An artificial intelligence approach for modeling the rejection of anti-inflammatory drugs by nanofiltration and reverse osmosis membranes using kernel support vector machine and neural networks

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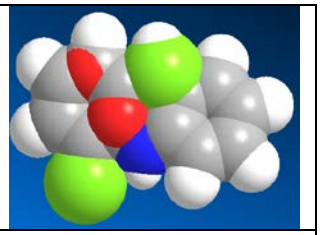
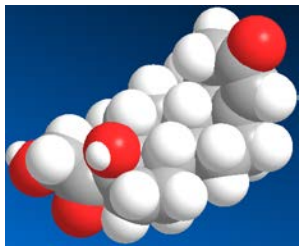
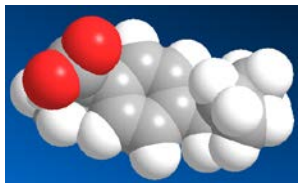
03	**Diclofenac**	$C_{14}H_9Cl_2NO$	296.16	
04	**Hydrocortisone**	$C_{21}H_{30}O_5$	362.460	
05	**Ibuprofen**	$C_{13}H_{18}O_2$	206.29	

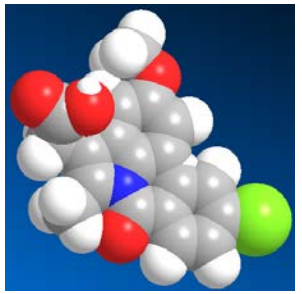
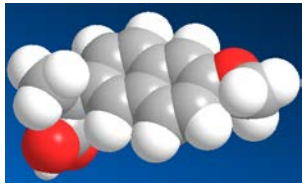
06	**Indomethacin**	$C_{19}H_{16}ClNO_4$	357.788	
07	**Naproxen**	$C_{14}H_{14}O_3$	230.259	

Table 2. Statistical analysis of inputs and output.

		Min (Train)	Max (Train)	Mean (Train)	STD (Train)	Min (Test)	Max (Test)	Mean (Test)	STD (Test)	Max (Overall)	Mean (Overall)	STD (Overall)	Max (Overall)
Inputs	**d_c(g/mol)**	0.5855	0.8892	0.7669	0.1116	0.5855	0.8892	0.7566	0.1142	0.5855	0.8892	0.7648	0.1120
	LogD	-2.5900	1.9200	1.1264	0.7264	-2.5900	1.9200	1.0515	0.8248	-2.5900	1.9200	1.1114	0.7463
	Dipole moment (Debye)	0.0000	5.2300	3.2694	1.4900	0.0000	5.2300	3.3107	1.4748	0.0000	5.2300	3.2776	1.4846
	Length (nm)	0.1719	1.5070	1.3347	0.1875	0.1719	1.5070	1.3077	0.2155	0.1719	1.5070	1.3293	0.1934
	Eqwidth (nm)	0.2932	1.1290	0.3855	0.0910	0.2932	1.0230	0.3845	0.0969	0.2932	1.1290	0.3853	0.0920
	MWCO (Dalton)	100.0000	405.0000	184.9583	90.8088	100.0000	405.0000	203.7500	91.5619	100.0000	405.0000	188.7167	91.1178
	SR (NaCl)	0.1360	0.9950	0.8046	0.2564	0.2053	0.9950	0.7865	0.2701	0.1360	0.9950	0.8010	0.2589
	Zeta potential (mv)	-77.8600	0.4900	-28.1020	16.3902	-77.8600	0.4900	-30.0060	15.2482	-77.8600	0.4900	-28.4828	16.1615
	Contact angle (°)	15.1200	67.5000	42.9740	14.2406	15.1200	67.5000	46.7020	13.1119	15.1200	67.5000	43.7196	14.0803
	pH	3.0000	9.0000	6.2952	1.1560	3.0000	8.0000	6.1848	0.9555	3.0000	9.0000	6.2731	1.1181
	Pressure (kPa)	280.0000	4100.0000	1127.0830	580.7110	280.0000	3000.0000	989.3330	469.2580	280.0000	4100.0000	1099.5330	562.1860
	Recovery (%)	0.0589	98.4800	15.7466	24.0704	0.1038	86.5500	8.8809	14.5309	0.0589	98.4800	14.3734	22.6352
	Temperature (C°)	20.0000	45.0000	27.6875	9.1487	20.0000	45.0000	27.7500	9.8366	20.0000	45.0000	27.7000	9.2734
Output	**Rejection (%)**	1.2900	100.0000	90.3796	16.0213	34.1224	100.0000	92.5237	12.2419	1.2900	100.0000	90.8084	15.3455

logD : [20]

Dipole moment : ChemBio3D Ultra 12.0 software

Molecular size (length, width, and depth) : [20]

$eqwidth = \sqrt{molecular\ width * molecular\ depth}$ [20]

$d_c = 0.065Mw^{0.438}$ [31]

Table 3. Weights and bias of the optimized NN model.

Input-Hidden layer connections														Hidden layer -Output connections	
Weights													Biais	Weights	Biais
$w_{j,1}^{I}$	$w_{j,2}^{I}$	$w_{j,3}^{I}$	$w_{j,4}^{I}$	$w_{j,5}^{I}$	$w_{j,6}^{I}$	$w_{j,7}^{I}$	$w_{j,8}^{I}$	$w_{j,9}^{I}$	$w_{j,10}^{I}$	$w_{j,11}^{I}$	$w_{j,12}^{I}$	$w_{j,13}^{I}$	b_j^H	$w_{I,j}^{H}$	b_1^0
-0.5669	-0.6087	0.1294	0.0142	0.1986	0.0215	0.2086	-0.1355	0.9975	0.2086	-0.2682	-0.0931	-0.0461	0.9257	0.8200	
0.3787	0.0008	-0.2904	0.0511	0.0214	0.1173	-0.0600	0.1362	0.1449	1.2332	-0.1092	0.0262	0.2470	-0.0945	-0.5322	
0.1104	0.0655	-0.2213	0.0153	-0.0047	-0.1381	0.1931	-0.3186	-0.9262	0.7103	-0.3230	-0.0127	-0.0496	0.1983	0.3022	
0.8364	0.0514	-0.0368	-0.6535	-0.2428	0.1859	0.1881	-0.4735	-1.2572	1.2405	-0.2520	0.1007	-0.0576	0.0529	0.3764	
0.0845	0.0705	0.0356	0.2015	-0.0305	-0.6224	-0.1103	0.6070	0.4671	-0.0254	-0.2142	0.0851	-0.1775	0.2644	0.3929	
-0.9890	0.0517	0.3822	-0.4052	-0.0742	-0.1409	-0.1041	-1.4026	-0.0288	0.2704	-0.0789	0.1205	0.0438	-0.2744	-0.0408	
-0.7197	0.2669	0.1188	-0.6876	0.1144	-0.0930	-0.2672	0.4558	0.5826	-0.7077	-0.2013	0.1958	-0.1015	0.0186	1.2155	
-1.6049	0.4786	0.0495	-0.0679	-0.1717	0.4532	-0.0953	-1.0772	-0.5268	-0.1683	0.0894	-0.0576	0.0737	0.2466	0.1903	
0.4124	0.4520	0.2245	-1.4758	-0.0547	0.0265	-0.6731	-0.3656	-0.1948	-0.8147	-0.1026	0.0937	0.0517	-0.0794	-0.0358	
-0.0759	0.1039	0.5073	1.7859	0.0021	-0.0414	-0.3816	-1.3632	0.5145	-0.0064	0.3656	-0.0260	0.0119	-0.0945	0.6142	
0.3968	0.0202	-0.0079	-0.7833	-0.2357	0.3279	0.0132	-0.1369	0.1447	-0.0016	0.3933	0.2690	-0.0275	-0.1068	-0.0377	

0.3338	-0.0572	-0.5135	-1.7252	-0.0566	-0.1225	-0.1010	-0.4223	-0.5777	0.1092	0.1285	0.1703	0.0330	-0.2301	0.6548	
0.1984	0.0211	-0.4062	0.0433	-0.1828	0.3570	0.5516	-0.7523	-0.0225	0.0938	0.6749	0.0517	0.1551	-0.3427	0.5529	0.6149
0.1251	0.0965	0.2957	0.4272	-0.1542	-0.3990	-0.1098	1.3610	0.4978	-0.0109	0.5853	-0.7339	0.0652	1.1144	0.9415	
0.0965	-0.2596	-0.0383	-0.5160	0.0374	0.1421	-1.0058	-0.3770	-0.3084	-0.0625	-0.0198	0.0482	-0.0058	0.8634	-1.1687	
0.3814	-0.1225	0.0393	0.2760	-0.0082	-0.0680	-0.0720	-0.0301	0.3673	0.0890	0.3371	0.1266	-0.0167	0.0271	-1.1166	
-0.6209	0.1306	-0.0755	0.1328	0.0225	0.1535	0.4195	-0.2601	-0.7324	-0.0869	-0.8443	0.0956	0.0370	-0.1135	0.9290	
-0.0546	0.0692	-0.0380	0.1775	-0.1446	-0.1111	-0.3152	-0.1001	-1.4555	0.1631	0.0136	-0.2202	0.0137	-0.5594	1.4205	
0.4321	0.0055	-0.1652	0.2391	-0.0766	-0.4236	0.2914	0.0937	-0.1600	0.2463	0.5560	-0.3218	-0.2475	0.2125	0.2439	
-0.1220	0.2263	-0.0085	0.2437	0.0080	-0.3137	0.9830	0.1502	-0.7210	0.0883	0.1070	0.2764	-0.0592	-0.2114	-0.5522	
0.8557	0.0906	-0.1392	0.0233	0.1814	-0.6863	0.4231	1.0988	-0.4535	0.0380	-0.3243	0.0296	-0.0940	0.5017	-0.5784	
0.0012	0.1768	-0.2177	0.1119	0.1164	0.0296	-0.6950	-0.3282	0.8951	0.1781	0.3780	0.0041	-0.0007	0.1321	-0.0670	
-1.2107	0.0906	-0.0929	0.2719	0.2351	0.0643	0.9254	0.8481	0.3196	-0.1560	-0.4216	0.1169	-0.0527	-0.0277	0.3992	
0.2542	-0.0598	-0.1295	0.0784	0.2570	0.7652	0.0287	0.7726	0.3354	-0.1699	-0.1555	0.3316	0.1792	0.0917	0.0539	
-0.3442	-0.1059	-0.1828	0.1765	0.0887	-0.2642	-0.4817	0.0074	-0.7848	-0.1170	-0.1030	-0.0377	-0.0286	-0.0222	-0.0419	