

**Remediation of Hexavalent Chromium, and Pharmaceuticals from aquatic environment
employing Oxygen -doped porous carbon adsorbent; Antifungal activity**

Sajad Ur Rehman Beig, Umar Ali Dar, Sajad Ahmad Sheergugri, Shakeel A. Shah

*Department of Chemistry, National Institute of Technology, Srinagar Hazratbal, Srinagar, J&K
190006, India*

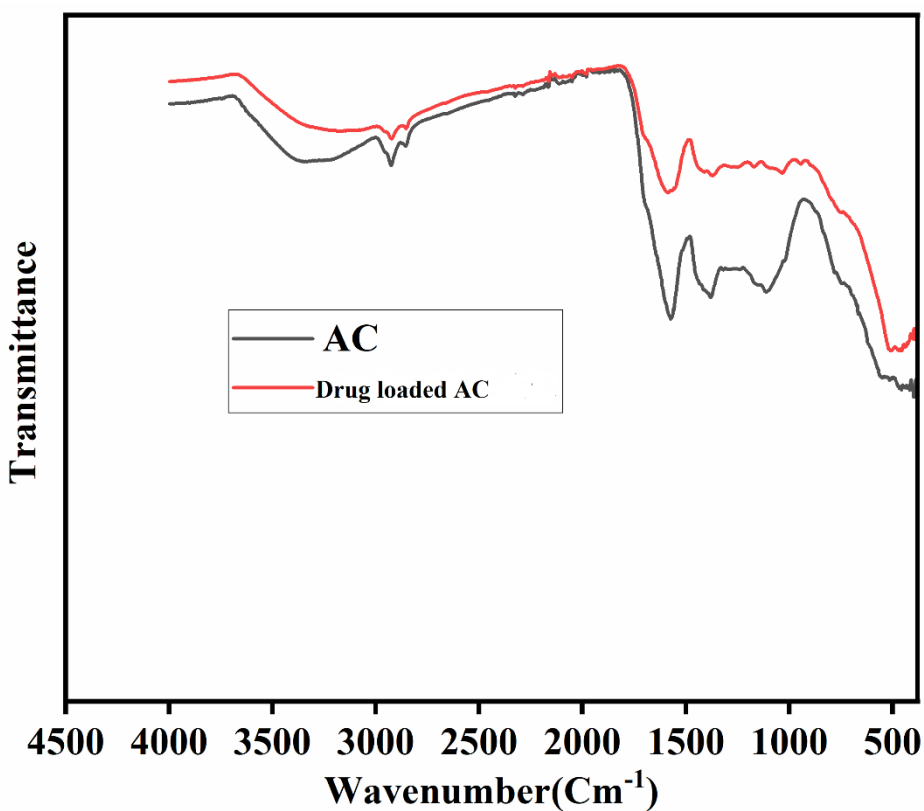


Fig S1 FT-IR spectra of AC before and after drug adsorption

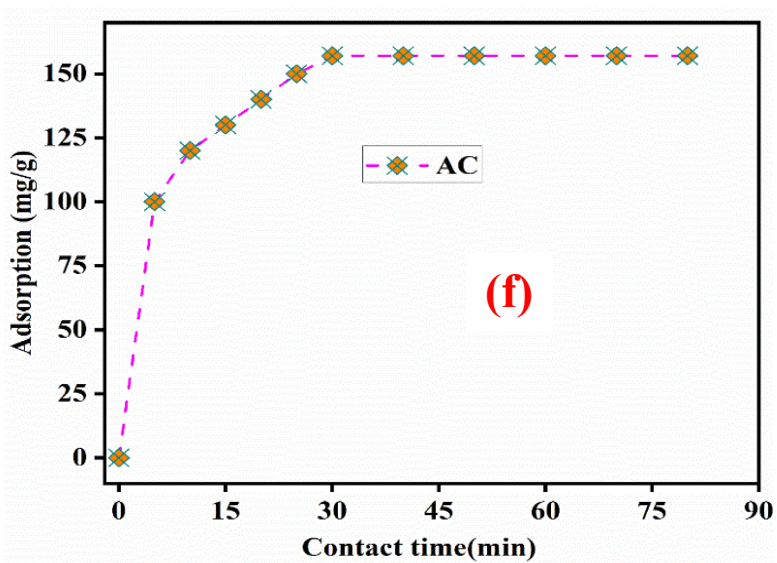
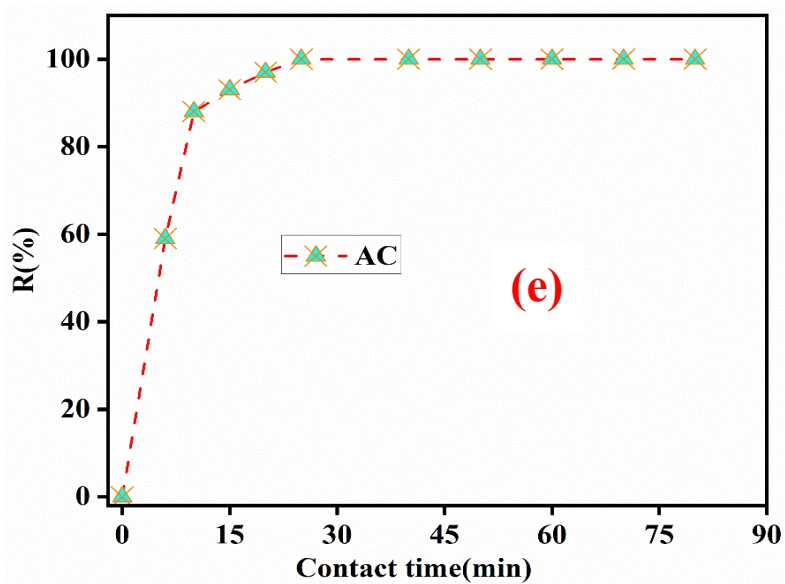
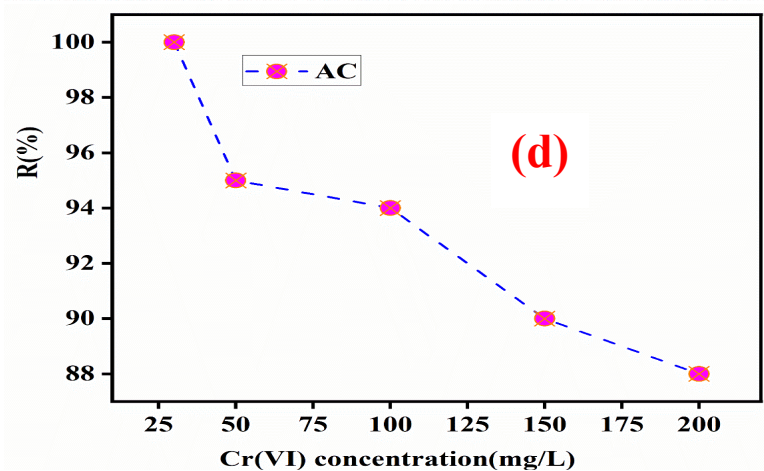
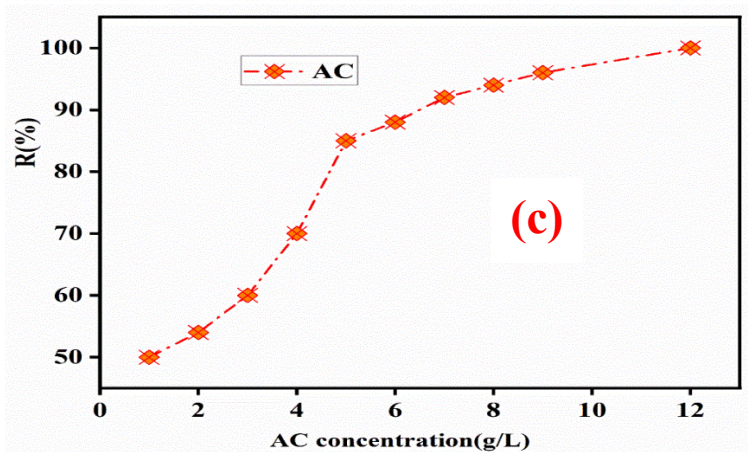
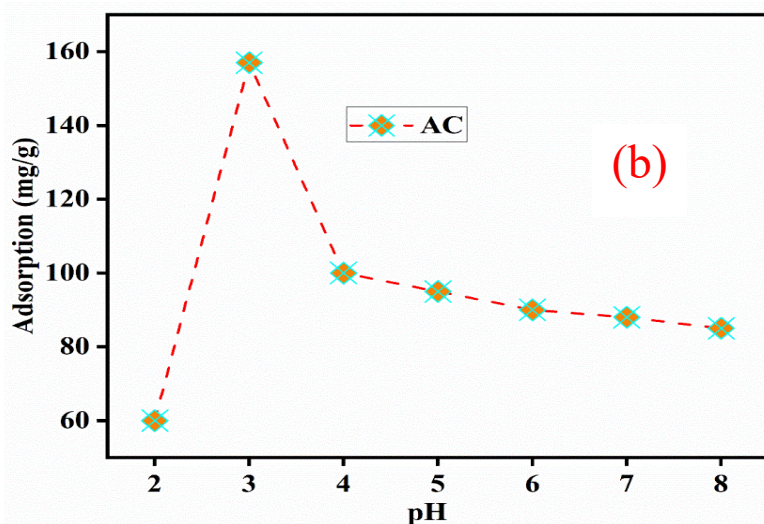
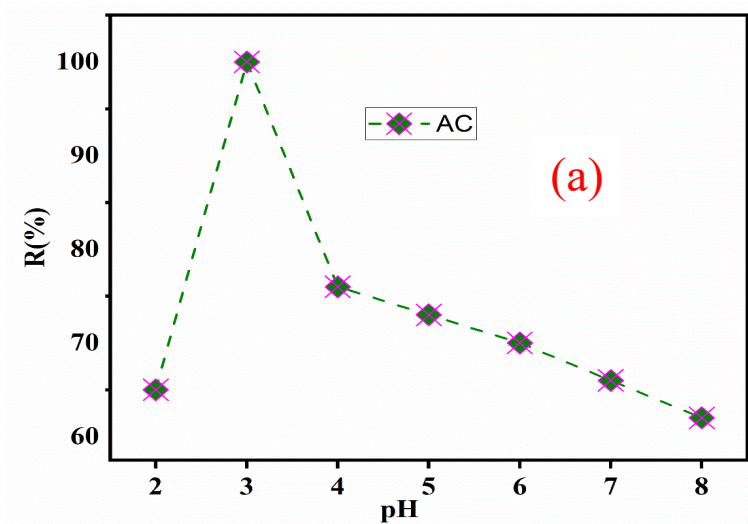


Fig S2 effect of pH on removal percentage (a) adsorption capacity (b); effect of dosage on removal percentage (c); effect of Cr (VI) concentration on removal percentage (d); effect of contact time on removal percentage (e) adsorption capacity

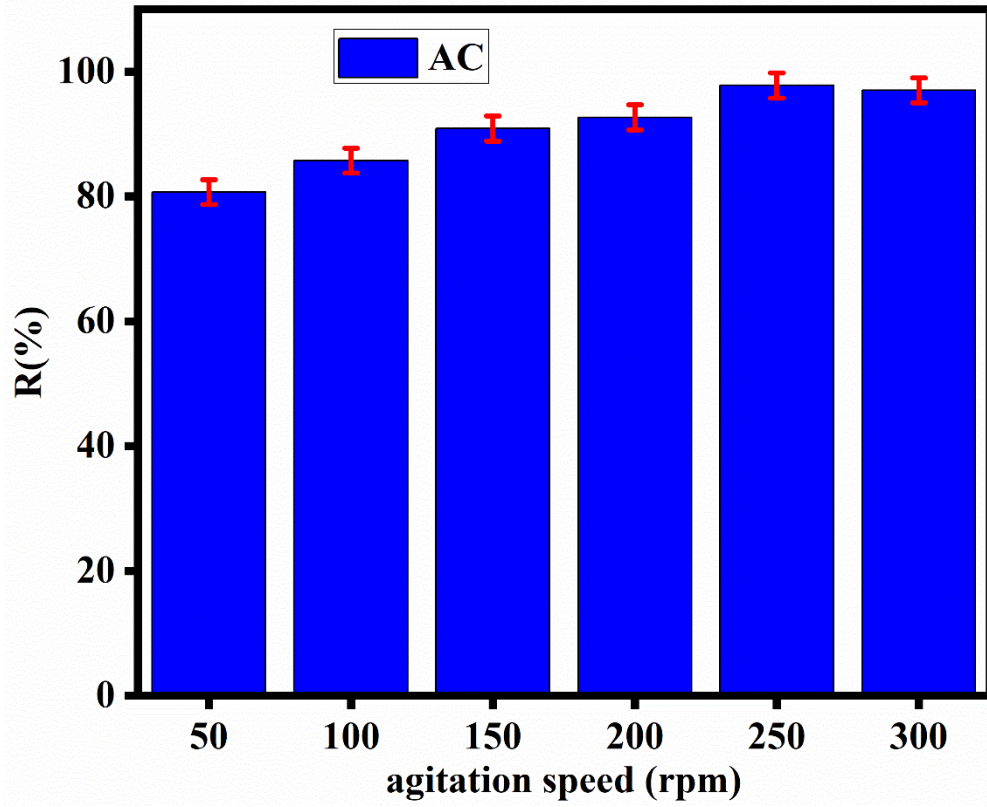


Fig S3 effect of agitation speed on removal percentage R(%)

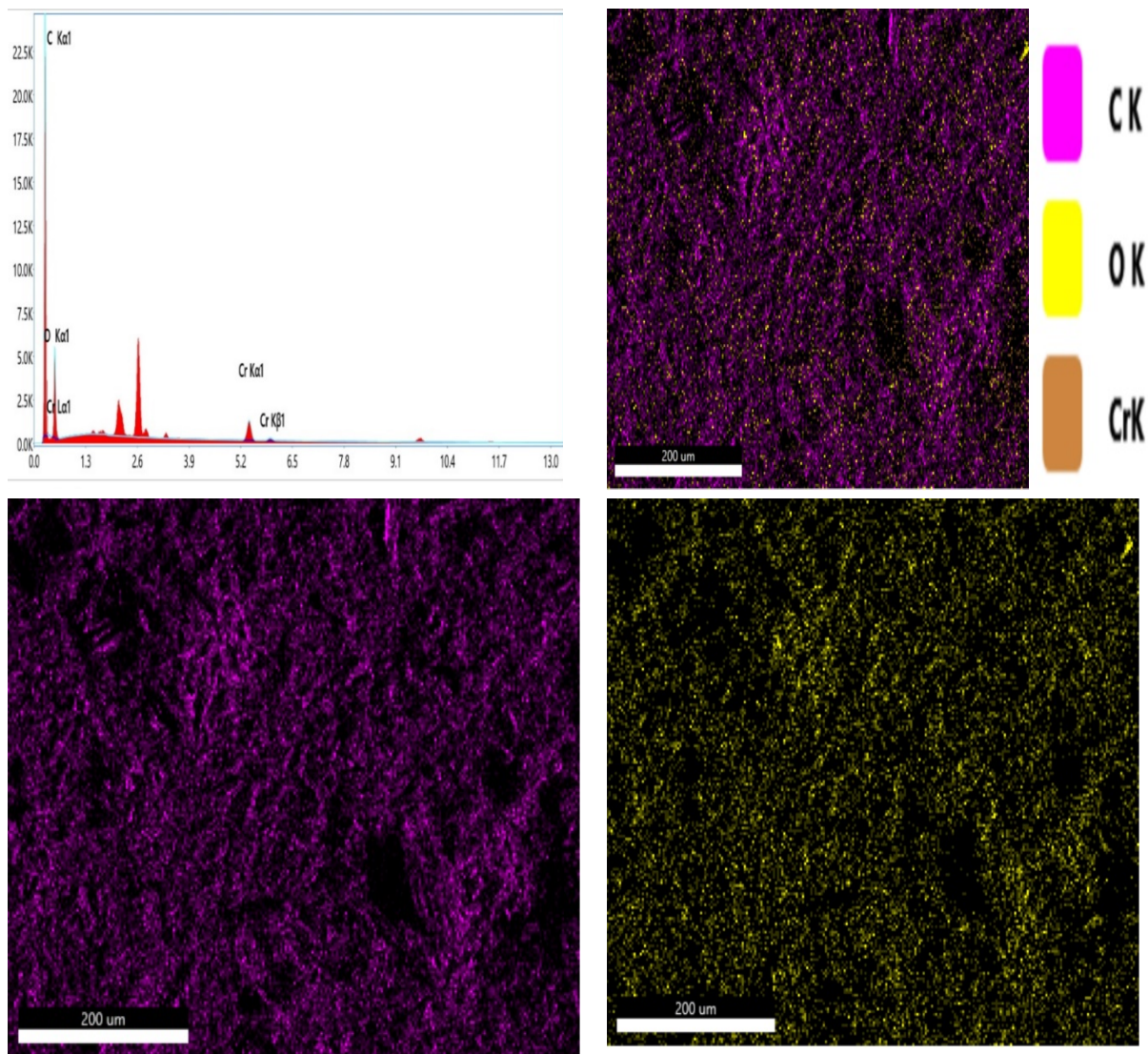


Fig S4. EDAX- mapping of AC after Cr (VI) adsorption

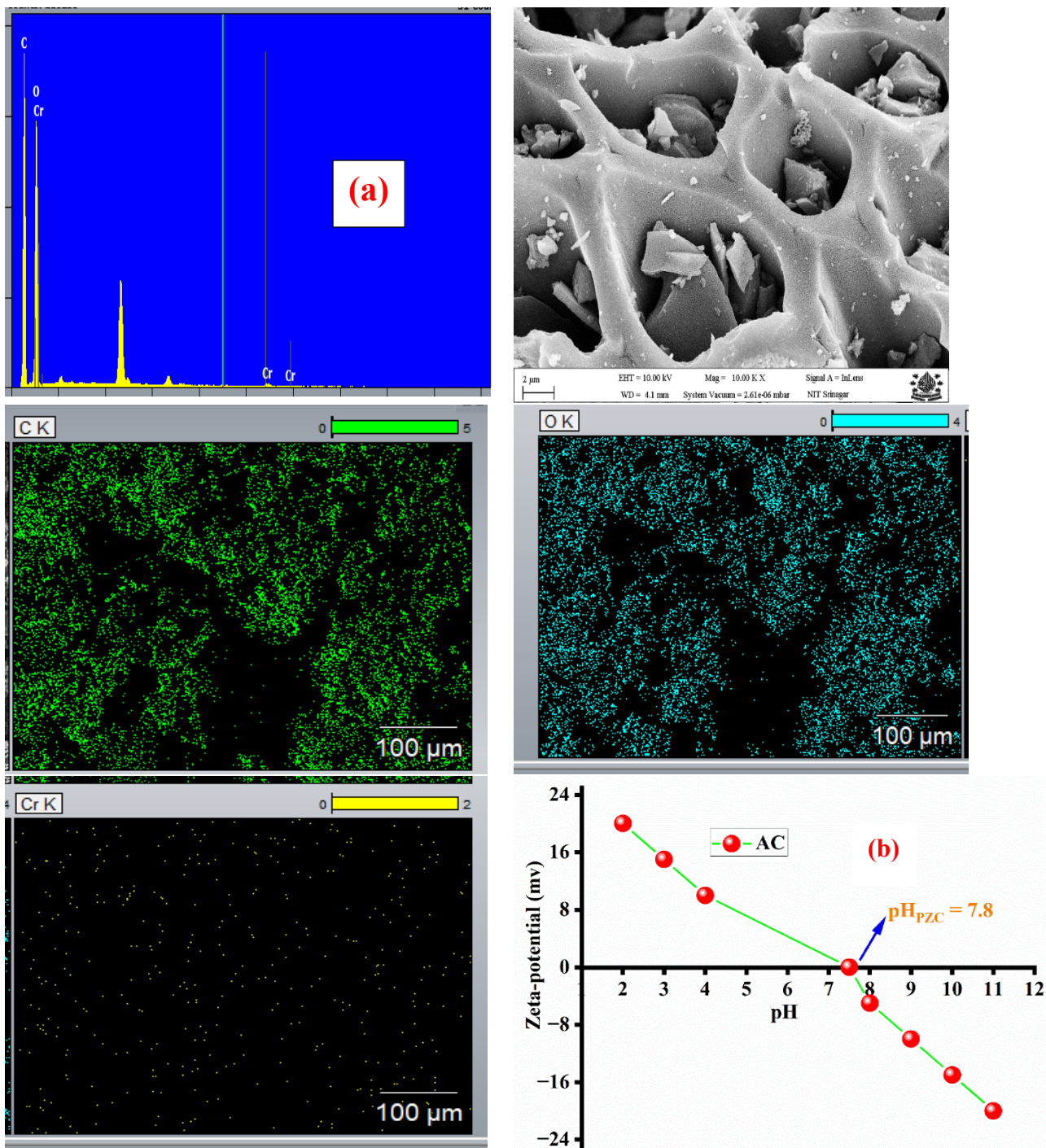


Fig.S5 (a) EDAX- mapping of CDPL after Cr (VI) adsorption; (b) point of zero charge analysis

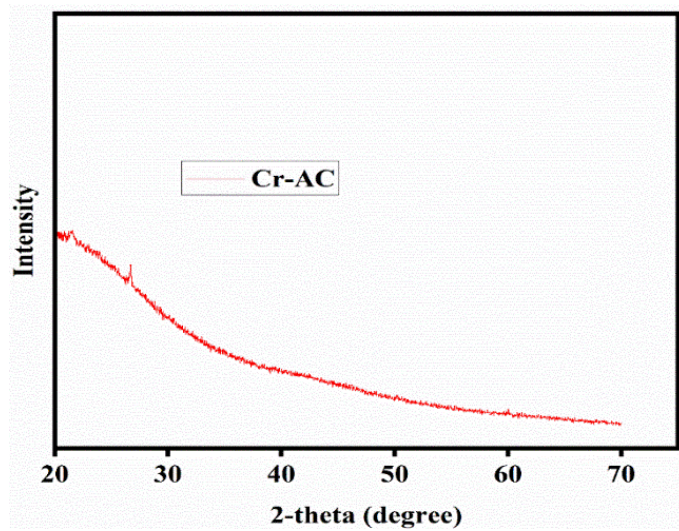
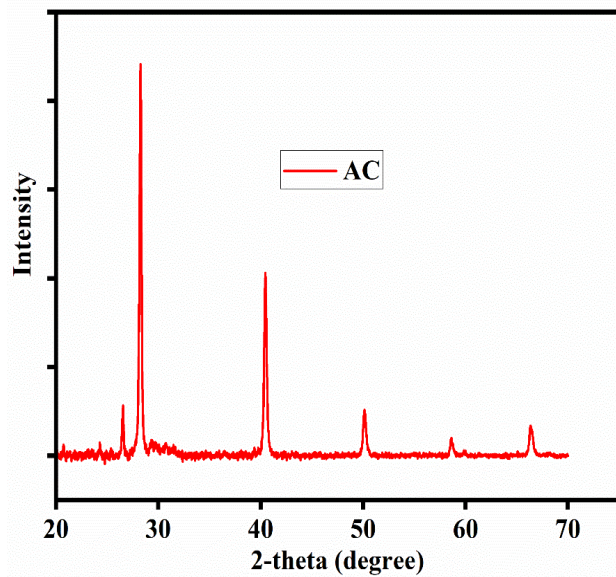
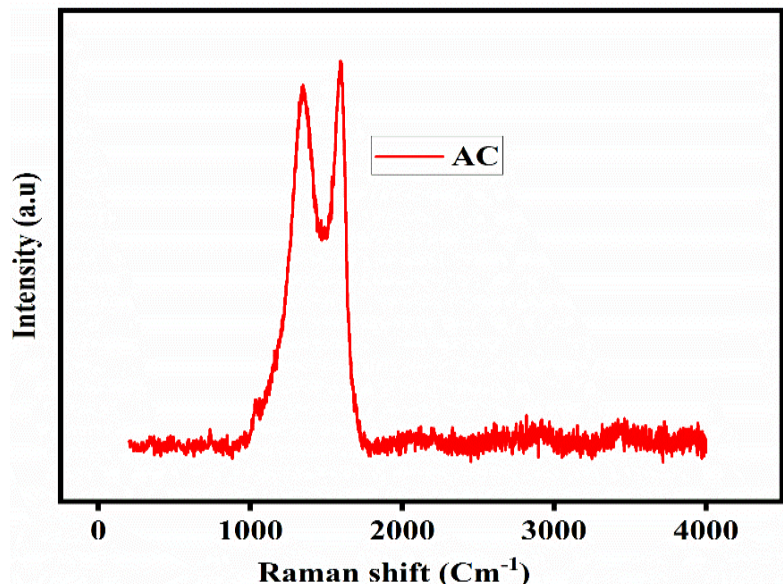


Fig.S6 Raman spectra of AC (a) XRD before (c) after (d) Cr (VI) adsorption

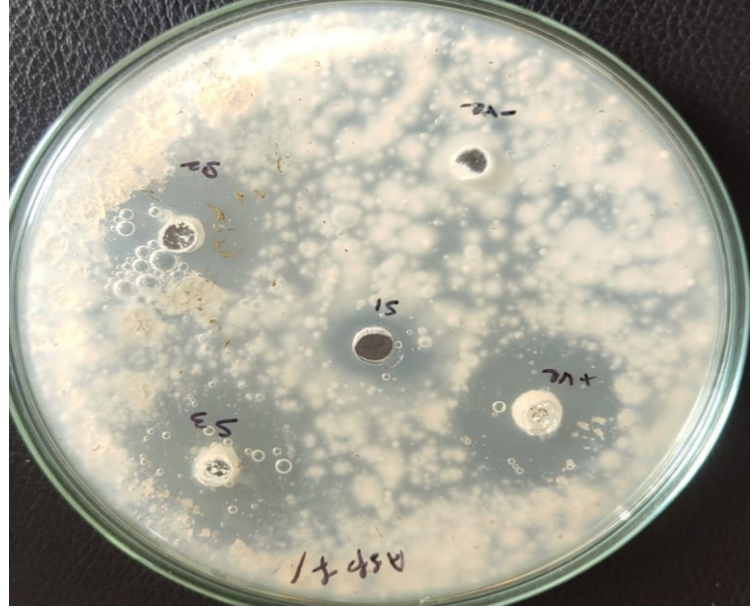
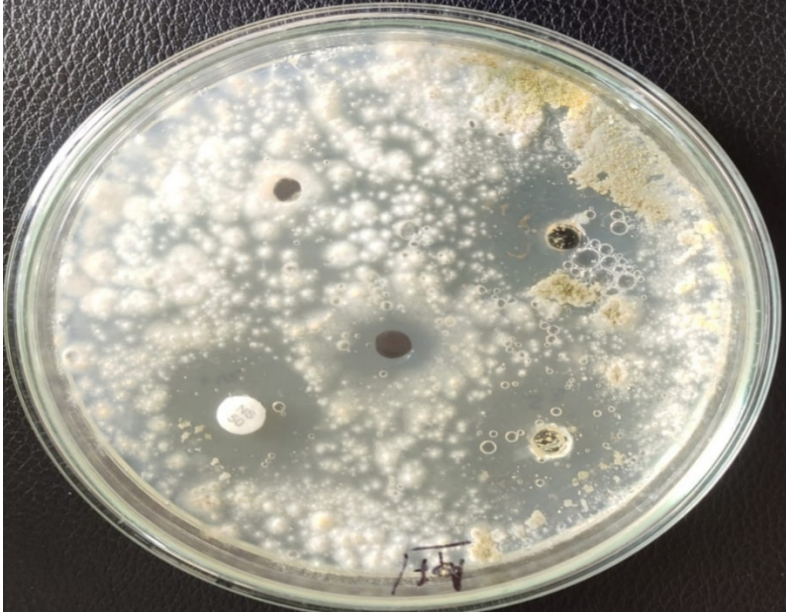


Fig. S7 Antifungal activity of AC in combination with silver

Table S1 Isothermal adsorption fitting curve data at different temperatures for Cr (VI), Acetaminophen, Ibuprofen, and Orudis KT adsorption onto AC

Isotherm model	Parameters	Cr (VI)	Acetaminophen	Ibuprofen	Orudis KT
Langmuir	Q _{max} (mg/g)	156.946±0.452	248.349 ± 8.23E-6	216.138 ± 7.415E-6	201.725 ± 7.739E-6
	K _L (L/mg)	1.473±0.013	0.149 ± 2.65E-8	0.119 ± 1.93E-8	0.104 ± 1.750E-8
	RMSE	0.107	1.05769E-10	6.9739E-11	6.59197E-11
	R ²	0.999	0.999	0.999	0.999
Freundlich	K _F ((mg/g)/(L/mg) ^(1/n))	89.181±2.142	94.497±7.027	69.923±5.774	58.62±5.117
	1/n	0.367±0.030	0.214±0.0201	0.247±0.222	0.269±0.0234
	RMSE	26.557	57.508	46.787	41.526
	R ²	0.966	0.9437	0.9499	0.9537
Temkin	A (L/g)	13.775±0.910	3.806±1.047	2.037±0.415	1.477±0.247
	B (j/mol)	35.086±0.770	41.714±2.358	40.020±1.923	39.314±1.694
	RMSE	2.646	25.429	16.911	12.825
	R ²	0.998	0.994	0.995	0.995
Radke Prausnitz	Q _{max} (mg/g)	190.115±52.325	217.378 ± 39.554	208.056 ± 42.039	156.858 ± 35.200
	K _{RP}	1.100±0.608	0.192 ± 0.069	0.129 ± 0.044	0.155 ± 0.062
	n	1.540±0.215	0.972 ± 0.0416	0.994 ± 0.0461	0.944 ± 0.0505
	RMSE	50.580	14.762	10.680	9.574
Toth isotherm	q _m (mg/g)	222.108±89.502	221.434 ± 35.763	209.363 ± 32.250	165.322 ± 32.191
	K _T	1.089±0.533	0.183 ± 0.055	0.127 ± 0.032	0.139 ± 0.044
	t	1.153±0.2165	0.972 ± 0.0414	0.994 ± 0.045	0.944 ± 0.050
	RMSE	50.580	14.762	10.680	9.574
	R ²	0.971	0.997	0.997	0.997

Table S2 Calculated values of parameters for kinetic models of Cr (VI) onto AC

Adsorbent	C _o (mg/L)	Q _e (exp) (mg/g)	Pseudo-first-order			Pseudo- second -order		
			K ₁ (min ⁻¹)	Q _e (cal) (mg/g)	R ²	K ₂ (g/mg min)	Q _e (cal) (mg/g)	R ²
AC	0.5	29.98	0.107	16.53	0.94	0.0435	30.31	0.999
	1.0	58.71	0.17	23.89	0.96	0.0036	60.62	0.990
	2.0	118.39	0.24	36.31	0.98	0.00073	119.047	0.994
	3.0	127.89	0.028	38.01	0.94	0.0069	129.87	0.992
	4.0	144.69	0.0197	56.22	0.77	0.00806	146.19	0.998

Table S3 Calculated values of parameters for kinetic models of Acetaminophen, Ibuprofen, and Orudis KT on to AC

Kinetic model	Parameters	Acetaminophen	Ibuprofen	Orudis KT
Pseudo-first-order	Q _e (mg/g)	91.716 ± 0.759	57.00 ± 0.054	47.230 ± 0.049
	K ₁ (min ⁻¹)	0.323 ± 0.026	0.24551 ± 0.002	0.190 ± 0.002
	RMSE	5.776	2.723	2.144
	R ²	0.987	0.919	0.965
Pseudo-second -order	Q _e (mg/g)	94.948 ± 1.280E-6	58.928 ± 1.241E-6	49.189 ± 1.299E-6
	K ₂ (min ⁻¹)	0.008 ± 1.695E-9	0.007 ± 1.883E-9	0.005 ± 1.798E-9
	RMSE	9.157E-12	7.766E-12	7.858E-12
	R ²	0.998	0.997	0.995

Adsorbate	ΔG ⁰ (kJ mol ⁻¹) 298K ,312K,320K	ΔH ⁰ (kJmol ⁻¹)	ΔS ⁰ (jmol ⁻¹)
Cr (VI)	-0.003, -0.342, -1.03	72.853	21.021
Acetaminophen	-85.6, -86.4, -87.9	-37.32	162.12
Ibuprofen	-84.2, -84.9, -86.3	-37.08	157.96
Orudis KT	-81.8, -82.6, -84.1	-33.50	161.01

Table.S4 Thermodynamic parameters of adsorption of Cr (VI), Acetaminophen, Ibuprofen, and Orudis KT by AC

Contami				
Cr (VI)	Hexanediamide - modified biochar	80.85	2.0	1
	Melamine – modified biochar	62.26	2.0	1
	L-glutathione modified biochar	55.66	2.0	1
	AC	156.9	3.0	This study
	Natural peach gum polysaccharide	188.32	2.0	26
Acetaminophen (paracetamol)	AC derived from the oak acorn	45.45	3.0	3
	NH ₄ Cl -induced AC	233	7.1	4
	Sludge-based activated carbon	145.4	8.0	5
	AC	248.16	8.0	This study
Ibuprofen	AC from vegetable	115.1	2.0	6
	AC from agricultural by product	12.6	4.1	7
	AC from oak acorn	96.15	3.0	3
	AC	216.10	4.0	This study
Orudis KT (Ketoprofen)	AC from agricultural by-products	24.7	4.0	7
	AC from vegetable	79.1	2.0	6
	graphene oxide/MOF composites	59	7.0	8
	AC	201.7	6.0	This study

Table. S5 Adsorption capacities of various adsorbents reported in literature

Strains	AC with silver	Fluconazole
<i>Aspergillus Niger</i>	>512	1.25
<i>Asp</i>	---	---
Table .S6 Outcomes of antifungal activity by AC with silver		
<i>Ca.....</i>	---	---
<i>Candida par psilosis</i>	> 200	2.5
<i>Candida glabrata</i>	>512	2.5