



Research article

Pyridopyrazine derivatives as highly selective histamine H4 receptor antagonist for the treatment of atopic dermatitis: QSAR modeling and molecular docking studies

Mohamed El Yaqoubi^{1,*}, Mouad Lahyaoui¹, Yousra Seqqat¹, Taoufiq Saffaj¹, Bouchaib Ihssane¹, Nabil Saffaj², Rachid Mamouni², Fouad Ouazzani Chahdi¹, Fahad M Alshabrmi⁴, Alaa Abdulaziz Alnahari³, Saad M. Howladar³, Ammar AL-Farga^{3,*} and Youssef Kandri Rodi¹

¹ Laboratory of Applied Organic Chemistry, Faculty of Science and Technology, Sidi Mohamed Ben Abdellah University, USMBA, Po. Box 2626 Fez, Morocco

² Laboratory of Biotechnology, Materials and Environment, IbnZohr University, BP 8106-BP 32/S, Riad Salam, CP 80000 Agadir, Morocco

³ University of Jeddah, College of Science, Department of Biological science, Jeddah, Saudi Arabia

⁴ Department of Medical Laboratories, College of Applied Medical Sciences, Qassim University, Buraydah 51452, Saudi Arabia

* **Correspondence:** E-mail: mohamed.elyaqaoubi@usmba.ac.ma, amalfarga@uj.edu.sa.

Supplementary

Table S1. Values of molecular descriptors.

Compounds	pIC50	PEOE_VSA_FPNEG	weinerPol	zagreb	VAdjEq	vsurf_CP	vsurf_CW4	vsurf_HL1	vsurf_HL2	rsynth	ASA_P	ast_violation	ASA+	ASA-
1	3.000	0.042	33.000	112	0.515	0.113	0.551	0.161	0.065	0.650	10.963.396	1.000	40.373.944	12.762.859
2	3.000	0.041	33.000	112	0.515	0.153	0.525	0.145	0.079	0.700	95.851.654	1.000	38.741.055	10.712.401
3	0.077	0.039	35.000	118	0.496	0.122	0.502	0.154	0.082	0.619	10.899.474	2.000	39.229.434	16.030.385
4	0.067	0.037	35.000	118	0.496	0.116	0.479	0.164	0.091	0.619	10.779.842	2.000	39.263.477	17.985.321
5	0.034	0.037	35.000	118	0.496	0.224	0.334	0.080	0.035	0.619	14.639.209	2.000	40.919.955	2.255.936
6	0.510	0.039	35.000	118	0.496	0.117	0.498	0.155	0.080	0.714	14.806.596	1.000	42.989.026	16.112.144
7	0.280	0.037	41.000	136	0.449	0.086	0.790	0.239	0.128	0.750	19.742.375	2.000	33.231.342	18.631.187
8	0.240	0.038	37.000	122	0.479	0.090	0.623	0.204	0.101	0.727	22.222.356	1.000	39.924.231	18.415.219
9	0.180	0.037	38.000	124	0.479	0.183	0.443	0.117	0.070	0.636	10.805.282	2.000	33.300.653	21.151.329
10	0.520	0.041	41.000	132	0.449	0.094	0.598	0.170	0.064	0.667	19.151.152	2.000	43.342.398	19.576.657
11	0.240	0.039	44.000	150	0.410	0.094	0.609	0.199	0.096	0.704	26.586.453	2.000	40.536.575	29.583.435
12	0.270	0.036	40.000	128	0.463	0.114	0.540	0.148	0.067	0.565	20.297.386	2.000	38.960.272	22.022.089
13	0.300	0.035	39.000	124	0.479	0.117	0.483	0.165	0.091	0.591	13.385.425	2.000	41.745.453	1.990.751
14	0.130	0.044	33.000	112	0.515	0.103	0.713	0.212	0.106	0.600	12.597.466	1.000	31.316.394	16.590.276
15	10.000	0.038	39.000	134	0.475	0.130	0.477	0.159	0.075	0.652	1.663.562	2.000	37.750.897	23.258.298
16	0.380	0.037	38.000	124	0.479	0.110	0.479	0.133	0.046	0.500	21.252.779	2.000	42.368.903	27.310.751
17	0.760	0.041	35.000	118	0.496	0.098	0.562	0.186	0.087	0.476	16.768.111	2.000	35.295.078	22.605.206
18	2.900	0.037	39.000	122	0.479	0.127	0.477	0.147	0.071	0.636	19.196.291	2.000	42.580.161	23.737.079

Continued on next page

Compounds	pIC50	PEOE_VSA_FPNEG	weinerPol	zagreb	VAdjEq	vsurf_CP	vsurf_CW4	vsurf_HL1	vsurf_HL2	rsynth	ASA_P	ast_violation	ASA+	ASA-
19	10.00	0.041	37.000	116	0.496	0.100	0.534	0.157	0.060	0.619	16.648.996	2.000	4.188.558	20.293.745
20	4.800	0.037	36.000	124	0.479	0.151	0.330	0.105	0.048	0.636	19.974.908	2.000	47.871.603	23.745.012
21	4.100	0.037	36.000	124	0.479	0.107	0.427	0.155	0.075	0.636	18.712.567	2.000	48.113.913	23.333.781
22	6.300	0.069	32.000	114	0.515	0.082	0.640	0.238	0.123	0.600	21.842.752	1.000	34.884.082	20.185.214
23	1.200	0.039	34.000	120	0.496	0.081	0.556	0.186	0.084	0.286	20.004.114	2.000	38.821.274	18.902.292
24	0.065	0.043	32.000	114	0.515	0.077	0.609	0.205	0.070	0.300	23.614.592	1.000	32.701.877	2.747.536
25	5.200	0.074	30.000	110	0.535	0.078	0.866	0.299	0.129	0.316	18.440.018	1.000	17.979.361	20.146.872
26	0.430	0.040	36.000	132	0.492	0.098	0.617	0.202	0.107	0.409	12.855.392	2.000	35.076.929	18.783.318
27	0.490	0.046	33.000	126	0.510	0.109	0.568	0.176	0.082	0.381	16.860.704	2.000	34.444.046	22.149.731
28	0.052	0.038	39.000	134	0.475	0.134	0.450	0.141	0.064	0.652	13.564.815	2.000	39.993.179	23.060.422
29	10.000	0.040	39.000	134	0.475	0.105	0.512	0.179	0.082	0.261	13.211.986	2.000	39.457.718	22.093.919
30	0.062	0.040	35.000	118	0.496	0.119	0.490	0.166	0.085	0.476	13.696.535	2.000	39.103.784	16.004.063
31	0.028	0.039	35.000	118	0.496	0.078	0.599	0.204	0.092	0.476	16.272.374	2.000	42.271.979	20.183.499
32	0.053	0.045	32.000	114	0.515	0.059	0.816	0.342	0.199	0.150	14.409.018	1.000	23.354.417	17.382.526
33	0.027	0.043	32.000	114	0.515	0.055	0.887	0.354	0.183	0.150	17.170.274	2.000	22.451.479	2.046.132



AIMS Press

© 2024 the Author(s), licensee AIMS Press. This is an open access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>)