Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - algorithms scores

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Table S1. Classification algorithms' A, K, and E scores along with their APD values and ROC curves.

Algorithm	Database	Dataset	A (%)	K	E (%)	APD leverage (%)	APD similarity (%)	ROC curve
DT	FlavStr	Tr	80.76	0.61	19.23	96.40	100.00	Active: 0.86
		Ts	82.14	0.63	17.85			Active: 0.86
		CV	73.07	0.45	26.92			Active: 0.64
	FabG	Tr	100.00	1.00	0.00	80.00	100.00	Active: 1.00
		Ts	80.00	0.61	20.00			Active: 0.83
		CV	87.50	0.75	12.50			Active: 0.80
	FabZ	Tr	90.00	0.80	10.00	100.00	100.00	Active: 0.91
		Ts	100.00	1.00	0.00			Active: 1.00
		CV	70.00	0.40	30.00			Active: 0.50
	FabI	Tr	100.00	1.00	0.00	100.00	100.00	Active: 1.00
		Ts	80.00	0.54	20.00			Active: 0.75
		CV	100.00	1.00	0.00			Active: 1.00
$DT_{S_{AR}}$	FlavStr	Tr	100.00	1.00	0.00	-	-	-
		Ts	60.71	0.23	39.29			-

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Algorithm	Database	Dataset	A (%)	K	E (%)	APD leverage (%)	APD similarity (%)	ROC curve
		CV	69.23	0.57	21.15			-
		Tr	100.00	1.00	0.00			-
	FabG	Ts	100.00	1.00	0.00	-	-	-
		CV	87.50	0.71	12.50			-
		Tr	100.00	1.00	0.00			-
	FabZ	Ts	66.66	0.33	33.33	-	-	-
		CV	90.00	0.78	10.0			-
		Tr	100.00	1.00	0.00			-
	FabI	Ts	80.00	0.54	20.00	-	-	-
		CV	100.00	1.00	0.00			-
RF		Tr	76.92	0.51	23.07			Active: 0.83
	FlavStr	Ts	82.14	0.62	17.85	96.04	100.00	Active: 0.79
		CV	75.00	0.48	25.00			Active: 0.74
	FabG	Tr	100.00	1.00	0.00	100.00	100.00	Active: 1.00
		Ts	100.00	1.00	0.00			Active: 1.00
		CV	87.50	0.71	12.50			Active: 1.00

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Algorithm	Database	Dataset	A (%)	K	E (%)	APD leverage (%)	APD similarity (%)	ROC curve
		Tr	80.00	0.54	20.00			Active: 0.87
	FabZ	Ts	83.33	0.66	16.66	100.00	100.00	Active: 0.88
		CV	80.00	0.58	20.00			Active: 0.75
		Tr	100.00	1.00	0.00			Active: 1.00
	FabI	Ts	80.00	0.61	20.00	100.00	100.00	Active: 0.83
		CV	100.00	1.00	0.00			Active: 1.00
SVM		Tr	75.00	0.48	25.00			Active: 0.77
	FlavStr	Ts	67.85	0.36	32.14	96.04	100.00	Active: 0.69
		CV	73.07	0.44	26.92			Active: 0.67
		Tr	100.00	1.00	0.0			Active: 1.00
	FabG	Ts	100.00	1.00	0.0	80.00	100.00	Active: 1.00
		CV	87.50	0.71	12.50			Active: 0.83
		Tr	100.00	1.00	0.0			Active: 1.00
	FabZ	Ts	100.00	1.00	0.0	100.00	100.00	Active: 1.00
		CV	100.00	1.00	0.0			Active: 1.00
	FabI	Tr	100.00	1.00	0.0			Active: 1.00

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Algorithm	Database	Dataset	A (%)	K	E (%)	APD leverage (%)	APD similarity (%)	ROC curve
		Ts	80.00	0.54	20.00	100.00	100.00	Active: 0.75
		CV	100.00	1.00	0.0			Active: 1.00
MLP	FlavStr	Tr	86.53	0.72	13.46	96.40	100.00	Active: 0.92
		Ts	92.85	0.85	7.14			Active: 0.98
		CV	73.07	0.45	26.92			Active: 0.72
	FabG	Tr	75.00	0.38	25.00	100.00	100.00	Active: 1.00
		Ts	100.00	1.00	0.00			Active: 1.00
		CV	75.00	0.38	25.00			Active: 0.93
	FabZ	Tr	60.00	0.00	40.00	100.00	100.00	Active: 1.00
		Ts	50.00	0.00	50.00			Active: 1.00
		CV	75.00	0.28	30.00			Active: 0.95
	FabI	Tr	87.50	0.75	12.50	100.00	100.00	Active: 1.00
		Ts	100.00	1.00	0.00			Active: 1.00
		CV	87.50	0.75	12.50			Active: 1.00
KNN	FlavStr	Tr	96.15	0.92	3.84	96.40	100.00	Active: 0.99
		Ts	85.71	0.71	14.28			Active: 0.95

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Algorithm	Database	Dataset	A (%)	K	E (%)	APD leverage (%)	APD similarity (%)	ROC curve
		CV	73.07	0.44	26.92			Active: 0.67
	FabG	Tr	100.00	1.00	0.00	80.00	100.00	Active: 1.00
		Ts	80.00	0.61	20.00			Active: 1.00
		CV	87.50	0.71	12.50			Active: 1.00
	FabZ	Tr	80.00	0.61	20.00	100.00	83.33	Active: 1.00
		Ts	83.33	0.66	16.67			Active: 1.00
		CV	100.00	1.00	0.00			Active: 1.00
	FabI	Tr	100.00	1.00	0.00	100.00	100.00	Active: 1.00
		Ts	100.00	1.00	0.00			Active: 1.00
		CV	87.50	0.75	12.50			Active:0.81

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Table S2. Regression algorithms' R^2, RMSE, and acceptability criteria along with their APD values.

Algorithm	Database	Dataset	R^2	RMSE	MAE	Acceptability criteria	APD leverage (%)	APD similarity (%)
DT	FlavStr	Tr	0.79	0.55	0.36	Failed	100.00	100.00
		Ts	0.23	1.27	0.77			
		CV	0.25	1.06	0.73			
	FabG	Tr	1.00	0.00	0.00	Failed	80.00	100.00
		Ts	-2.86	0.85	0.74			
		CV	0.38	0.62	0.53			
	FabZ	Tr	1.00	0.00	0.00	Passed	100.00	83.33
		Ts	0.79	0.31	0.20			
		CV	0.90	0.22	0.16			
	FabI	Tr	0.78	0.37	0.32	Passed	100.00	100.00
		Ts	0.63	0.36	0.32			
		CV	0.68	0.49	0.42			
RF	FlavStr	Tr	0.87	0.43	0.33	Failed	100.00	100.00
		Ts	0.53	0.99	0.70			
		CV	0.47	0.80	0.67			
	FabG	Tr	0.91	0.22	0.18	Failed	80.00	100.00

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Algorithm	Database	Dataset	R^2	RMSE	MAE	Acceptability criteria	APD leverage (%)	APD similarity (%)
		Ts	0.78	0.19	0.13			
		CV	0.48	0.57	0.44			
		Tr	0.97	0.11	0.10			
	FabZ	Ts	0.80	0.30	0.25	Passed	100.00	83.33
		CV	0.76	0.34	0.33			
		Tr	0.90	0.25	0.22			
	FabI	Ts	0.13	0.56	0.51	Failed	100.00	100.00
		CV	0.40	0.61	0.51			
SVM		Tr	0.65	0.72	0.55			
	FlavStr	Ts	0.64	0.86	0.65	Passed	100.00	100.00
		CV	0.54	0.83	0.62			
		Tr	0.99	0.07	0.06			
	FabG	Ts	0.93	0.11	0.09	Passed	80.00	100.00
		CV	0.97	0.12	0.09			
	FabZ	Tr	0.99	0.01	0.01	Passed	100.00	83.33
		Ts	0.97	0.11	0.09			

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Algorithm	Database	Dataset	R^2	RMSE	MAE	Acceptability criteria	APD leverage (%)	APD similarity (%)
MLP	FabI	CV	0.99	0.03	0.02	Passed	100.00	100.00
		Tr	0.99	0.07	0.05			
		Ts	0.93	0.15	0.12			
		CV	0.97	0.13	0.12			
	FlavStr	Tr	0.68	0.69	0.55	Passed	100.00	100.00
		Ts	0.59	0.92	0.69			
		CV	0.68	0.69	0.54			
	FabG	Tr	0.97	0.13	0.11	Passed	80.00	100.00
		Ts	0.95	0.09	0.08			
		CV	0.94	0.19	0.16			
	FabZ	Tr	0.99	0.03	0.02	Passed	100.00	83.3
		Ts	0.97	0.10	0.08			
		CV	0.99	0.03	0.02			
	FabI	Tr	0.98	0.10	0.07	Passed	100.00	100.00
		Ts	0.91	0.17	0.14			
		CV	0.93	0.19	0.18			

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Algorithm	Database	Dataset	R^2	RMSE	MAE	Acceptability criteria	APD leverage (%)	APD similarity (%)
PLS	FlavStr	Tr	0.70	0.67	0.53	Passed	100.00	100.00
		Ts	0.58	0.94	0.68			
		CV	0.70	0.67	0.53			
	FabG	Tr	0.99	0.07	0.05	Passed	80.00	100.00
		Ts	0.92	0.12	0.09			
		CV	0.99	0.07	0.05			
	FabZ	Tr	0.99	0.01	0.01	Passed	100.00	83.33
		Ts	0.97	0.11	0.09			
		CV	0.99	0.01	0.01			
	FabI	Tr	0.99	0.07	0.06	Passed	100.00	100.00
		Ts	0.94	0.14	0.11			
		CV	0.99	0.07	0.06			