Supplementary Information

for

A green and facile modification of red mud waste with MIL-100 (Fe) for multi-pollutant adsorption from wastewater: Isotherms, kinetics, and thermodynamics

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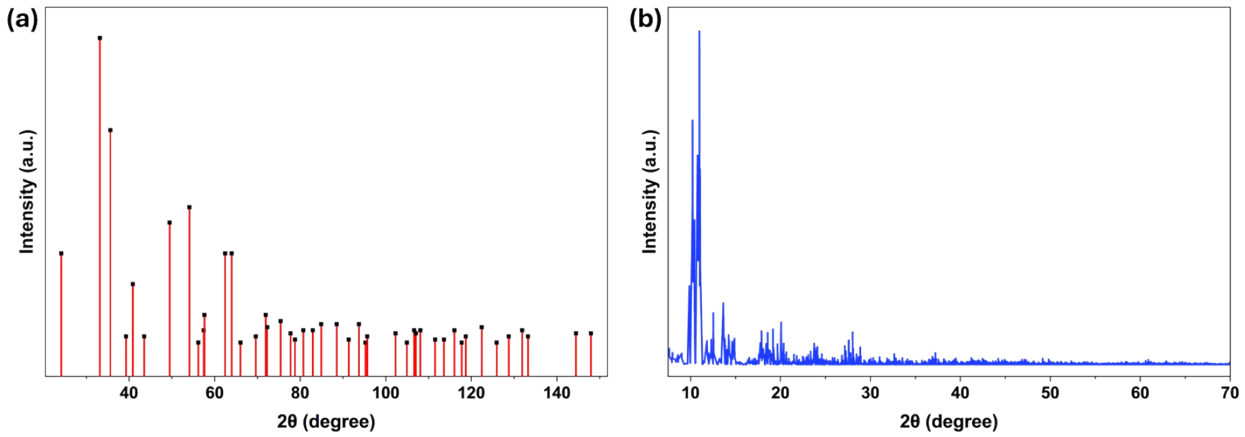

Fig. S1 (a) Standard XRD pattern of α-Fe_2O_3 (Reference code - 00-033-0664, extracted using software X'Pert HighScore Plus), and (b) simulated XRD pattern of MIL-100 (Fe) (CIF file no. - 7102029, extracted from Crystallography Open Database, further analyzed using software VESTA).

ISO 25178			
Height Parameters			
Sq	6.87	nm	*Root mean square height*
Ssk	7.29		*Skewness*
Sku	68.2		*Kurtosis*
Sp	127	nm	*Maximum peak height*
Sv	23.7	nm	*Maximum pit height*
Sz	150	nm	*Maximum height*
Sa	2.27	nm	*Arithmetic mean height*

Fig. S2 Height parameters of MARM-II composite determined through atomic force microscopy (AFM) spectroscopy.

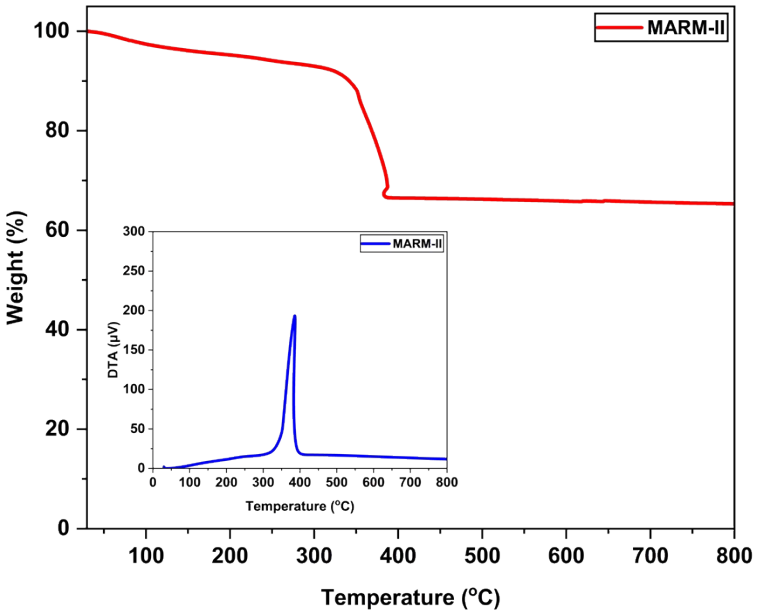

Fig. S3 Thermogravimetric analysis (TGA) and differential thermal analysis (DTA) (inset) profile of MARM-II composite.

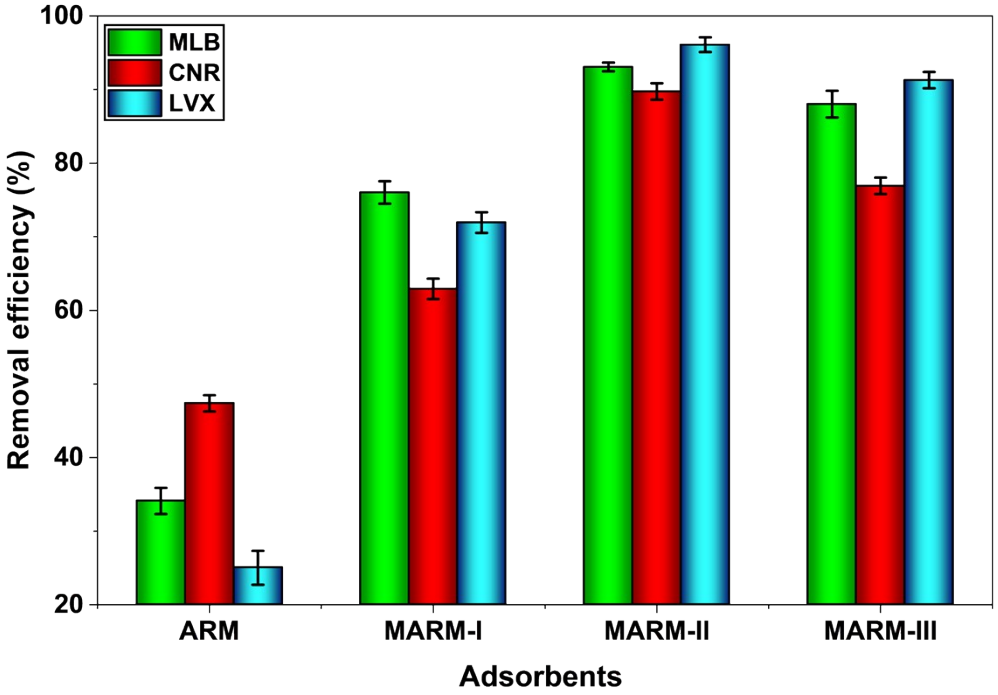

Fig. S4 Adsorptive removal of methylene blue (MLB), congo red (CNR), and levofloxacin (LVX) using pristine activated red mud (ARM), and ARM/MIL-100 (Fe) (MARM) variants.

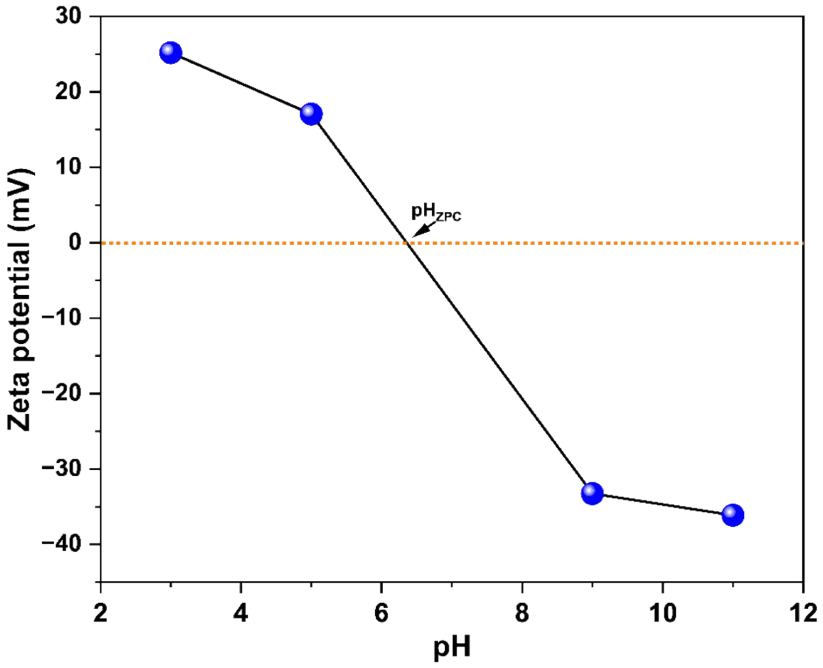

Fig. S5 Surface charge profile of MARM-II composite obtained through zeta potential analysis.

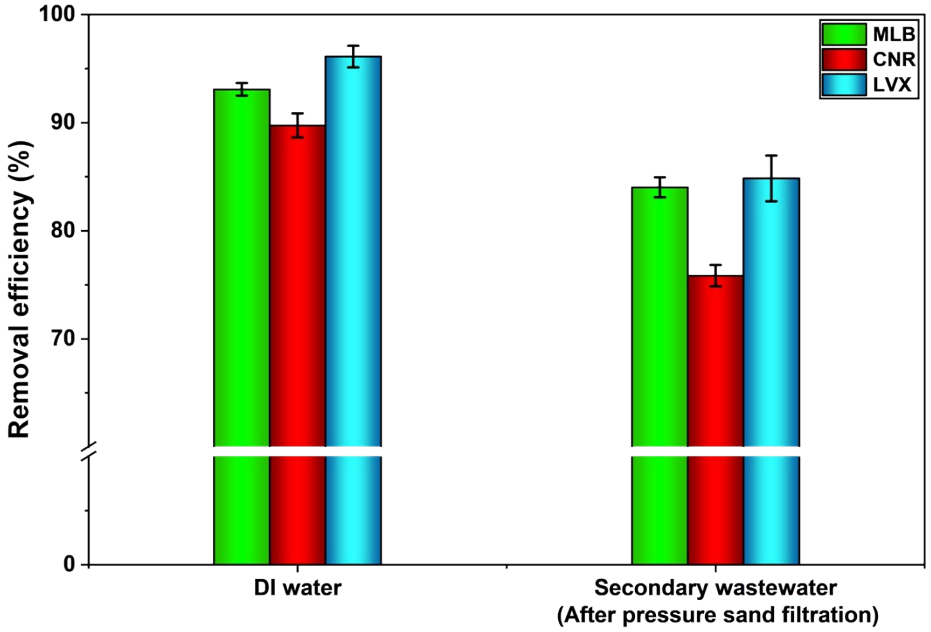

Fig. S6 Effect real wastewater matrix on the adsorptive removal of MLB, CNR, and LVX.

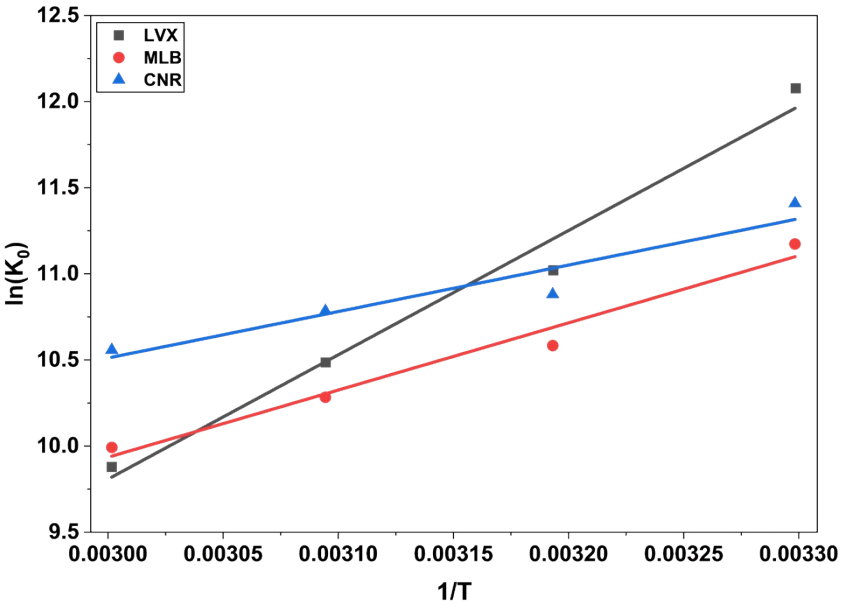

Fig. S7 Van't Hoff plots for LVX, MLB, and CNR adsorption onto the MARM-II composite.

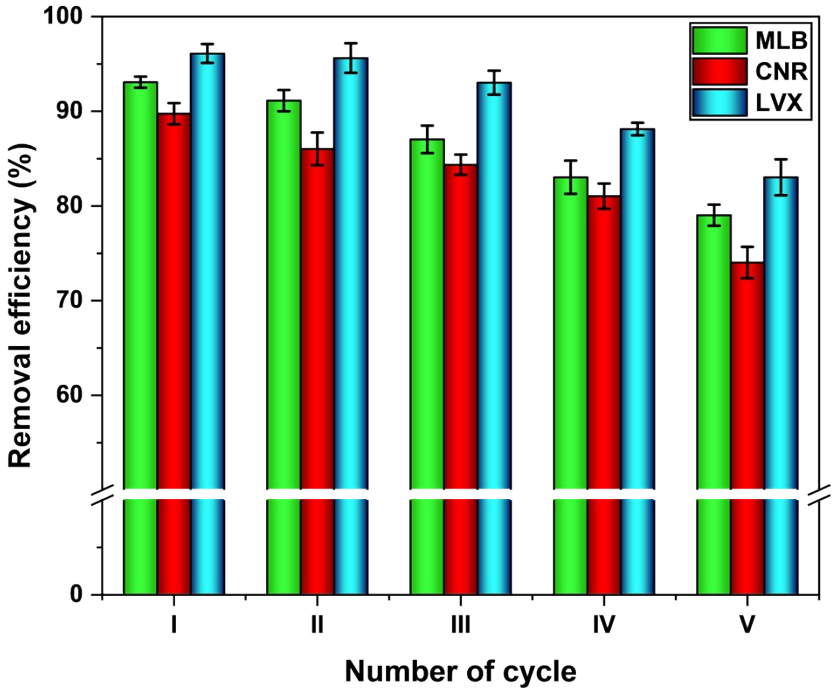

Fig. S8 Effect of number of cycles on the adsorptive removal of MLB, CNR, and LVX (Contact time: 150 min, initial MLB, CNR, and LVX concentration: 10 mg/L each, MARM-II dose: 0.4 g/L, solution pH: 7, and temperature: 27±3 °C)

Table S1 Details of chemicals used in the present study.

S. No.	Name	Chemical formula (Price)	Purity	Company
1	Ferrous sulfate heptahydrate	$FeSO_4 \cdot 7H_2O$ (₹230.00 per 500 g)	≥98%	SRL, India
2	Trimesic acid	$C_9H_6O_6$ (₹6,220.00 per 100 g)	≥98%	Merck, India
3	Ethanol	C_2H_5OH (₹620.00 per 1 L)	99%	SRL, India
4	Hydrochloric acid	HCl	37%	SRL, India
5	Sodium hydroxide pellets	NaOH (₹290.00 per 500 g)	98%	SRL, India
6	Levofloxacin	$C_{18}H_{20}FN_3O_4$	HPLC grade, ≥98%	Sigma-Aldrich
7	Congo Red	$C_{32}H_{22}N_6Na_2O_6S_2$	High Purity	Sigma-Aldrich
8	Methylene Blue	$C_{16}H_{18}N_3SCl$	(C.I. 52015)	Merck, India
9	Sodium chloride	NaCl	≥99.0%	Merck, India
10	Sodium bicarbonate	$NaHCO_3$	≥99.7%	Merck, India
11	Sodium nitrate	$NaNO_3$	≥99.0%	Merck, India
12	Sodium sulfate	Na_2SO_4	≥99.0%	Merck, India
13	Calcium chloride	$CaCl_2$	≥98.0 %	Merck, India
14	Magnesium sulfate	$MgSO_4$	≥98.0 %	Merck, India
15	Alumina refinery residue	Red mud (RM) (₹600.00 per 2 kg)		

Table S2 Instrumentation techniques used in the present study.

S. No.	Instrument	Company
1	X-ray diffraction (XRD) analysis	D2 Phaser, Bruker, USA
2	Micro-Raman spectroscopy	LabRAM HR Evolution, HORIBA Scientific
3	Fourier-transform infrared spectroscopy (FT-IR)	Bruker Alpha II
4	Field emission gun scanning electron microscopy (FEG-SEM)	Zeiss Merlin Gemini II, Germany
5	Atomic force microscopy (AFM)	Agilent 5500 Atomic Force Microscope
6	X-ray photoelectron spectroscopy (XPS)	PHI 5000 VersaProbe III, ULVAC PHI Inc., USA
7	High-resolution transmission electron microscopy (HRTEM)	JEOL (JEM-ARM300F2) (Double Aberration-corrected 300 kV HRTEM)
8	Inductively coupled plasma mass spectrometry	iCAP Q, ICP-MS, Thermo Scientific, USA
9	UV-Vis Spectrophotometer	Cary 60 UV-Vis Spectrophotometer
10	Thermo-gravimetric and Differential Thermal Analysis (TGA-DTA)	Perkin Elmer Pyris Diamond

Table S3 Textural properties of MIL-100 (Fe), ARM, and MARM-II composite, as obtained by Brunauer-Emmett-Teller (BET) and Barrett-Joyner-Halenda (BJH) analysis.

Adsorbent	**BET surface area (m^2/g)**	**Cumulative pore volume (cm^3/g)**	**Average pore size (diameter, nm)**
MIL-100 (Fe)	1845.522	0.108	3.599
ARM	21.339	0.064	3.829
MARM-II	651.741	0.161	3.626

Table S4 Performance comparison of MARM-II composite for the adsorptive removal of LVX, CNR, and MLB, with other reported adsorbents.

S. No.	**Adsorbent**	**Targeted pollutants**	**Operation conditions**	Q_{max} **(mg/g)**	**Removal efficiency**	**Reference**
1	(PNHM)/MnO_2/Fe_3O_4	CNR	Initial concentration: 20 mg/L; Dose: 1 g/L; pH: 6.75; Contact time: 180 min	599.49	98%	[1]
2	GS/PANI/Fe_3O_4	CNR	Initial concentration:	248.76	92.4%	[2]

			100 mg/L; Dose: 1 g/L; Contact time: 120 min			
3	PANI/Fe_3O_4	CNR	Initial concentration: 20 mg/L; Dose: 2 g/L; Contact time: 50 min	8.93	89.62%	[3]
4	C/Fe_3C/γ-Fe_2O_3	CNR	Initial concentration: 50 mg/L; pH: 2; Dose: 0.04 g/L; Contact time: 24 min	531.9	96%	[4]
5	SW-ZnO-PANI	MLB	Initial concentration: 25 mg/L; pH: 7; Dose: 0.5 g/L; Contact time: 100 min	20.55	95%	[5]
6	NBent-NTiO_2-Chit	LVX	Initial concentration: 25 mg/L; pH:	90.91	90.2%	[6]

			4; Dose: 0.5 g/L; Contact time: 10 min			
7	Fe_3O_4@SiO_2	LVX	Initial concentration: 20 mg/L; pH: 6.5; Dose:1 g/L; Contact time: 240 min	6.848	80.2%	[7]
8	Fe-pillared montmorillonite (Fe-P-Mt)	LVX	Initial concentration: 20mg/L; pH: 7; Dose: 0.5 g/L; Contact time: 48 h	48.61	-	[8]
9	PANI/Bi_2WO_6	CNR	Initial concentration: 25 mg/L; pH: 6; Dose: 0.5 g/L; Contact time: 90 min	142.92	92.03%	[9]
10	Polyaniline/chitosan	CNR	Initial concentration: 100 mg/L; pH: 3; Dose: 0.1	322.58	95.4%	[10]

			g/L; Contact time: 60 min			
11	MIL-101(Fe)	MLB	Initial concentration: 10 mg/L; Adsorbent dose: 2 g/L; Solution pH: 9; Contact time: 10 min	94%	58.82 mg/g	[11]
12	Magnetic iron oxide/kaolinite (MK)	CNR	Initial concentration: 50 mg/L; Adsorbent dose: 1 g/L; Solution pH: 5.5-5.8 (natural pH); Contact time: 30 min	~90%	45.59 mg/g	[12]
13	UiO-66/MIL-101(Fe)	MLB	Initial concentration: 100 mg/L; Adsorbent dose: 0.5 g/L; Solution pH: 9; Contact time: 60 min	99.2%	448.71 mg/g	[13]
14	RM/TCA-MOF	Methyl orange (MO)	Initial concentration:	95.2%	39.52 mg/g	[14]

			6.0 mg/L; Adsorbent dose: 0.07 g; Solution pH: 2.33; Contact time: 61 min			
15	Coral-like mesoporous carbon aluminosilicate composite from RM waste	MLB	Initial concentration: 40 mg/L; Adsorbent dose: 5 mg; Solution pH: Unadjusted; Contact time: 120 min	82.94%	94.02 mg/g	[15]
16	RM derived α-Fe_2O_3	CNR	Initial concentration: 50 mg/L; Adsorbent dose: 0.5 g/L; Solution pH: 5; Contact time: 240 min	93%	342.57 mg/g	[16]
17	Nanocomposites prepared from RM and durian husk (bp-Fe_3O_4)	MLB	Initial concentration: 50 mg/L; Adsorbent dose: 3 g/L; Solution pH: 7; Contact time: 60 min	>90%	37.5 mg/g	[17]

18	**MARM-II**	**MLB**	**Initial concentration: 10 mg/L; Dose: 0.4 g/L; pH: 7; Contact time: 60 min**	**123.021**	**~ 93%**	**This study**
		CNR	**Initial concentration: 10 mg/L; Dose: 0.4 g/L; pH: 7; Contact time: 105 min**	**143.934**	**~ 90%**	
		LVX	**Initial concentration: 10 mg/L; Dose: 0.4 g/L; pH: 7; Contact time: 60 min**	**97.657**	**~ 96%**	

Table S5 Water quality parameters of secondary wastewater matrix.

Parameters	**Secondary wastewater (After pressure sand filter)**
pH	6.4 ± 0.2
Turbidity (NTU)	8.1 ± 0.4
TSS (mg/L)	56 ± 3
TDS (mg/L)	328 ± 3
Electrical conductivity (µS/cm)	511 ± 6
Chloride (Cl^-, mg/L)	56.3 ± 3.8
Bicarbonate (HCO_3^-, mg/L)	119.4 ± 6.5
Sulfate (SO_4^{2-}, mg/L)	24.2 ± 1.6
Nitrate (NO_3^-, mg/L)	68.2 ± 0.7
Phosphate (PO_4^{3-}, mg/L)	13.3 ± 1.8
COD (mg/L) (Without addition of MLB+CNR+LVX)	77.2 ± 4.50
TOC (mg/L) (Without addition of MLB+CNR+LVX)	26.41 ± 3.17
COD (mg/L) (With addition of MLB+CNR+LVX, each having a concentration of 10 mg/L)	181.0 ± 3.26
TOC (mg/L) (With addition of MLB+CNR+LVX, each having a concentration of 10 mg/L)	58.53 ± 2.05

Table S6 Various kinetic model constants for MLB, CNR, and LVX adsorption on MARM-II composite.

Kinetic models		Parameters	MLB	CNR	LVX
Pseudo-first-order (PFO) kinetic model		q_e (mg/g)	27.277±0.076	25.976±0.215	31.586±0.082
		k_1 (min^{-1})	0.119	0.091	0.142
		R^2	0.999	0.995	0.999
Pseudo-second-order (PSO) kinetic model		q_e (mg/g)	28.299	27.653±0.09	32.459±0.127
		k_2 (g/mg.min)	0.011	0.006	0.014
		R^2	0.998	0.999	0.999
Elovich model		α (mg/g.min)	3.262×10^5	497.883	9.3654×10^7
		β (g/mg)	0.614	0.378	0.714
		R^2	0.992	0.995	0.999
Intraparticle diffusion (IPD) model	Stage 1	c	0.847±3.541	0.614±2.567	1.175±4.915
		k_i ($mg/g.min^{0.5}$)	4.950±0.914	4.462±0.663	5.886±1.269
		R^2	0.967	0.978	0.955
	Stage 2	c	22.725±1.873	19.027±0.405	28.082±0.365
		k_i ($mg/g.min^{0.5}$)	0.613±0.279	0.823±0.06	0.462±0.054
		R^2	0.828	0.995	0.986
	Stage 3	c	27.225±0.033	23.729±0.433	31.373±0.106
		k_i ($mg/g.min^{0.5}$)	0.009±0.003	0.238±0.042	0.031±0.01
		R^2	0.615	0.864	0.641

Table S7 Isotherm models for LVX, MLB, and CNR adsorption on MARM-II composite.

S. No.	Model	Parameters	Contaminants		
			LVX	**MLB**	**CNR**
1	Langmuir isotherm	Q_{max} (mg/g)	89.895±7.318	123.021±11.926	143.934±24.248
		K_L (L/mg)	0.486±0.125	0.222±0.053	0.129±0.045
		χ^2	27.726	23.754	38.622
	303.15 K	R^2	0.979	0.986	0.977
		Q_{max} (mg/g)	97.657±5.686	120.488±11.390	131.708±27.694
		K_L (L/mg)	0.169±0.025	0.123±0.026	0.076±0.031
	313.15 K	χ^2	10.173	11.989	34.084
		R^2	0.992	0.991	0.963
		Q_{max} (mg/g)	91.042±11.673	98.423±9.481	98.613±16.654
		K_L (L/mg)	0.099±0.028	0.091±0.013	0.069±0.024
	323.15 K	χ^2	17.111	8.413	18.617
		R^2	0.973	0.991	0.977
		Q_{max} (mg/g)	84.736±17.607	69.812±10.154	70.543±13.082
		K_L (L/mg)	0.054±0.022	0.068±0.021	0.055±0.021
	333.15 K	χ^2	16.787	9.965	11.425
		R^2	0.969	0.978	0.973
2	Freundlich isotherm	K_F	25.868±4.951	21.894±4.421	16.998±4.339

	303.15 K	(mg/g).(L/mg)$^{1/n}$			
		n	2.454±0.455	1.784±0.275	1.539±0.255
		χ^2	80.112	67.619	76.934
		R^2	0.939	0.96	0.955
	313.15 K	K_F (mg/g).(L/mg)$^{1/n}$	16.013±3.345	14.771±3.059	10.749±3.421
		n	1.907±0.286	1.649±0.219	1.479±0.26
		χ^2	43.053	38.608	62.264
		R^2	0.962	0.971	0.95
	323.15 K	K_F (mg/g).(L/mg)$^{1/n}$	10.302±3.175	10.331±2.463	8.175±2.725
		n	1.728±0.323	1.668±0.235	1.57±0.283
		χ^2	49.133	29.083	42.457
		R^2	0.941	0.968	0.947
	333.15 K	K_F (mg/g).(L/mg)$^{1/n}$	5.823±2.260	6.178±2.185	5.166±1.936
		n	1.535±0.3	1.672±0.322	1.589±0.304
		χ^2	33.69	27.807	24.165
		R^2	0.939	0.939	0.942
3	Sips isotherm	Q_m (mg/g)	92.506±16.885	108.519±18.625	100.662±11.126
	303.15 K	K_s (L/mg)^m	0.463±0.183	0.250±0.067	0.149±0.035
		m	0.941±0.291	1.185±0.313	1.584±0.378
		χ^2	40.6829	29.540	23.412
		R^2	0.979	0.988	0.991

	313.15 K	Q_m (mg/g)	87.745±7.654	100±17.763	95±39.954
		K_s (L/mg)^m	0.172±0.023	0.132±0.028	0.1±0.038
		m	1.182±0.174	1.197±0.275	1.2±0.618
		χ^2	6.079	15.745	44.003
		R^2	0.996	0.992	0.976
	323.15 K	Q_m (mg/g)	77.913±15.574	83.369±13.407	75.517±39.174
		K_s (L/mg)^m	0.0954±0.027	0.0899±0.02	0.066±0.037
		m	1.2±0.349	1.203±0.253	1.2±0.714
		χ^2	13.096	9.137	37.235
		R^2	0.979	0.986	0.938
	333.15 K	Q_m (mg/g)	68.706±27.047	56.152±8.083	58.181±19.308
		K_s (L/mg)^m	0.051±0.024	0.057±0.019	0.051±0.025
		m	1.2±0.525	1.3±0.288	1.2±0.465
		χ^2	15.756	4.990	11.487
		R^2	0.981	0.993	0.963
4	Redlich-Peterson isotherm 303.15 K	K_{RP} (L/mg)	51.259±28.282	23.809±9.633	18.543±14.608
		α_{RP} (L/mg)$^\beta$	0.729±0.861	0.1±0.269	0.129±0.611
		β	0.918±0.218	1.234±0.833	1±1.4
		χ^2	38.743	32.999	57.934
		R^2	0.98	0.987	0.977
	313.15 K	K_{RP} (L/mg)	13.826±3.089	13.18±4.438	10.024±9.59
		α_{RP} (L/mg)$^\beta$	0.059±0.094	0.0545±0.148	0.076±0.532
		β	1.273±0.433	1.225±0.779	1±1.836

		χ^2	7.286	16.663	51.127
		R^2	0.996	0.992	0.973
	323.15 K	K_{RP} (L/mg)	9.014±6.338	7.612±2.261	6.866±5.486
		α_{RP} (L/mg)$^{\beta}$	0.099±0.365	0.023±0.073	0.07±0.363
		β	1±0.855	1.353±0.855	1±1.241
		χ^2	25.668	10.709	27.926
		R^2	0.979	0.992	0.977
	333.15 K	K_{RP} (L/mg)	4.566±4.264	4.728±3.218	3.866±3.031
		α_{RP} (L/mg)$^{\beta}$	0.054±0.355	0.068±0.264	0.055±0.279
		β	1±1.515	1±0.857	1±1.132
		χ^2	25.198	14.948	17.138
		R^2	0.94	0.978	0.973

Table S8 Thermodynamic parameters for LVX, MLB, and CNR adsorption on MARM-II composite.

Pollutant	**Temperature (K)**	K_e°	ΔG° **(kJ/mol)**	ΔH° **(kJ/mol)**	ΔS° **(kJ/K.mol)**	**R²**
MLB	303.15	71017.8	-28.154	-32.474±3.71	-0.015±0.012	0.974
	313.15	39347.7	-27.546			
	323.15	29110.9	-27.616			
	333.15	21753.2	-27.664			
CNR	303.15	89874.3	-28.748	-22.434±4.881	0.002±0.015	0.913

	313.15	52949.2	-28.319			
	323.15	48072.3	-28.964			
	333.15	38318.5	-29.232			
LVX	303.15	175640.4	-30.437	-60.043±5.924	-0.098±0.002	0.981
	313.15	61076.6	-28.691			
	323.15	35778.6	-28.170			
	333.15	19515.6	-27.363			

Table S9 Cost analyses of synthesis of MARM-II composite and MLB+CNR+LVX solution treatment

Cost assessment of MARM-II for research purpose
Chemical cost **i) For synthesis of MARM-II** = 2.25 g of $FeSO_4.7H_2O$ + 1.42 g of H_3BTC + 0.80 g of NaOH (pellets) + 2.84 g of ARM = ₹ (1.035 + 88.324 + 0.464 + 0.852) = ₹ 90.675 **ii) For washing of MARM-II** = 10 mL of ethanol = ₹ 6.2

Energy cost (Instruments not utilized to full capacity)

i) Producing 5 g ARM using muffle furnace (1500 W) for 4 h
= (1500/1000) × 4 × 7.12* = ₹ 42.72

ii) Stirring (100 W) for 20 h (Using single point of multi-point magnetic stirrer)
= (100/1000) × 20 × 7.12 = ₹ 14.24

iii) Drying (60 ^{o}C) using hot air oven (800 W) for total of 8 h
= (800/1000) × 8 × 7.12 = ₹ 45.568

iv) Heating (150 ^{o}C) using hot air oven (800 W) for total of 6 h
= (800/1000) × 6 × 7.12 = ₹ 34.176

**Average tariff for electricity as per West Bengal State Electricity Distribution Company Limited (WBSEDCL) = 712 Paise/kWh.*[18]

Average experimental yield of MARM-II = 4.63 g

Chemical cost = ₹ 96.875

Energy cost = ₹ 136.70

Total cost incurred for per unit wt. synthesis of MARM-II = ₹ 50.45/g (0.56 US $/g)

Scaling possibility (Using multi-point magnetic stirrer)

Chemical cost

i) For synthesis of MARM-II (10 points)
= [2.25 g of $FeSO_4.7H_2O$ + 1.42 g of H_3BTC + 0.80 g of NaOH (pellets) + 2.84 g of ARM] × 10
= [₹ (1.035 + 88.324 + 0.464 + 0.852)] × 10
= ₹ 906.75

ii) For washing of MARM-II
= [10 mL of ethanol] × 10
= ₹ 62

Energy cost (Instruments utilization capacity enhanced)

i) Producing 30 g ARM using muffle furnace (1500 W) for 4 h
= (1500/1000) × 4 × 7.12 = ₹ 42.72

ii) Stirring (100 W) for 20 h (10 points of multi-point magnetic stirrer)
= (100/1000) × 20 × 7.12 = ₹ 14.24

iii) Drying (60 ^{o}C) using hot air oven (800 W) for total of 8 h
= (800/1000) × 8 × 7.12 = ₹ 45.568

iv) Heating (150 ^{o}C) using hot air oven (800 W) for total of 6 h
= (800/1000) × 6 × 7.12 = ₹ 34.176

Average experimental yield of MARM-II = 46.3 g

Chemical cost = ₹ 968.75

Energy cost = ₹ 136.70

Total cost incurred for per unit wt. synthesis of MARM-II = ₹ 23.87/g (0.27 US $/g)

Therefore, total cost incurred (after scale-up) for treatment of 1 L (100 mL × 10) of MLB+CNR+LVX solution (each having a concentration of 10 mg/L);

= Adsorbent cost + stirring cost

= [(0.4 g/L) × 1L × 23.87] + [(100/1000) × (150/60) × 7.12]

= ₹ 11.328/L (0.13 US $/L)

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