Journal of Applied Pharmaceutical Science
Available online at http://www.japsonline.com

Field and Gaussian-based 3D-QSAR models on 8-amino-imidazo [1, 5a] pyrazine derivatives as Bruton's tyrosine kinase inhibitors

Seethalakshmi Sakthivel, Julie Rebecca Joseph Mathari, Mursaleen Baba, Habeeb Shaik Mohideen

Department of Genetic Engineering, Bioinformatics and Integrative Omics Lab, School of Bioengineering, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chengalpattu, Chennai – 603203, Tamil Nadu, India.

Doi: https://doi.org/10.7324/JAPS.2025.176784

SUPPLEMENTARY MATERIAL

Supplementary Files

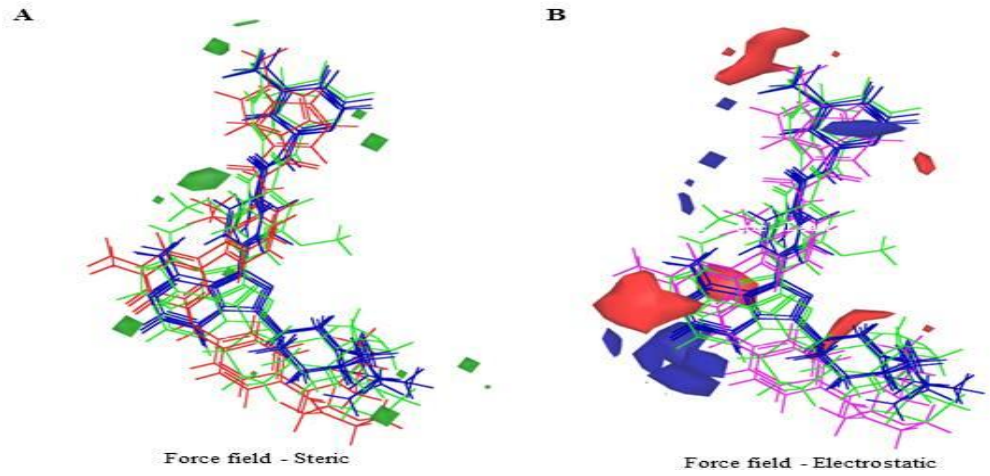

Figure S1. Compounds were shown in line and the line color represents the activity of the compound. (A) Force field steric contour map (Green: highly active, blue: moderate and red: least active). (B) Electrostatic force field (Green: highly active, blue: moderate and magenta: least active).

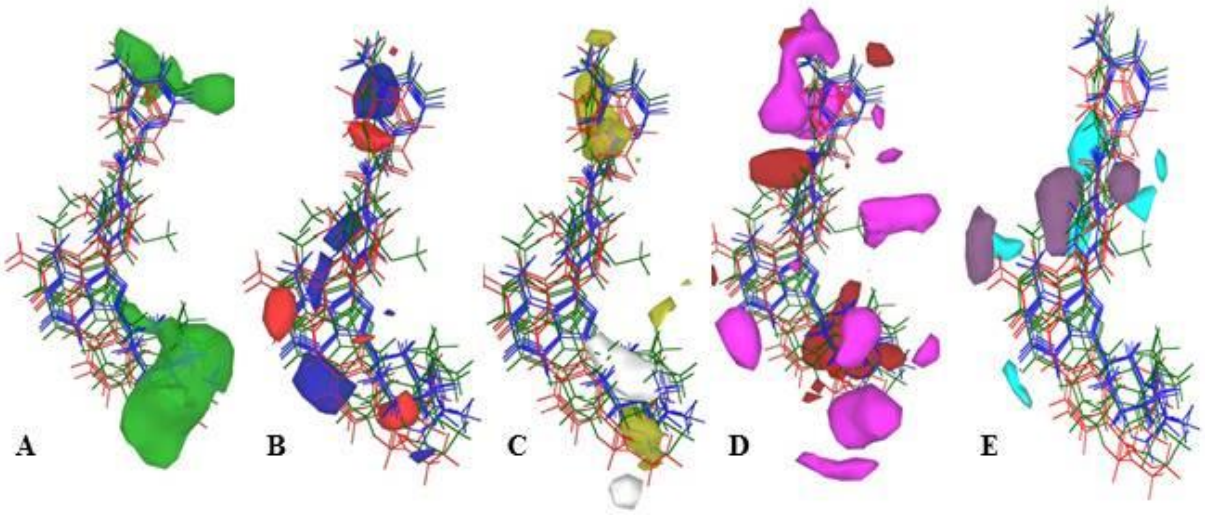

Figure S2. (A) Gaussian Steric, (B) Gaussian Electrostatic, (C) Gaussian Hydrophobic, (D) Gaussian Hbond Acceptor and (E) Gaussian Hbond Donor (Compounds were shown in lines and the color indicates activity. Green : highly active, blue: moderate and red: least active).

Table S1. Statistical Details of Force Field QSAR

# Factors	SD	R^2	R^2 CV	R^2 Scramble	Stability	F	P	RMSE	Q^2	Pearson-r
1	0.7411	0.6135	0.555	0.1363	0.996	73	4.73E-11	0.74	0.6319	0.8539
2	0.4762	0.8439	0.6616	0.3577	0.896	121.6	7.14E-19	0.6	0.7598	0.8813
3	0.3904	0.8974	0.695	0.5281	0.802	128.3	8.97E-22	0.67	0.7028	0.8576
4	0.3529	0.9181	0.6863	0.6419	0.821	120.4	9.06E-23	0.67	0.6999	0.8563
5	0.332	0.9292	0.6952	0.7226	0.823	110.2	5.10E-23	0.7	0.6737	0.8473

Table S2. Steric and Electrostatic field interaction in force field based QSAR

# Factors	Force Field Steric	Force Field Electrostatic
1	0.643	0.357
2	0.665	0.335
3	0.717	0.283
4	0.727	0.273
5	0.73	0.27

Table S3. Statistical summary Gaussian QSAR with five PLS factors.

# Factors	SD	R^2	R^2 CV	R^2 Scramble	Stability	F	P	RMSE	Q^2	Pearson-r
1	0.6879	0.6669	0.6223	0.1092	0.997	92.1	1.48E-12	0.65	0.7164	0.853
2	0.5067	0.8232	0.7002	0.2764	0.964	104.8	1.17E-17	0.64	0.7316	0.8759
3	0.4639	0.8551	0.6952	0.4556	0.927	86.6	1.74E-18	0.73	0.6439	0.8432
4	0.3741	0.9079	0.675	0.6046	0.844	106	1.10E-21	0.7	0.6723	0.8467
5	0.3216	0.9335	0.675	0.7084	0.818	118	1.34E-23	0.77	0.6079	0.8207

Table S4. Contribution of different fields in Gaussian QSAR.

# Factors	Gaussian Steric	Gaussian Electrostatic	Gaussian Hydrophobic	Gaussian Hbond Acceptor	Gaussian Hbond Donor
1	0.424	0.129	0.238	0.118	0.091
2	0.46	0.112	0.237	0.114	0.077
3	0.45	0.087	0.275	0.127	0.062
4	0.391	0.093	0.31	0.154	0.051
5	0.385	0.099	0.293	0.161	0.063