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SUPPLEMENTARY MATERIAL TO

Application of genetic algorithm – multiple linear regressions to predict the activity of RSK inhibitors

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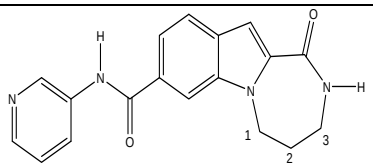
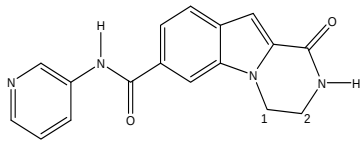
TABLE S-I. Chemical structures and the observed pIC_{50} values and those predicted by the GA–MLR method

No.	General structure	Substituent	Experimental	Predicted
1		–	6.62	6.00
2		1-Me	7.39	6.96
3		2-Me	5.92	5.37
4		2-CH_2NH_2	5.74	6.15
5		1,2-*cis*-DiMe	6.62	6.72
6[a]		1,2-*trans*-DiMe	5.96	6.39
7		2,2-DiMe	5.34	5.21
8		2,2-DiF	5.77	6.07
9[a]		2-spiro-c-Pr	6.39	5.83
10		2-spiro-c-Bu	5.48	5.40
11		3-Me	5.60	5.85
12		–	6.14	6.61
13		1-Me	6.77	7.06
14		1,1-DiMe	6.68	6.98
15		1,2-*cis*-DiMe	7.35	6.67
16		1,2-*trans*-DiMe	6.06	6.39
17		2-Me	6.46	6.14
18		2-CH_2NH_2	6.01	6.21

* Corresponding author. E-mail: pourbasheer@ut.ac.ir

TABLE S-I. Continued

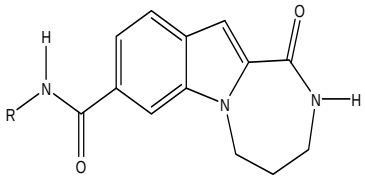
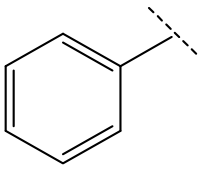
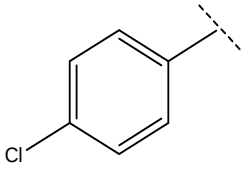
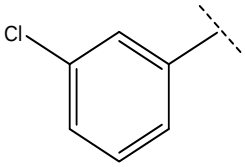
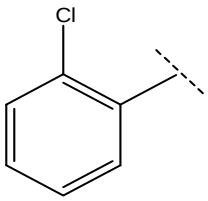
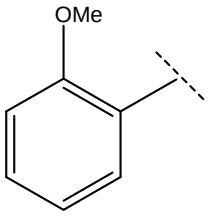
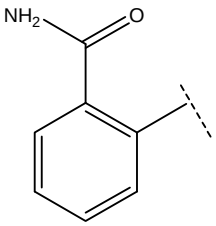
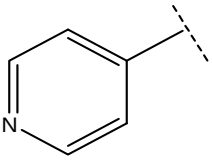
No.	General structure	Substituent	Experimental	Predicted
19		H	5.04	5.90
20			6.54	6.42
21[a]			6.74	6.67
22[a]			6.57	7.43
23[a]			5.22	5.77
24			6.40	6.97
25			7.68	7.97
26			7.47	7.12

TABLE S-I. Continued

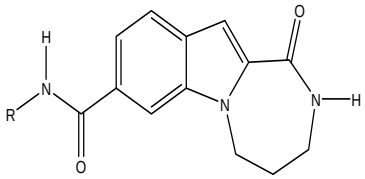
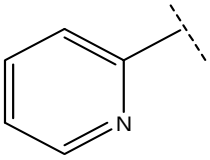
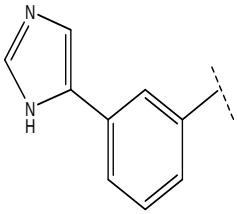
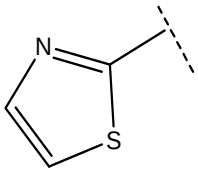
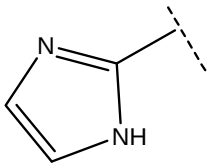
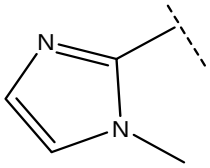
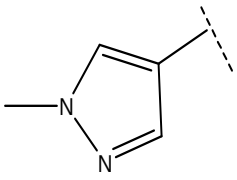
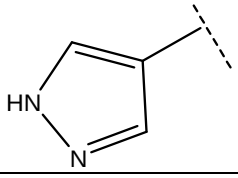
No.	General structure	Substituent	Experimental	Predicted
27			6.66	6.75
28			7.28	6.91
29[a]			5.66	6.41
30			7.59	6.72
31			5.66	5.91
32[a]			7.96	7.95
33			7.37	7.56

TABLE S-I. Continued

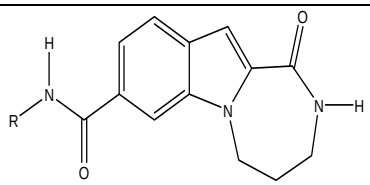
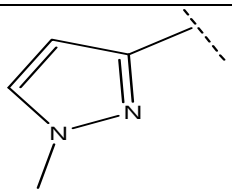
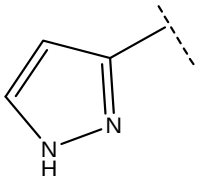
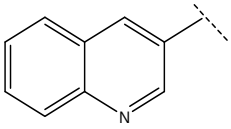
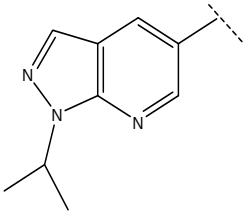
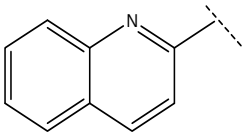
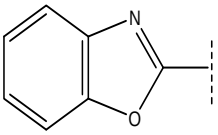
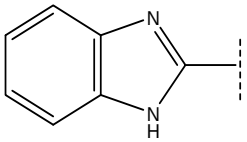
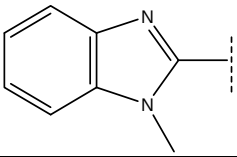
No.	General structure	Substituent	Experimental	Predicted
34			6.27	7.03
35			7.03	6.51
36			7.47	7.12
37			7.28	7.56
38			7.17	7.29
39			6.44	7.23
40			8.40	8.21
41			8.05	7.60

TABLE S-I. Continued

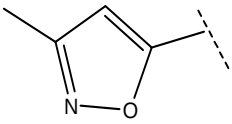
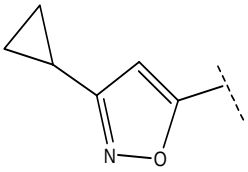
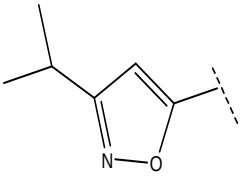
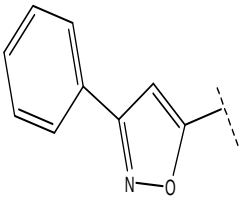
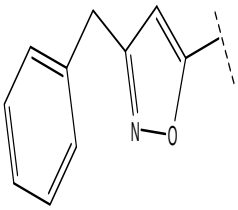
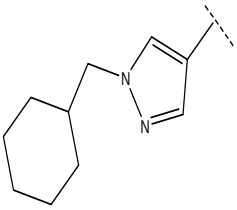
No.	General structure	Substituent	Experimental	Predicted
42			7.72	7.59
43			7.74	7.91
44[a]			7.59	8.00
45			7.07	7.42
46			7.89	7.77
47[a]			8.15	8.56

TABLE S-I. Continued

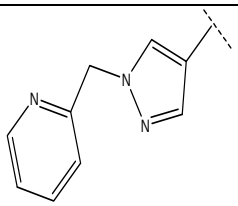
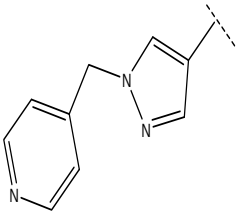
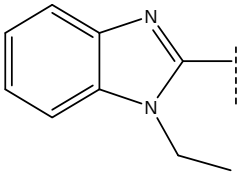
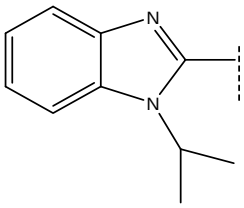
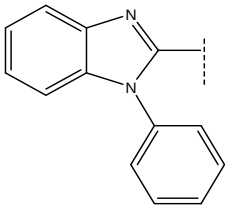
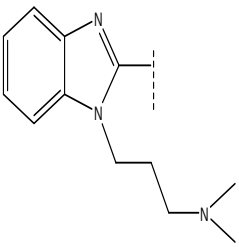
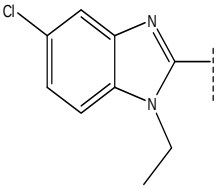
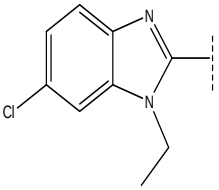
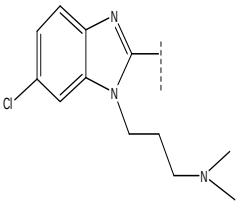
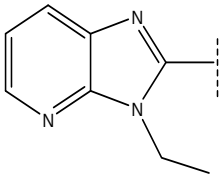
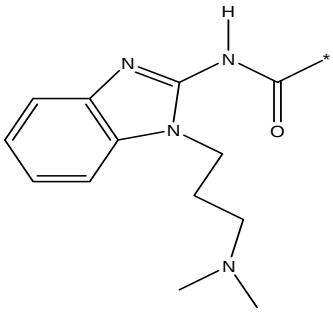
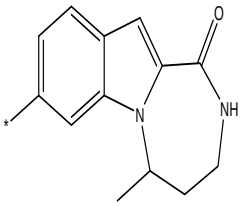
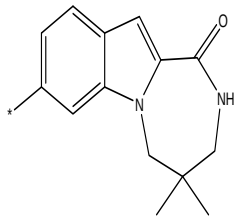
No.	General structure	Substituent	Experimental	Predicted
48			8.00	7.90
49			8.70	8.25
50[a]			9.00	8.83
51			7.70	7.90
52[a]			7.21	7.50
53			7.68	7.39

TABLE S-I. Continued

No.	General structure	Substituent	Experimental	Predicted
54			8.22	7.64
55			7.92	7.72
56			7.70	7.71
57			8.40	8.35
58			9.00	9.22
59			7.57	7.66

[a]Test set

TABLE S-II. *K*-means clustering of the compounds

Cluster	No. of compounds	Serial number of compounds in different clusters									
1	1					58					
2	38	5	8	9[a]	12	13	14	15	17	18	20
		21[a]	24	25	26	27	28	29[a]	30	31	33
		34	35	40	41	42	43	44[a]	45	46	47[a]
		48	49	52[a]	53	56	57	58	59		
						62					
3	18	1	2	3	4	6[a]	7	10	11	16	19
		22[a]	23[a]	32[a]	36	37	39	51	54		
4	2	38	50[a]								

[a]Test set