APPENDIX

SPSS Output

Regression

Variables Entered/Removed[a]

Model	Variables Entered	Variables Removed	Method
1	Zscore(VAR00631)(RDF_PiChg_86)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
2	Zscore(VAR00493)(RDF_SigChg_76)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
3	Zscore(VAR00238)(3DACorr_TotChg_9)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
4	Zscore(VAR01111)(RDF_LpEN_54)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
5	Zscore(VAR00226)(3DACorr_PiChg_9)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
6	Zscore(VAR00474)(RDF_SigChg_57)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
7	Zscore(VAR00136)(2DACorr_PiChg_9)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).
8	Zscore(VAR00742)(RDF_TotChg_69)	.	Stepwise (Criteria: Probability-of-F-to-enter <= .050, Probability-of-F-to-remove >= .100).

a. Dependent Variable: pFAR

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.657[a]	.432	.405	.47939
2	.783[b]	.613	.574	.40532
3	.851[c]	.725	.681	.35076
4	.902[d]	.813	.772	.29673
5	.937[e]	.879	.843	.24600
6	.963[f]	.927	.900	.19688
7	.977[g]	.955	.934	.15914
8	.987[h]	.975	.961	.12336

a. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86)

b. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76)

c. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9)

d. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54)

e. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9)

f. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57)

g. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57), Zscore(VAR00136)(2DACorr_PiChg_9)

h. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57), Zscore(VAR00136)(2DACorr_PiChg_9), Zscore(VAR00742)(RDF_TotChg_69)

ANOVA[i]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	3.667	1	3.667	15.954	.001[a]
	Residual	4.826	21	.230		
	Total	8.493	22			
2	Regression	5.207	2	2.604	15.848	.000[b]
	Residual	3.286	20	.164		
	Total	8.493	22			
3	Regression	6.155	3	2.052	16.676	.000[c]
	Residual	2.338	19	.123		
	Total	8.493	22			
4	Regression	6.908	4	1.727	19.613	.000[d]
	Residual	1.585	18	.088		
	Total	8.493	22			
5	Regression	7.464	5	1.493	24.669	.000[e]
	Residual	1.029	17	.061		
	Total	8.493	22			
6	Regression	7.873	6	1.312	33.849	.000[f]
	Residual	.620	16	.039		
	Total	8.493	22			
7	Regression	8.113	7	1.159	45.766	.000[g]

	Residual	.380	15	.025		
	Total	8.493	22			
8	Regression	8.280	8	1.035	68.012	.000[h]
	Residual	.213	14	.015		
	Total	8.493	22			

a. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86)

b. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76)

c. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9)

d. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54)

e. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9)

f. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57)

g. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57), Zscore(VAR00136)(2DACorr_PiChg_9)

h. Predictors: (Constant), Zscore(VAR00631)(RDF_PiChg_86), Zscore(VAR00493)(RDF_SigChg_76), Zscore(VAR00238)(3DACorr_TotChg_9), Zscore(VAR01111)(RDF_LpEN_54), Zscore(VAR00226)(3DACorr_PiChg_9), Zscore(VAR00474)(RDF_SigChg_57), Zscore(VAR00136)(2DACorr_PiChg_9), Zscore(VAR00742)(RDF_TotChg_69)

i. Dependent Variable: pFAR

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients		
		B	Std. Error	Beta	t	Sig.
1	(Constant)	-.416	.100		-4.158	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.408	.102	-.657	-3.994	.001
2	(Constant)	-.416	.085		-4.918	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.488	.090	-.785	-5.406	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.276	.090	.445	3.062	.006
3	(Constant)	-.416	.073		-5.683	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.355	.092	-.571	-3.875	.001
	Zscore(VAR00493)(RDF_SigChg_76)	.337	.081	.542	4.156	.001
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.263	.095	-.423	-2.776	.012
4	(Constant)	-.416	.062		-6.718	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.457	.085	-.735	-5.377	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.401	.072	.646	5.569	.000
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.334	.084	-.537	-3.987	.001
	Zscore(VAR01111)(RDF_LpEN_54)	.234	.080	.377	2.924	.009
5	(Constant)	-.416	.051		-8.103	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.675	.101	-1.087	-6.702	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.364	.061	.586	5.967	.000
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.277	.072	-.446	-3.862	.001
	Zscore(VAR01111)(RDF_LpEN_54)	.250	.067	.402	3.752	.002
	Zscore(VAR00226)(3DACorr_PiChg_9)	-.253	.083	-.407	-3.032	.008
6	(Constant)	-.416	.041		-10.125	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.613	.083	-.987	-7.396	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.461	.057	.742	8.053	.000
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.283	.058	-.456	-4.924	.000
	Zscore(VAR01111)(RDF_LpEN_54)	.207	.055	.333	3.775	.002
	Zscore(VAR00226)(3DACorr_PiChg_9)	-.284	.067	-.458	-4.214	.001

	Zscore(VAR00474)(RDF_SigChg_57)	-.197	.061	-.318	-3.246	.005
7	(Constant)	-.416	.033		-12.526	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.815	.094	-1.311	-8.699	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.477	.047	.768	10.252	.000
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.318	.048	-.512	-6.646	.000
	Zscore(VAR01111)(RDF_LpEN_54)	.319	.057	.513	5.566	.000
	Zscore(VAR00226)(3DACorr_PiChg_9)	-.362	.060	-.583	-6.025	.000
	Zscore(VAR00474)(RDF_SigChg_57)	-.201	.049	-.323	-4.082	.001
	Zscore(VAR00136)(2DACorr_PiChg_9)	.176	.057	.283	3.081	.008
8	(Constant)	-.416	.026		-16.159	.000
	Zscore(VAR00631)(RDF_PiChg_86)	-.705	.080	-1.134	-8.832	.000
	Zscore(VAR00493)(RDF_SigChg_76)	.439	.038	.707	11.589	.000
	Zscore(VAR00238)(3DACorr_TotChg_9)	-.364	.040	-.586	-9.190	.000
	Zscore(VAR01111)(RDF_LpEN_54)	.351	.045	.565	7.724	.000
	Zscore(VAR00226)(3DACorr_PiChg_9)	-.322	.048	-.519	-6.699	.000
	Zscore(VAR00474)(RDF_SigChg_57)	-.237	.040	-.382	-5.981	.000
	Zscore(VAR00136)(2DACorr_PiChg_9)	.161	.045	.259	3.613	.003
	Zscore(VAR00742)(RDF_TotChg_69)	-.135	.041	-.217	-3.311	.005

a. Dependent Variable: pFAR

ลิขสิทธิ์มหาวิทยาลัยเชียงใหม่
Copyright© by Chiang Mai University
All rights reserved

CURRICULUM VITAE

Author's Name	Mr. Pathomwat Wongrattanakamon	
Date/Year of Birth	4 August 1980	
Place of Birth	Chiang Mai Province, Thailand	
Education	2016	Doctor of Philosophy, Pharmacy, Faculty of Pharmacy, Chiang Mai University
	2009	Master of Science, Pharmacology, Department of Pharmacology, Faculty of Science, Mahidol University
	2004	Bachelor of Pharmacy, Faculty of Pharmacy, Silpakorn University
Scholarship	2016	The Graduate School, Chiang Mai University

Publications

Wongrattanakamon, P., Lee, V. S., Nimmanpipug, P., & Jiranusornkul, S. (2016). Nucleotide-binding domain 1 modelling: A novel molecular docking approach for screening of P-glycoprotein inhibitory activity of bioflavonoids. *Chemical Data Collections*, 2, 10-16.

Wongrattanakamon, P., Lee, V. S., Nimmanpipug, P., & Jiranusornkul, S. (2016). 3D-QSAR modelling dataset of bioflavonoids for predicting the potential modulatory effect on P-glycoprotein activity. *Data Brief*, 9, 35-42.

Wongrattanakamon, P., Lee, V. S., Nimmanpipug, P., & Jiranusornkul, S. (2016). Nucleotide binding domain 1 pharmacophore modeling for visualization and analysis of P-glycoprotein–flavonoid molecular interactions. *Front Biol (Beijing)*, 11(5), 391-395.

ลิขสิทธิ์มหาวิทยาลัยเชียงใหม่
Copyright© by Chiang Mai University
All rights reserved

Wongrattanakamon, P., Lee, V. S., Nimmanpipug, P., Chansakaow, S., & Jiranusornkul, S. (2017). Insight into the molecular mechanism of P-glycoprotein mediated drug toxicity induced by bioflavonoids: an integrated computational approach. *Toxicol Mech Methods*, (in press).

Oral presentation

Prediction of modulatory effects of flavonoids on P-glycoprotein by multiple linear regression analysis. The 3rd International Conference on Computation for Science and Technology 2014 (ICCST-3), Bali, Indonesia, 23-25 September 2014

Conferences

Wongrattanakamon, P., Yamanont, P., Poopairachapong, N., Sanvarinda, Y., Sibmooh, N., Kuptniratsaikul, V., Unchern, S. (2009). Effect of *Derris scandens* Extract on Oxidative Stress Status and Platelet Function of the Knee Osteoarthritis Patients. The 3rd UBU Research Conference 28-29 July 2009 Ubon Ratchathani University, 320-326.

ลิขสิทธิ์มหาวิทยาลัยเชียงใหม่
Copyright© by Chiang Mai University
All rights reserved