	Gradient Boosting Machine	**RF**	Random Forest
GEP	Gene Expression Programming	**RMSE**	Root Mean Squared Error
GNN	Graph Neural Network	**RNN**	Recurrent Neural Network
GPR	Gaussian Process Regression	**RSM**	Response Surface Methodology
GRNN	General Regression Neural Network	**SHAP**	SHapley Additive exPlanations
IQR	Interquartile Range	**SVM**	Support Vector Machine
kNN	k-Nearest Neighbors	**SVR**	Support Vector Regression
LightGBM	Light Gradient Boosting Machine	**XAI**	Explainable Artificial Intelligence
LSTM	Long Short-Term Memory	**XGBoost**	Extreme Gradient Boosting
MAE	Mean Absolute Error		

S1. PRISMA 2020 Checklist

Table S1 presents the completed PRISMA 2020 checklist for this systematic review, indicating where each item is reported.

Table S1: PRISMA 2020 checklist indicating where each item is reported.

Section and Topic	Item	Checklist item	Location
TITLE			
Title	1	Identify the report as a systematic review.	Title
ABSTRACT			
Abstract	2	See the PRISMA 2020 for Abstracts checklist.	Abstract
INTRODUCTION			
Rationale	3	Describe the rationale for the review in the context of existing knowledge.	Section 1, paragraphs 1–4
Objectives	4	Provide an explicit statement of the objective(s) or question(s) the review addresses.	Section 1, paragraph 5
METHODS			
Eligibility criteria	5	Specify the inclusion and exclusion criteria for the review and how studies were grouped for the syntheses.	Section 2.1, Table 1
Information sources	6	Specify all databases, registers, websites, organisations, reference lists and other sources searched or consulted to identify studies. Specify the date when each source was last searched or consulted.	Section 2.2

Section and Topic	**Item**	**Checklist item**	**Location**
Search strategy	7	Present the full search strategies for all databases, registers and websites, including any filters and limits used.	Section 2.3; SI Section S2.1
Selection process	8	Specify the methods used to decide whether a study met the inclusion criteria of the review, including how many reviewers screened each record and each report retrieved, whether they worked independently, and if applicable, details of automation tools used in the process.	Section 2.4; tool performance evaluated in Section 2.6.1
Data collection process	9	Specify the methods used to collect data from reports, including how many reviewers collected data from each report, whether they worked independently, any processes for obtaining or confirming data from study investigators, and if applicable, details of automation tools used in the process.	Section 2.5; tool performance evaluated in Section 2.6.2; SI Section S2.4
Data items	10a	List and define all outcomes for which data were sought. Specify whether all results that were compatible with each outcome domain in each study were sought, and if not, the methods used to decide which results to collect.	Section 2.5; SI Section S2.4
	10b	List and define all other variables for which data were sought. Describe any assumptions made about any missing or unclear information.	Sections 2.5 and 2.8

Section and Topic	Item	Checklist item	Location
Study risk of bias assessment	11	Specify the methods used to assess risk of bias in the included studies, including details of the tool(s) used, how many reviewers assessed each study and whether they worked independently, and if applicable, details of automation tools used in the process.	Not assessed; rationale in Section 2.7
Effect measures	12	Specify for each outcome the effect measure(s) (e.g., risk ratio, mean difference) used in the synthesis or presentation of results.	Section 2.8
Synthesis methods	13a	Describe the processes used to decide which studies were eligible for each synthesis.	Section 2.8
	13b	Describe any methods required to prepare the data for presentation or synthesis, such as handling of missing summary statistics, or data conversions.	Sections 2.5.3 and 2.8
	13c	Describe any methods used to tabulate or visually display results of individual studies and syntheses.	Section 3, Figs. 2–10
	13d	Describe any methods used to synthesize results and provide a rationale for the choice(s). If meta-analysis was performed, describe the model(s), method(s) to identify the presence and extent of statistical heterogeneity, and software package(s) used.	Section 2.8; SI Section S3

Section and Topic	Item	Checklist item	Location
	13e	Describe any methods used to explore possible causes of heterogeneity among study results.	SI Section S3
	13f	Describe any sensitivity analyses conducted to assess robustness of the synthesized results.	Not applicable
Reporting bias assessment	14	Describe any methods used to assess risk of bias due to missing results in a synthesis.	Section 2.7; funnel plot and Egger's test, Section 3.5.1
Certainty assessment	15	Describe any methods used to assess certainty (or confidence) in the body of evidence for an outcome.	Not assessed; rationale in Section 2.7
RESULTS			
Study selection	16a	Describe the results of the search and selection process, from the number of records identified in the search to the number of studies included in the review, ideally using a flow diagram.	Sections 2.3–2.4; Fig. 1
	16b	Cite studies that might appear to meet the inclusion criteria, but which were excluded, and explain why they were excluded.	Sections 2.1 and 2.6.1, Table 1
Study characteristics	17	Cite each included study and present its characteristics.	SI Section S8; SI dataset
Risk of bias in studies	18	Present assessments of risk of bias for each included study.	Not assessed; rationale in Section 2.7
Results of individual studies	19	For all outcomes, present, for each study: (a) summary statistics for each group and (b) an effect estimate and its precision.	SI dataset

Section and Topic	Item	Checklist item	Location
Results of syntheses	20a	For each synthesis, briefly summarise the characteristics and risk of bias among contributing studies.	Sections 3.1–3.7
	20b	Present results of all statistical syntheses conducted. If meta-analysis was done, present for each the summary estimate and its precision and measures of statistical heterogeneity.	Section 3.5; SI Section S3
	20c	Present results of all investigations of possible causes of heterogeneity among study results.	Section 3.5; SI Section S3
	20d	Present results of all sensitivity analyses conducted to assess the robustness of the synthesized results.	Not applicable
Reporting biases	21	Present assessments of risk of bias due to missing results for each synthesis assessed.	Section 3.5.1 (funnel plot, Egger's test)
Certainty of evidence	22	Present assessments of certainty (or confidence) in the body of evidence for each outcome assessed.	Not assessed; rationale in Section 2.7
DISCUSSION			
Discussion	23a	Provide a general interpretation of the results in the context of other evidence.	Section 4 (Conclusions)
	23b	Discuss any limitations of the evidence included in the review.	Section 3.10
	23c	Discuss any limitations of the review processes used.	Sections 2.6 and 3.10

Section and Topic	Item	Checklist item	Location
	23d	Discuss implications of the results for practice, policy, and future research.	Sections 3.9 and 4
Other Information			
Registration and protocol	24a	Provide registration information for the review, including register name and registration number, or state that the review was not registered.	Not registered
	24b	Indicate where the review protocol can be accessed, or state that a protocol was not prepared.	Protocol not prepared
	24c	Describe and explain any amendments to information provided at registration or in the protocol.	Not applicable
Support	25	Describe sources of financial or non-financial support for the review, and the role of the funders or sponsors in the review.	Acknowledgements
Competing interests	26	Declare any competing interests of review authors.	Declaration of Competing Interest
Availability of data, code, and other materials	27	Report which of the following are publicly available and where they can be found: template data collection forms; data extracted from included studies; data used for all analyses; analytic code; any other materials used in the review.	SI Section S8

S2. Search Strategy and Screening Protocol

S2.1. Database and Search String

The systematic literature search was conducted on two databases: Scopus and PubMed.

Scopus. (accessed February 23, 2026). The following Boolean search string was used:

```
TITLE-ABS-KEY( ( "machine learning" OR "deep learning" OR "artificial intelligence"
OR "neural network" OR "random forest" OR "support vector" OR "gradient boosting"
OR "XGBoost" OR "decision tree" OR "ensemble learning" ) AND ( "adsorption" OR
"adsorb*" OR "biosorption" ) AND ( "emerging contaminant*" OR "emerging pollutant*"
OR "pharmaceutical*" OR "antibiotic*" OR "endocrine disrupt*" OR "PFAS" OR "PFOA" OR
"PFOS" OR "microplastic*" OR "pesticide*" OR "personal care product*" ) )
```

This search returned 1,337 records. No date restriction was applied.

PubMed. (accessed February 23, 2026). The following search string, combining title/abstract fields (`[tiab]`) and MeSH headings (`[mh]`), was used:

```
(("machine learning"[tiab] OR "deep learning"[tiab] OR "artificial intelligence"[tiab]
OR "neural network"[tiab] OR "neural networks"[tiab] OR "artificial neural
network"[tiab] OR "random forest"[tiab] OR "random forests"[tiab] OR "support
vector"[tiab] OR "gradient boosting"[tiab] OR "XGBoost"[tiab] OR "CatBoost"[tiab]
OR "LightGBM"[tiab] OR "ensemble learning"[tiab] OR "transfer learning"[tiab]
OR "decision tree"[tiab] OR "decision trees"[tiab] OR "convolutional neural
network"[tiab] OR "recurrent neural network"[tiab] OR "LSTM"[tiab] OR "graph
neural network"[tiab] OR "ANFIS"[tiab] OR "SHAP"[tiab] OR "explainable AI"[tiab]
OR "Bayesian optimization"[tiab] OR "genetic algorithm"[tiab] OR "predictive
model"[tiab] OR "data-driven"[tiab] OR "Machine Learning"[mh]) AND ("adsorption"[tiab]
OR "sorption"[tiab] OR "biosorption"[tiab] OR "removal"[tiab] OR "uptake"[tiab]
OR "isotherm"[tiab] OR "adsorbent"[tiab] OR "adsorbents"[tiab] OR "activated
carbon"[tiab] OR "biochar"[tiab] OR "metal-organic framework"[tiab] OR "MOF"[tiab]
OR "zeolite"[tiab] OR "Adsorption"[mh]) AND ("emerging contaminant"[tiab]
OR "emerging contaminants"[tiab] OR "emerging pollutant"[tiab] OR "emerging
pollutants"[tiab] OR "micropollutant"[tiab] OR "micropollutants"[tiab] OR "PFAS"[tiab]
OR "PFOA"[tiab] OR "PFOS"[tiab] OR "perfluoroalkyl"[tiab] OR "polyfluoroalkyl"[tiab]
OR "pharmaceutical"[tiab] OR "pharmaceuticals"[tiab] OR "antibiotic"[tiab]
OR "antibiotics"[tiab] OR "tetracycline"[tiab] OR "ciprofloxacin"[tiab] OR
"amoxicillin"[tiab] OR "sulfamethoxazole"[tiab] OR "ibuprofen"[tiab] OR
"diclofenac"[tiab] OR "carbamazepine"[tiab] OR "naproxen"[tiab] OR "levofloxacin"[tiab]
OR "microplastic"[tiab] OR "microplastics"[tiab] OR "nanoplastic"[tiab] OR
"nanoplastics"[tiab] OR "endocrine disruptor"[tiab] OR "endocrine disruptors"[tiab]
OR "endocrine disrupting"[tiab] OR "bisphenol"[tiab] OR "BPA"[tiab] OR "phthalate"[tiab]
OR "phthalates"[tiab] OR "antibiotic resistance gene"[tiab] OR "antibiotic resistance
```

```
genes"[tiab] OR "personal care product"[tiab] OR "personal care products"[tiab]
OR "triclosan"[tiab] OR "paraben"[tiab] OR "parabens"[tiab] OR "Water Pollutants,
Chemical"[mh] OR "Microplastics"[mh])) AND (2015/01/01:2025/12/31[dp]) AND (English[la])
AND ("Journal Article"[pt] OR "Review"[pt])
```

This search returned 827 records. Results were restricted to journal articles and reviews published in English between January 2015 and December 2025.

Combined results.. The two databases yielded a total of 2,164 records (Scopus: 1,337; PubMed: 827). After removing 419 duplicates (identified by DOI, PMID, and title matching), 1,745 unique records remained for screening.

S2.2. Inclusion Criteria

Studies were included if they met all three of the following criteria:

1. **ML/AI as core methodology:** Machine learning or artificial intelligence must be the primary analytical tool, not merely mentioned or used peripherally.
2. **Adsorption as primary mechanism:** The study must focus on adsorption (or biosorption) as the primary removal mechanism, not membrane filtration, photocatalysis, or biological degradation.
3. **Emerging contaminant as target:** The target pollutant must be classified as an emerging contaminant (pharmaceuticals, antibiotics, EDCs, PFAS, microplastics, pesticides, personal care products, or other emerging pollutants).

S2.3. Screening Process

Screening was conducted in two phases:

- **Phase 1, title/abstract screening:** All 1,337 records were screened against the three inclusion criteria using a combination of automated keyword matching and manual review, yielding 383 candidate papers.

- **Phase 2, full-text screening:** Full texts were extracted from 383 PDFs using the `pypdf` library (92.1% good-quality extraction). A section-aware scoring algorithm evaluated each paper across the three criteria, and the borderline cases ($n = 66$) were resolved by manual inspection. No language model was used at any screening stage. This phase yielded 204 included studies, of which two were identified during revision as review articles and removed, leaving the 202 studies analysed (main text, Section 2.6.1).

S2.4. Data Extraction Protocol

A structured data extraction framework captured 40 fields from each study, organized into five categories:

1. **Bibliographic metadata:** DOI, title, authors, journal, year, country
2. **ML methodology:** algorithms used, best-performing model, task type, validation method, dataset size, number of input features, software
3. **Performance metrics:** R^2, RMSE, MAE, MSE, MAPE
4. **Adsorption system:** adsorbent material, adsorbent category, target contaminant, EC category, isotherm models, kinetic models
5. **Adsorption outcomes:** $q_{\max}$ (mg/g), removal efficiency (%), pH, temperature, water type, study type

Extraction was performed in two complementary phases: (1) regex-based automated extraction (55 ML algorithm patterns, 25+ adsorbent categories, 80+ contaminant patterns), and (2) re-extraction of context-dependent fields with a large language model. Results were merged using a systematic reconciliation protocol.

Table S2 records the configuration of the second phase. The operative instruction given to the model was not preserved verbatim and therefore cannot be reproduced here; what can be reproduced, and is given below, is the specification of the input the model received and the schema its output was confined to. The accuracy of that output was measured against the source PDFs and is reported in main text Section 2.6.2 and SI Section S11.2.

S3. Complete ML Algorithm Inventory

Table S3 lists all 59 unique machine learning algorithms identified across the 202 reviewed studies, with the number of studies employing each algorithm. Total algorithm mentions: 475.

Table S3: Complete inventory of ML algorithms identified in the 202 reviewed studies.

#	Algorithm	n	#	Algorithm	n
1	ANN	131	31	LSBoost	2
2	RF	52	32	PCA	2
3	RSM	47	33	RNN	2
4	XGBoost	23	34	RSML	2
5	ANFIS	22	35	ARDRegression	1

#	Algorithm	n	#	Algorithm	n
6	SVM	21	36	Bayesian Ridge	1
7	DT	18	37	Bayesian nonlinear regression	1
8	GBM	18	38	CGCNN	1
9	Linear Regression	18	39	Elastic Net	1
10	CatBoost	10	40	Ensemble	1
11	kNN	10	41	FFNN	1
12	SVR	9	42	FINN	1
13	CNN	7	43	Fuzzy Logic	1
14	GRNN	6	44	GFA	1
15	AdaBoost	5	45	LM	1
16	Extra Trees	5	46	LassoCV	1
17	LightGBM	5	47	MIC	1
18	GPR	4	48	Neuro-Fuzzy	1
19	Stacking	4	49	PCR	1
20	LASSO	3	50	PLS	1
21	LS-SVM	3	51	Polynomial Fitting	1
22	LSTM	3	52	Polynomial Regression	1
23	MLP	3	53	QML	1
24	PSO	3	54	QSAR (LFER)	1
25	Bagging	2	55	Ridge	1
26	Cubist	2	56	RidgeCV	1
27	DNN	2	57	TAN	1
28	Deep Learning	2	58	Tikhonov Regularization	1
29	GA	2	59	WGAN	1
30	GEP	2			

Table S2: Configuration of the language-model extraction phase (main text, Section 2.5.2).

Element	**Value**
Model	Claude Opus 4.6 (Anthropic)
Access date	February 2026
Interface	Interactive agent session, not a scripted API call
Sampling settings	Provider defaults; output is not deterministic
Prompt	Not preserved verbatim; not reproducible
Passes	One; no independent second language-model pass
Source of text	Each paper's own PDF, parsed with `pypdf`; no external source, and no reliance on the model's recall of the study
Input package per paper	Header (first 3,000 characters), abstract (up to 2,000), Methods (up to 4,000), Results and Discussion (up to 4,000), Conclusion (up to 2,000)
Batching	41 batches of 5 papers
Output schema	11 fields, null permitted in each: country, ML algorithms, best model, best R^2, RMSE, $q_{\max}$ (mg/g), removal percentage, dataset size, target contaminant, adsorbent material, study type
Reconciliation	Every field compared against the independent regex pass; 582 field-level disagreements logged
Human oversight	Output reviewed by the authors; accuracy audited on 180 cells (Section S11.2)

S4. Statistical Comparison of Algorithm Performance

To determine whether the differences in reported R^2 values across the five most frequently reported best-performing algorithms were statistically significant, a Kruskal–Wallis rank sum test was performed on the 82 studies reporting R^2 values with a best model among ANN, RF, ANFIS, XGBoost, or GBM (Table S4).

Table S4: Summary of R^2 values by best-performing algorithm (Kruskal–Wallis test).

Algorithm	n	Median R^2	IQR
ANFIS	8	0.997	0.989–0.999
ANN	48	0.991	0.980–0.999
GBM	6	0.990	0.979–0.997
XGBoost	9	0.970	0.966–0.980
RF	11	0.947	0.920–0.977
Kruskal–Wallis $\chi^2 = 19.39$, df = 4, $p = 6.6 \times 10^{-4}$			

The test revealed a highly significant difference ($\chi^2 = 19.39$, df = 4, $p = 6.6 \times 10^{-4}$), confirming that algorithm choice significantly affects reported model performance. ANFIS achieved the highest median R^2 (0.997), followed closely by ANN (0.991) and GBM (0.990). RF exhibited the lowest median R^2 (0.947) and the widest interquartile range, suggesting more variable performance across adsorption systems. However, these differences should be interpreted cautiously given the unequal sample sizes and potential confounding by study-specific factors (dataset size, contaminant type, adsorbent material).

S5. Machine-Extractable Reporting: Indicator Definitions

The score assigned to each study is the sum of eight binary indicators (Table S5). Each indicator was scored as 1 where the extraction recovered a value and 0 where it did not, yielding a composite score from 0 to 8. As the extraction audit shows (main text, Section 2.6.2), an empty cell is not evidence that the study omitted the item, so each rate is a lower bound on reporting.

The per-study scores are provided in the accompanying dataset file (`extracted_data_STANDARDIZED.csv`).

S6. Adsorption Capacity (q_{max}) Summary by Adsorbent Category

Table S6 summarizes the reported maximum adsorption capacities stratified by adsorbent category. Only categories with ≥ 2 studies reporting q_{max} values are shown.

Table S5: Definitions of the eight machine-extractable reporting indicators.

#	Indicator	Definition	Recovered (%)
1	R^2 reported	Best-model coefficient of determination reported	54.5
2	RMSE reported	Root mean squared error reported	25.7
3	MAE reported	Mean absolute error reported	7.9
4	Dataset size reported	Number of training/total data points stated	38.6
5	Validation method	Cross-validation or train/test split described	45.5
6	No. of input features	Number of predictor variables stated	9.4
7	Software/tool disclosed	ML software or programming language identified	61.9
8	Multi-algorithm comparison	Two or more algorithms benchmarked	53.5
	Mean composite score	**2.97** / **8** (SD = 1.74)	

Table S6: Summary of reported $q_{\max}$ (mg/g) by adsorbent category.

Adsorbent Category	n	Median	IQR
Microplastics	2	7,253	3,630–10,876
Nanocomposite	3	439	365–584
LDH	3	374	209–631
Chitosan	2	371	201–542
Graphene Oxide	4	227	101–418
Clay/Bentonite	2	190	185–196
MOF	3	192	98–221
Carbon Nanotubes	8	145	55–260
Biochar	16	121	70–312
Iron Oxide/Magnetic	3	74	69–180
Activated Carbon	16	69	53–159
Silica	3	51	26–322
Other	15	132	47–180
Agricultural Waste	4	4	2–7

S7. Complete Target Contaminant Inventory

Table S7 lists the 50 most frequently studied target contaminants (out of 147 unique compounds identified). Contaminants appearing in only one study are omitted for brevity; the complete list is available in the accompanying dataset file.

Table S7: Top 50 most frequently studied target contaminants.

#	Contaminant	n	#	Contaminant	n
1	Tetracycline	36	26	Sulfamethazine	5
2	Ciprofloxacin	32	27	Trimethoprim	5
3	Diclofenac	16	28	Acetaminophen	4
4	Ibuprofen	16	29	Amoxicillin	4
5	Carbamazepine	15	30	Atrazine	4
6	Bisphenol A	13	31	Cephalexin	4
7	Methylene blue	10	32	Erythromycin	4
8	Oxytetracycline	9	33	Metformin	4
9	PFOA	7	34	Methyl orange	4
10	Sulfamethoxazole	7	35	Naproxen	4
11	Doxycycline	6	36	Norfloxacin	4
12	Malachite green	6	37	Ofloxacin	4
13	Levofloxacin	5	38	17α-Ethinylestradiol	3
14	PFOS	5	39	17β-Estradiol	3
15	Congo red	5	40	Atenolol	3
16	Crystal violet	5	41	Chlortetracycline	3
17	Rhodamine B	5	42	Clofibric acid	3
18	Cd(II)	5	43	Enrofloxacin	3
19	Pb(II)	5	44	Estrone	3
20	As(III)/As(V)	5	45	Fluoxetine	3
21	Cr(VI)	5	46	Ketoprofen	3
22	Cu(II)	5	47	Metronidazole	3

#	Contaminant	n	#	Contaminant	n
23	Zn(II)	5	48	Propranolol	3
24	Ni(II)	5	49	Salicylic acid	3
25	Phenol	5	50	Triclosan	3

S8. Reporting Quality by Year

Table S8: Reporting quality score distribution by publication year.

Year	n	Mean	Median	Min	Max
2015	1	1.00	1.0	1	1
2016	4	2.00	2.5	0	3
2017	2	1.00	1.0	0	2
2018	1	1.00	1.0	1	1
2019	9	2.00	2.0	0	3
2020	6	2.50	2.0	1	4
2021	20	3.05	3.0	1	5
2022	22	2.64	3.0	0	5
2023	32	2.81	3.0	0	5
2024	41	3.15	3.0	0	7
2025	64	3.39	3.0	0	7

S9. Complete List of Included Studies

Table S9 lists all 202 studies included in this systematic review, sorted alphabetically by first author.

Table S9: Complete list of 202 studies included in this systematic review.

#	First Author	Year	Journal	Country	Best Model	Ref.
1	Adeola et al.	2025	ACS Sustainable Resource Management	Canada	ANFIS	[1]
2	Ahmadi et al.	2022	Environ Res	Iran	ANFIS	[2]
3	Ahmed et al.	2024	Journal of Environmental Management	Bangladesh	GBM	[3]
4	Ahmed et al.	2024	Journal of Water Process Engineering	Bangladesh	MLP	[4]
5	Akinola et al.	2025	Journal of Environmental Chemical En...	South Africa	ANN	[5]
6	Al-Howri et al.	2025	Biomass Conversion and Biorefinery	Malaysia	DT	[6]
7	Al-Jamimi et al.	2023	Journal of Molecular Liquids	Saudi Arabia	SVM	[7]
8	Al-Kizwini et al.	2021	International Journal of Environment...	Iraq	ANN	[8]
9	Almuntashiri et al.	2021	Chemosphere	Australia	ANN	[9]
10	Almuntashiri et al.	2022	Journal of Water Process Engineering	Australia	ANN	[10]
11	Almuntashiri et al.	2025	Process Safety and Environmental Pro...	Australia	ANN	[11]
12	Alver et al.	2024	Arabian Journal for Science and Engi...	Turkey	ANFIS	[12]
13	Anusi et al.	2025	Current Research in Green and Sustai...	Nigeria	ANN	[13]

Continued on next page

Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
14	Arshadi et al.	2019	Journal of Colloid and Interface Sci...	USA	ANN	[14]
15	Astray et al.	2023	Nanomaterials	Spain	ANN	[15]
16	Atta et al.	2024	Desalination and Water Treatment	Iraq	ANN	[16]
17	AttariKhasraghi et al.	2021	Journal of Molecular Liquids	Iran	ANN	[17]
18	Azizi et al.	2023	Research on Chemical Intermediates	Iran	DT	[18]
19	Balasubramani et al.	2020	Journal of Molecular Liquids	India	ANN	[19]
20	Balasubramani et al.	2023	Industrial and Engineering Chemistry...	India	SVM	[20]
21	Balasubramanian et al.	2024	Carbon Research	New Zealand	RSML	[21]
22	Beigzadeh et al.	2020	Water Sci Technol	Iran	RF	[22]
23	Bhattacharya et al.	2020	Sustainable Environment Research	India	RSM	[23]
24	Bhattacharya et al.	2021	Surfaces and Interfaces	India	RSM	[24]
25	Bhattacharya et al.	2022	Environmental Science and Pollution ...	India	—	[25]
26	Bhattacharya et al.	2024	Sadhana - Academy Proceedings in Eng...	India	RSM	[26]
27	Bhattacharyya et al.	2018	Desalination and Water Treatment	India	ANN	[27]

Continued on next page

Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
28	Bi et al.	2025	Journal of Hazardous Materials	China	RF	[28]
29	Bouhedda et al.	2019	Chemometrics and Intelligent Laborat...	Algeria	ANFIS	[29]
30	Bouzemlal et al.	2025	Environ Geochem Health	Algeria	XGBoost	[30]
31	Bulanga et al.	2025	Next Materials	South Africa	ANN	[31]
32	Chen et al.	2023	Desalination and Water Treatment	China	ANN	[32]
33	Chen et al.	2025	Journal of Cleaner Production	China	TAN	[33]
34	Cho et al.	2021	Environmental Research	South Korea	QSAR	[34]
35	Cho et al.	2022	Journal of Hazardous Materials	South Korea	Linear Regression	[35]
36	Cho et al.	2025	Journal of Hazardous Materials	South Korea	ANN	[36]
37	Chu et al.	2021	Journal of Environmental Chemical En...	South Korea	ANN	[37]
38	Ciğeroğlu et al.	2021	Journal of Molecular Structure	Turkey	RF	[38]
39	Costa et al.	2024	Environmental Research	Brazil	ANN	[39]
40	Costa et al.	2024	Journal of Water Process Engineering	Brazil	ANN	[40]
41	Costa et al.	2025	Environmental Science and Pollution ...	Brazil	ANN	[41]
42	Coutinho et al.	2025	Biomass and Bioenergy	Brazil	ANN	[42]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
43	Dagher et al.	2024	Separation and Purification Technology	France	RF	[43]
44	Deb et al.	2019	Environmental Science and Pollution . . .	India	—	[44]
45	Dehdashti et al.	2019	Journal of Environmental Health Scie. . .	Iran	ANN	[45]
46	Dehghani et al.	2020	Journal of Molecular Liquids	Iran	ANN	[46]
47	Deng et al.	2025	Applied Organometallic Chemistry	China	ANN	[47]
48	Devatha et al.	2019	Journal of Environmental Management	India	RSM	[48]
49	Ebere et al.	2023	Chemical Engineering Science	Japan	ANN	[49]
50	Ebere et al.	2025	Separation and Purification Technology	Japan	ANN	[50]
51	Ebrahimi et al.	2025	Environmental Technology and Innovat. . .	Iran	ANFIS	[51]
52	Ecevit et al.	2025	Journal of Water Process Engineering	Turkey	ANN	[52]
53	Edebali et al.	2023	Applied Surface Science Advances	Turkey	ANN	[53]
54	Enyoh et al.	2024	Cambridge Prisms: Plastics	Japan	ANN	[54]
55	Ersan et al.	2025	ACS ES and T Water	USA	PCR	[55]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
56	Fabregat-Palau et al.	2025	Environmental Science and Technology	Germany	Stacking	[56]
57	Faisal et al.	2024	Scientific Reports	Iraq	ANN	[57]
58	Fang et al.	2025	Water (Switzerland)	China	ANN	[58]
59	Farzinmanesh et al.	2024	Chemosphere	Iran	GRNN	[59]
60	Fasniuc-Pereu et al.	2025	Polymers	Romania	ANN	[60]
61	Fayyadh et al.	2025	Results in Chemistry	Malaysia	ANN	[61]
62	Firouzi et al.	2021	Journal of Environmental Chemical En...	Iran	ANN	[62]
63	Fu et al.	2025	Environmental Science and Technology	China	LightGBM	[63]
64	Gao et al.	2025	Journal of Cleaner Production	China	Stacking	[64]
65	Gholami et al.	2023	Alexandria Engineering Journal	Iran	LS-SVM	[65]
66	Goh et al.	2024	Environ Sci Pollut Res Int	Malaysia	ANN	[66]
67	Hafeez et al.	2024	Heliyon	Pakistan	ANN	[67]
68	Hamza et al.	2022	Adsorption Science and Technology	Saudi Arabia	GPR	[68]
69	He et al.	2025	Journal of Environmental Chemical En...	China	CatBoost	[69]
70	Hedayati et al.	2017	Journal of Applied Research and Tech...	Iran	ANFIS	[70]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
71	Henrique et al.	2021	Journal of Environmental Chemical En...	Brazil	ANN	[71]
72	Hou et al.	2023	Journal of Water Process Engineering	China	ANN	[72]
73	Huang et al.	2022	Bioresource Technology	China	—	[73]
74	INYINBOR et al.	2023	ACS Omega	Nigeria	ANN	[74]
75	Islam et al.	2024	Chemical Papers	Japan	RF	[75]
76	Islam et al.	2024	Water (Switzerland)	Japan	RF	[76]
77	Jafari et al.	2023	Heliyon	Iran	ANN	[77]
78	Jaffari et al.	2023	Chemical Engineering Journal	South Korea	CatBoost	[78]
79	Jha et al.	2025	Bioresour Technol	India	GBM	[79]
80	Ji et al.	2023	Water Supply	China	ANN	[80]
81	Jiang et al.	2024	Separation and Purification Technology	China	XGBoost	[81]
82	Jiang et al.	2025	Separation and Purification Technology	China	RF	[82]
83	Jin et al.	2023	Environmental Research	South Korea	Linear Regression	[83]
84	Jin et al.	2025	Separation and Purification Technology	China	LSTM	[84]
85	Jin et al.	2025	Sustainable Materials and Technologies	China	Deep Learning	[85]
86	Kang et al.	2021	Microporous and Mesoporous Materials	South Korea	ANN	[86]
87	Karbassiyazdi et al.	2022	Environmental Research	Australia	XGBoost	[87]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
88	Kassahun et al.	2021	Environmental Technology and Innovat...	Ethiopia	ANN	[88]
89	Khajavian et al.	2024	Journal of Industrial and Engineerin...	Russia	RF	[89]
90	Khanmohammadi et al.	2024	Chemosphere	Iran	ANN	[90]
91	Khazaie et al.	2023	Journal of the Taiwan Institute of C...	Iran	ANN	[91]
92	Khezerlou et al.	2021	Ceramics International	Iran	—	[92]
93	Kim et al.	2025	Journal of Water Process Engineering	South Korea	CatBoost	[93]
94	Kubar et al.	2025	Water, Air, and Soil Pollution	Pakistan	RF	[94]
95	Lee et al.	2024	International Journal of Biological ...	South Korea	ANN	[95]
96	Lee et al.	2025	Separation and Purification Technology	South Korea	Linear Regression	[96]
97	Li et al.	2021	Journal of Hazardous Materials	United Kingdom	RF	[97]
98	Li et al.	2024	Journal of Hazardous Materials	China	—	[98]
99	Li et al.	2025	J Hazard Mater	China	GBM	[99]
100	Liu et al.	2021	ACS Omega	China	ANFIS	[100]
101	Liu et al.	2023	Environmental Research	China	RF	[101]
102	Liu et al.	2024	Bioresource Technology	China	AdaBoost	[102]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
103	Liu et al.	2024	Journal of Hazardous Materials	China	Stacking	[103]
104	Lu et al.	2025	RSC Advances	China	GBM	[104]
105	M et al.	2025	Environmental Science and Pollution ...	Brazil	ANN	[105]
106	M.; et al.	2025	Environmental Research	China	—	[106]
107	Mahanty et al.	2024	Journal of Water Process Engineering	India	ANN	[107]
108	Mahmoud et al.	2024	Chemosphere	Egypt	ANN	[108]
109	Malhotra et al.	2024	Journal of Environmental Chemical En...	India	ANN	[109]
110	Mansab et al.	2024	Environ Sci Pollut Res Int	Pakistan	ANN	[110]
111	Mansoor et al.	2024	Journal of Environmental Science and...	South Africa	ANN	[111]
112	Manyazewal et al.	2025	Remediation	Ethiopia	—	[112]
113	Manzar et al.	2022	Separation and Purification Technology	Saudi Arabia	ANN	[113]
114	Megha et al.	2025	Microchemical Journal	India	FINN	[114]
115	Mhemid et al.	2023	Journal of Ecological Engineering	Iraq	ANN	[115]
116	Mijwel et al.	2025	Microporous and Mesoporous Materials	Malaysia	RNN	[116]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
117	Mojiri et al.	2019	Environmental Technology and Innovat...	Japan	ANN	[117]
118	Mojiri et al.	2019	Water (Switzerland)	Japan	ANN	[118]
119	Mojiri et al.	2020	Journal of Contaminant Hydrology	Japan	ANN	[119]
120	Mojiri et al.	2021	Microorganisms	Japan	ANN	[120]
121	Mondal et al.	2016	Ecological Engineering	India	ANN	[121]
122	Mondal et al.	2016	Journal of Environmental Management	India	ANN	[122]
123	Mondal et al.	2016	Desalination and Water Treatment	India	ANN	[123]
124	Mun et al.	2023	Journal of Environmental Management	South Korea	Linear Regression	[124]
125	Nagappan et al.	2025	Water, Air, and Soil Pollution	India	ANN	[125]
126	Nasrollahpour et al.	2024	iScience	Canada	DNN	[126]
127	Nguyen et al.	2022	Chemosphere	China	Cubist	[127]
128	Oh et al.	2022	Environmental Pollution	South Korea	—	[128]
129	Okolie et al.	2022	Total Environment Research Themes	Ireland	—	[129]
130	Oladipo et al.	2016	International Journal of Biological ...	Turkey	ANN	[130]
131	Oliveira et al.	2023	Environmental Research	Brazil	ANN	[131]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
132	Oliveira et al.	2024	Journal of Cleaner Production	Brazil	ANFIS	[132]
133	Oliveira et al.	2025	Environmental Science and Pollution ...	Brazil	ANN	[133]
134	Omidi et al.	2022	Chemosphere	Iran	ANN	[134]
135	Ovuoraye et al.	2023	Journal of Engineering and Applied S...	Nigeria	RF	[135]
136	Pauletto et al.	2021	Chemical Engineering Journal	Brazil	ANN	[136]
137	Polanco-Gamboa et al.	2025	Results in Engineering	Mexico	PCA	[137]
138	Prasad et al.	2025	Environmental Science: Water Researc...	India	RSML	[138]
139	Probst et al.	2020	Journal of Pharmaceutical Sciences	USA	CNN	[139]
140	Qarajehdaghi et al.	2023	Process Safety and Environmental Pro...	Iran	ANN	[140]
141	Radmehr et al.	2021	Journal of Environmental Chemical En...	Iran	ANFIS	[141]
142	Rangappa et al.	2024	Sustainability (Switzerland)	India	RF	[142]
143	Rasoulzadeh et al.	2025	Scientific Reports	Iran	Tikhonov Regular...	[143]
144	Reynel-Ávila et al.	2015	Journal of Molecular Liquids	Mexico	ANN	[144]
145	Rodríguez-Narváez et al.	2025	Journal of Water Process Engineering	Mexico	kNN	[145]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
146	Rushdi et al.	2025	Chemical Engineering Journal	Malaysia	—	[146]
147	Saawarn et al.	2024	Chemosphere	India	ANFIS	[147]
148	Saeidi et al.	2024	Chemical Engineering Journal	Germany	RF	[148]
149	Salawu et al.	2022	Journal of Hazardous Materials	USA	ANN	[149]
150	Selvaraj et al.	2024	Environmental Research	India	ANN	[150]
151	Shang et al.	2022	Chemical Engineering Journal	China	ANN	[151]
152	Sharma et al.	2023	ChemNanoMat	India	ANFIS	[152]
153	Sheikhmohammadi et al.	2025	Journal of the Taiwan Institute of C...	Iran	Polynomial Regre...	[153]
154	Show et al.	2022	Biomass Conversion and Biorefinery	India	RSM	[154]
155	Soleimanpour et al.	2021	Iranian Journal of Science and Techn...	Iran	ANFIS	[155]
156	Spaolonzi et al.	2022	Journal of Cleaner Production	Brazil	ANN	[156]
157	Tavassoli et al.	2025	Heliyon	Iran	GEP	[157]
158	Temiz et al.	2025	Biomass and Bioenergy	Turkey	ANN	[158]
159	Temiz et al.	2025	Journal of Environmental Chemical En...	Turkey	XGBoost	[159]
160	Thao et al.	2025	Chemosphere	Vietnam	—	[160]
161	Tian et al.	2025	ACS Omega	China	XGBoost	[161]
162	Tian et al.	2025	Scientific Reports	China	XGBoost	[162]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
163	Tréguier et al.	2019	mBio	France	—	[163]
164	Vakili et al.	2019	Journal of Environmental Management	Japan	ANN	[164]
165	Vera et al.	2024	Environmental Science and Pollution ...	Ecuador	ANN	[165]
166	Viet et al.	2022	Bioresource Technology	South Korea	ANN	[166]
167	Vinayagam et al.	2022	Bioresource Technology Reports	India	ANFIS	[167]
168	Vinayagam et al.	2023	Bioresource Technology Reports	India	ANFIS	[168]
169	Vinayagam et al.	2024	Chemosphere	India	ANN	[169]
170	Vukčević et al.	2024	Separations	Serbia	ANN	[170]
171	Wang et al.	2023	Applied Surface Science	China	ANN	[171]
172	Wang et al.	2023	Ceramics International	China	ANN	[172]
173	Wang et al.	2024	Colloids and Surfaces A: Physicochem...	China	GBM	[173]
174	Wang et al.	2024	Journal of Hazardous Materials	China	XGBoost	[174]
175	Wang et al.	2025	International Journal of Biological ...	China	CatBoost	[175]
176	Wang et al.	2025	Journal of Environmental Chemical En...	China	XGBoost	[176]
177	Wang et al.	2025	Journal of Environmental Chemical En...	China	RF	[177]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
178	Wang et al.	2025	Water Research	China	XGBoost	[178]
179	Xian et al.	2025	Journal of Water Process Engineering	China	RF	[179]
180	Xiao et al.	2025	Environmental Research	China	XGBoost	[180]
181	Xin et al.	2025	Journal of Hazardous Materials Advan...	China	QML	[181]
182	Yang et al.	2022	Environmental Research	South Korea	kNN	[182]
183	Yang et al.	2022	Process Safety and Environmental Pro...	South Korea	RSM	[183]
184	Yang et al.	2023	Science of the Total Environment	China	ANN	[184]
185	Yao et al.	2023	Journal of Hazardous Materials	China	GBM	[185]
186	Yavari et al.	2025	Current Research in Green and Sustai...	Iran	XGBoost	[186]
187	Yoo et al.	2023	Environmental Science and Pollution ...	South Korea	ANN	[187]
188	Yousefi et al.	2021	Journal of Environmental Chemical En...	Iran	LS-SVM	[188]
189	Yuan et al.	2023	Water Research	China	ANN	[189]
190	Yurtsever et al.	2017	Journal of Water Reuse and Desalinat...	Turkey	ANN	[190]
191	Zhai et al.	2025	Bioresource Technology	China	XGBoost	[191]
192	Zhang et al.	2023	Chemosphere	China	ANN	[192]
193	Zhang et al.	2023	Scientific Reports	China	RF	[193]
194	Zhang et al.	2024	Environmental Pollution	China	—	[194]

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Table S9: (continued)

#	First Author	Year	Journal	Country	Best Model	Ref.
195	Zhang et al.	2024	ACS Omega	China	RF	[195]
196	Zhang et al.	2025	Environmental Science and Technology	China	CatBoost	[196]
197	Zhang et al.	2025	J Colloid Interface Sci	United Kingdom	CGCNN	[197]
198	Zheng et al.	2022	Journal of Environmental Chemical En...	China	ANN	[198]
199	Zhongguan et al.	2023	Chemosphere	China	ANN	[199]
200	Zhou et al.	2025	Journal of Hazardous Materials	China	ANN	[200]
201	Zhu et al.	2021	Chemical Engineering Journal	China	RF	[201]
202	Zhu et al.	2022	Journal of Hazardous Materials	China	RF	[202]

S10. Post-hoc Pairwise Comparison of Algorithm Performance

The Kruskal–Wallis test reported in Section S4 establishes only that the five distributions are not interchangeable. Dunn's test with Holm correction was therefore applied to all ten pairs among the same 82 studies. Effect sizes are Cliff's δ, computed with the first-named algorithm as the reference group, so a positive value means the first algorithm reports the higher R^2. Magnitude labels follow the conventional thresholds (negligible < 0.147, small < 0.33, medium < 0.474, large ≥ 0.474). Significant pairs after correction are shown in bold.

Only two comparisons survive correction, both involving RF. The remaining eight, including ANN against ANFIS and ANN against XGBoost, are not distinguishable at the 5% level. Because GBM ($n = 6$) and ANFIS ($n = 8$) are represented by few studies, a non-significant result involving them indicates insufficient data rather than demonstrated equivalence.

Stratifying by dataset size was also attempted, in order to test whether algorithm ranking depends on sample size. It is not interpretable. Only 51 of the 110 studies with a usable R^2 also report a dataset size, and splitting those 51 leaves several algorithms represented by a single study in a stratum, as Table S11

Table S10: Dunn post-hoc pairwise comparisons of best-model R^2 with Holm correction ($n = 82$ studies).

Comparison	n_a	n_b	Median_a	Median_b	p (Holm)	Cliff's δ	Magnitude
ANN vs RF	48	11	0.991	0.947	**0.0053**	+0.64	large
RF vs ANFIS	11	8	0.947	0.997	**0.0124**	-0.77	large
ANN vs XGBoost	48	9	0.991	0.970	0.0661	+0.61	large
ANFIS vs XGBoost	8	9	0.997	0.970	0.0661	+0.67	large
RF vs GBM	11	6	0.947	0.990	0.2015	-0.70	large
XGBoost vs GBM	9	6	0.970	0.990	0.4836	-0.50	large
ANN vs ANFIS	48	8	0.991	0.997	1.0000	-0.23	small
ANN vs GBM	48	6	0.991	0.990	1.0000	+0.07	negligible
RF vs XGBoost	11	9	0.947	0.970	1.0000	-0.30	small
ANFIS vs GBM	8	6	0.997	0.990	1.0000	+0.21	small

shows. The p values are reported for completeness and should not be interpreted as evidence about algorithm ranking.

Table S11: Kruskal–Wallis test stratified by dataset size, among studies reporting both R^2 and dataset size.

Stratum	Studies	In top-5 set	Algorithms with $n \geq 2$	Median R^2	χ^2	p
n<50	16	9	3	0.964	0.12	0.939
n>=50	35	23	4	0.977	7.87	0.049

Across the two strata, reported R^2 does not differ (Mann–Whitney $U = 260$, $p = 0.70$; Cliff's $\delta = -0.07$, negligible), and the proportion of studies reporting $R^2 > 0.99$ is statistically indistinguishable (3/16 versus 6/35; Fisher exact $p = 1.0$).

S11. Audit of Screening and Extraction

S11.1 Screening audit

The 993 records excluded at the title/abstract stage were stratified by the route through which the exclusion was reached and sampled proportionally ($n = 101$, 10.2%; random seed 20260912, recorded in the audit log). Each sampled record was re-assessed from title and abstract against the same criteria by an assessor blind to the screeners' stated reasons. Confidence intervals are Wilson intervals on the combined INCLUDE + UNCERTAIN proportion, which is the conservative reading.

Table S12: Screening audit results by exclusion route. INCLUDE denotes a record the assessor judged should have proceeded to full text; UNCERTAIN denotes one the abstract cannot settle.

Exclusion route	Population	Sampled	INCLUDE	UNCERTAIN	EXCLUDE	% I+U	95% CI
One EXCLUDE, one UNCERTAIN	503	51	0	3	48	5.9	2.0–15.9
Both screeners EXCLUDE	405	41	0	1	40	2.4	0.4–12.6
Prescreening filter	85	9	0	0	9	0.0	0.0–29.9
Total	**993**	**101**	**0**	**4**	**97**	**4.0**	1.6–9.7

"% I+U" is the combined INCLUDE and UNCERTAIN proportion; the confidence interval is a Wilson interval on that proportion.

No record was judged a clear false exclusion (0/101; 95% Wilson CI 0–3.7%). The four unsettled records are: *Analysis and modelling of powdered activated carbon dosing for taste and odour removal* (10.1016/j.watres.2018.04.023), where the target compounds are not named and fall outside the emerging-contaminant categories used here; *A machine learning framework to predict PPCP removal through various wastewater and water reuse treatment trains* (10.1039/d4ew00892h), which models removal at the level of whole treatment trains without naming an adsorption unit process; *Recent advances in layered double hydroxides for pharmaceutical wastewater treatment* (10.1080/10643389.2025.2488808); and *Modeling, optimization and understanding of adsorption process for pollutant removal via machine learning* (10.1016/j.chemosphere.2022.137044). The last two are review articles, which the tightening phase excludes on separate grounds.

S11.2 Extraction audit

Thirty studies were drawn at random from the 198 with available full text (same seed), and six fields were checked cell by cell against the source PDF (180 cells). "Accuracy when populated" is correct/(correct + incorrect); "omission rate when empty" is the proportion of empty cells for which the paper does report the quantity.

Where a value was recorded it was correct in 112 of 120 cells (93.3%, 95% Wilson CI 87.4–96.6%); active errors were 4.4% of all 180 cells. The three descriptive fields were correct in all 87 populated cells and were never wrongly empty. All eight errors are listed below.

Four of the eight errors are the same failure, in which a three-way 60/20/20 partition is compressed to "60:40 split"; this string occurs in six records across the full dataset, and the four that entered the audit sample were all wrong. Two further errors attach a ratio from an unrelated part of the paper to the data split, and one imports a kinetic-model R^2 into the machine-learning column. Reading the 30 papers in full also

Table S13: Extraction accuracy by field, from 30 studies audited against their source PDFs.

Field	Correct	Incorrect	Omission	Correctly empty	Unverifiable	Acc. (%)	Omis. (%)
Best model	27	0	0	3	0	100.0	0.0
Best-model R^2	13	1	11	5	0	92.9	68.8
Dataset size	6	1	9	13	1	85.7	40.9
Adsorbent material	30	0	0	0	0	100.0	—
Target contaminant	30	0	0	0	0	100.0	—
Validation method	6	6	15	3	0	50.0	83.3
All fields	**112**	**8**	**35**	**24**	**1**	**93.3**	**59.3**

"Acc." is accuracy when populated, correct/(correct + incorrect). "Omis." is the omission rate when empty, the proportion of empty cells for which the paper does report the quantity.

Table S14: Complete list of extraction errors identified in the audit.

Study	Field	Extracted	Source value
B03	Validation method	2:1 split	85:15 train/test for the Bayesian-regularisation ANN; 70:15:15 for the Levenberg–Marquardt networks
B04	Dataset size	27	29 experimental runs (Box–Behnken matrix)
B09	Validation method	60:40 split	60% training / 20% validation / 20% testing
B11	Validation method	60:40 split	60% training / 20% validation / 20% testing
B19	Validation method	60:40 split	80% training / 20% validation (shuffle and split, $n = 5$); the 60/40 in the text is an HPLC mobile-phase ratio
B22	Validation method	60:40 split	60% training / 20% validation / 20% testing
B23	Best-model R^2	0.9998	R^2 of an Elovich kinetic fit; the ANN reports a test correlation coefficient of 0.979 and no R^2
B23	Validation method	1:3 split	Random division of 40 runs into training/validation/test; the 1:3 in the text is a char:NaOH activation ratio

establishes the validation practice relied upon in the main text: 27 of 30 (90%, 95% CI 74–97%) state a validation scheme, every one of which is an internal partition of the same experimental dataset; one study additionally checks four extra experimental conditions in duplicate; none validates against an independent dataset.

Per-record judgements for both audits are available from the corresponding author on request.

S12. Minimum Reporting Checklist for Machine Learning in Adsorption Studies (MRCAS)

The checklist proposed in Section 3.7 of the main text is reproduced below. It comprises 22 items in five categories. It is intended to be completed by authors and submitted alongside a manuscript reporting a machine-learning model of an adsorption system; the reporting rates documented in this review indicate that most of these items are currently left unstated.

S13. Data Availability

The complete extracted dataset (`extracted_data_STANDARDIZED.csv`) containing all 202 studies × 40 fields is available as a supplementary data file. This dataset includes:

- Bibliographic metadata (DOI, title, authors, journal, year, country)
- ML methodology fields (algorithms, best model, validation method, dataset size, software)
- Performance metrics (R^2, RMSE, MAE, MSE, MAPE)
- Adsorption system details (adsorbent material/category, target contaminant, EC category)
- Adsorption outcomes (q_{max}, removal %, isotherm/kinetic models)
- Per-study reporting quality scores (8 binary indicators + composite score)

Researchers are encouraged to use this dataset for meta-analyses, benchmarking, and the development of standardized reporting guidelines for ML-assisted adsorption studies.

References

[1] A. O. Adeola, G. Fuoco, K. A. Adegoke, O. Adeleke, A. K. Oyebamiji, L. Paramo, R. Naccache, Experimental, machine-learning, and computational studies of the sequestration of pharmaceutical mixtures using lignin-derived magnetic activated carbon, ACS Sustainable Resource Management 2 (1) (2025) 219–230. doi:10.1021/acssusresmgt.4c00451.

Table S15: Proposed Minimum Reporting Checklist for Machine Learning in Adsorption Studies (MRCAS). Items are organized into five categories. Studies should report all applicable items to ensure reproducibility and enable cross-study comparison.

No.	Category	Item	Reported?
A. Data Description			
1	Data	Total dataset size (number of samples)	☐
2	Data	Data source (single experiment vs. multi-study compilation)	☐
3	Data	Number and names of input features	☐
4	Data	Target variable(s) and units (e.g., q_e in mg/g)	☐
5	Data	Data preprocessing steps (normalization, log-transform, outlier removal)	☐
B. Model Specification			
6	Model	Algorithm(s) used with full names and abbreviations	☐
7	Model	Software/library and version (e.g., Python scikit-learn 1.3)	☐
8	Model	Key hyperparameters and tuning method (grid search, Bayesian, etc.)	☐
9	Model	Network architecture details (for ANN: layers, neurons, activation)	☐
10	Model	Baseline model for comparison (e.g., linear regression)	☐
C. Validation Protocol			
11	Validation	Train/test split ratio and method (random, stratified, temporal)	☐
12	Validation	Cross-validation strategy (k-fold, LOO, nested CV) and k value	☐
13	Validation	Random seed for reproducibility	☐
14	Validation	Data leakage prevention measures (e.g., group-aware splitting for isotherms)	☐
D. Performance Metrics			
15	Metrics	R^2 (coefficient of determination) on test set	☐
16	Metrics	RMSE and/or MAE on test set	☐
17	Metrics	Performance on both training and test sets (to assess overfitting)	☐
18	Metrics	Confidence intervals or standard deviation across CV folds	☐
E. Interpretability & Reproducibility			
19	XAI	Feature importance analysis (SHAP, permutation, or built-in)	☐
20	XAI	Comparison of ML-derived insights with physicochemical theory	☐
21	Reproducibility	Code and/or data availability statement	☐
22	Reproducibility	Trained model availability or deployment details	☐

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