

Article

Bivariate Correlation Analysis of the Chemometric Profiles of Chinese Wild *Salvia miltiorrhiza* Based on UPLC-Qqq-MS and Antioxidant Activities

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Table S1. Chemical profiles of 50 wild *Salvia miltiorrhiza* varieties

Sample code	Investigated compounds																		
	Twelve phenolic acids (mg/g, DW)													Five tanshinones (mg/g, DW)					
	1	2	3	4	5	6	7	8	9	10	11	12	Total	13	14	15	16	17	Total
S1	1.79	0.017	0.047	0.064	0.003	0.009	5.43	3.31	39.04	0.28	0.029	0.093	50.12	1.40	1.20	2.85	2.02	0.64	8.11
S2	1.07	0.013	0.016	0.150	0.003	0.004	7.63	3.55	40.49	0.12	0.028	0.062	53.13	0.53	0.30	0.75	0.28	0.13	1.99
S3	1.19	0.009	0.014	0.071	0.002	0.001	5.41	2.08	39.05	0.14	0.035	0.047	48.05	1.28	0.97	1.12	0.77	0.10	4.23
S4	1.65	0.020	0.038	0.077	0.003	0.019	5.78	3.62	42.36	0.30	0.041	0.131	54.04	1.77	1.73	3.15	2.16	0.80	9.62
S5	0.49	0.011	0.027	0.039	0.002	0.014	2.02	1.50	25.13	0.17	0.032	0.012	29.45	3.52	2.04	4.91	3.79	0.46	14.73
S6	0.66	0.004	0.004	0.046	0.001	0.004	5.50	3.06	38.51	0.13	0.029	0.031	47.98	1.77	2.13	2.34	2.58	0.01	8.83
S7	0.64	0.002	0.002	0.066	0.001	0.002	5.13	3.79	36.11	0.10	0.032	0.048	45.94	0.82	0.39	0.64	0.30	0.09	2.23
S8	0.50	0.003	0.012	0.114	0.001	0.013	8.66	2.11	45.76	0.09	0.028	0.000	57.30	0.32	0.26	0.65	0.21	0.08	1.54
S9	0.74	0.007	0.009	0.110	0.003	0.003	7.06	3.26	39.16	0.11	0.028	0.049	50.53	0.17	0.18	0.12	0.13	0.01	0.61
S10	1.05	0.004	0.004	0.055	0.002	0.001	8.20	4.15	40.93	0.13	0.027	0.094	54.64	0.16	0.14	0.21	0.12	0.03	0.65
S11	0.41	0.015	0.024	0.034	0.002	0.004	1.19	1.10	22.57	0.08	0.036	0.008	25.48	4.13	1.30	2.56	1.65	0.17	9.81
S12	1.18	0.009	0.019	0.031	0.001	0.005	6.62	3.00	44.66	0.12	0.027	0.014	55.69	1.48	0.84	2.40	1.37	0.77	6.86
S13	0.82	0.015	0.024	0.043	0.003	0.006	5.48	3.18	42.25	0.20	0.029	0.023	52.08	7.49	1.45	9.82	8.70	0.95	28.40
S14	0.65	0.002	0.003	0.039	0.002	0.005	5.99	3.01	37.85	0.12	0.028	0.030	47.72	0.10	0.14	0.06	0.10	0.01	0.41

S15	0.59	0.006	0.021	0.089	0.002	0.011	11.12	2.88	44.79	0.10	0.028	0.006	59.64	0.24	0.35	0.17	0.13	0.02	0.91
S16	1.63	0.019	0.029	0.059	0.002	0.004	5.79	4.26	43.41	0.20	0.029	0.082	55.52	1.30	0.42	2.03	1.06	0.41	5.21
S17	1.00	0.013	0.028	0.041	0.002	0.010	5.03	2.84	40.69	0.17	0.028	0.029	49.88	2.96	0.80	4.69	2.27	0.09	10.81
S18	0.69	0.004	0.003	0.029	0.001	0.015	6.74	3.01	39.08	0.15	0.032	0.028	49.77	0.22	0.30	0.14	0.26	0.01	0.94
S19	2.36	0.022	0.028	0.069	0.002	0.014	4.57	3.62	43.30	0.42	0.037	0.054	54.50	1.64	0.83	2.60	1.79	0.32	7.18
S20	0.68	0.009	0.019	0.032	0.002	0.002	3.39	1.91	33.37	0.20	0.028	0.022	39.67	1.14	0.62	1.58	0.98	0.45	4.77
S21	0.74	0.005	0.016	0.036	0.001	0.004	7.03	2.75	38.98	0.13	0.027	0.008	49.73	2.47	0.37	5.77	1.35	0.94	10.90
S22	1.30	0.007	0.009	0.031	0.003	0.004	5.57	3.29	45.09	0.18	0.027	0.011	55.52	0.51	0.36	1.14	0.45	0.30	2.77
S23	0.84	0.003	0.004	0.032	0.002	0.004	6.62	3.17	39.26	0.12	0.026	0.006	50.09	1.56	1.30	3.38	1.77	0.45	8.47
S24	2.15	0.035	0.030	0.061	0.003	0.008	2.74	4.04	36.41	0.40	0.031	0.201	46.11	1.09	0.62	2.07	0.94	0.19	4.91
S25	0.71	0.007	0.046	0.065	0.001	0.005	7.84	1.92	36.85	0.09	0.030	0.001	47.56	1.05	0.90	0.93	1.14	0.09	4.10
S26	0.56	0.005	0.019	0.047	0.003	0.003	5.94	2.14	38.61	0.09	0.034	0.004	47.45	0.47	0.49	0.47	0.46	0.04	1.93
S27	0.75	0.004	0.018	0.091	0.001	0.002	7.42	3.00	43.94	0.09	0.045	0.012	55.37	0.21	0.26	0.22	0.18	0.02	0.89
S28	0.82	0.005	0.011	0.039	0.001	0.002	6.87	2.70	43.39	0.11	0.027	0.007	53.98	0.38	0.35	0.65	0.27	0.13	1.78
S29	0.75	0.006	0.024	0.099	0.002	0.003	9.00	2.05	39.47	0.07	0.028	0.001	51.51	0.14	0.25	0.17	0.12	0.02	0.69
S30	0.56	0.003	0.009	0.057	0.001	0.003	5.21	1.94	39.55	0.10	0.028	0.001	47.46	1.73	1.54	2.76	2.11	0.99	9.14
S31	0.51	0.003	0.010	0.113	0.002	0.008	4.21	2.00	35.02	0.10	0.030	0.001	42.01	0.88	0.45	1.86	0.57	0.53	4.29
S32	1.10	0.005	0.009	0.041	0.002	0.005	5.60	3.65	41.19	0.18	0.028	0.033	51.84	4.68	0.62	6.24	2.34	0.10	13.99

S33	0.98	0.006	0.014	0.069	0.002	0.005	7.43	3.92	46.63	0.14	0.030	0.022	59.25	1.36	0.64	2.38	1.00	0.43	5.80
S34	0.41	0.002	0.001	0.027	0.001	0.006	6.43	2.43	37.66	0.14	0.034	0.012	47.14	1.56	1.14	2.47	1.13	0.93	7.22
S35	0.58	0.004	0.006	0.030	0.001	0.010	6.82	2.43	39.56	0.12	0.030	0.009	49.60	0.13	0.23	0.11	0.20	0.02	0.69
S36	0.92	0.008	0.010	0.049	0.002	0.003	7.47	3.11	40.26	0.12	0.031	0.034	52.03	0.45	0.48	0.38	0.45	0.06	1.83
S37	0.91	0.025	0.018	0.069	0.002	0.005	6.05	3.14	38.00	0.20	0.028	0.073	48.51	0.37	0.37	0.47	0.26	0.10	1.57
S38	0.53	0.008	0.030	0.021	0.001	0.013	0.70	1.02	21.12	0.15	0.028	0.009	23.64	1.24	0.71	2.57	0.96	0.59	6.07
S39	1.17	0.022	0.034	0.061	0.003	0.007	4.95	2.87	39.93	0.16	0.033	0.029	49.26	3.12	1.98	5.40	3.73	0.80	15.04
S40	0.89	0.004	0.008	0.036	0.002	0.005	5.07	2.73	39.74	0.15	0.029	0.007	48.67	2.37	0.57	4.20	1.51	0.87	9.52
S41	0.81	0.012	0.028	0.071	0.003	0.015	5.38	1.28	34.16	0.08	0.028	0.000	41.87	1.59	0.53	2.33	0.94	0.20	5.59
S42	1.00	0.016	0.037	0.037	0.002	0.011	4.59	2.68	41.40	0.17	0.028	0.028	50.00	1.96	0.89	4.34	1.99	0.48	9.65
S43	1.15	0.011	0.008	0.029	0.002	0.007	3.59	2.87	40.66	0.34	0.029	0.016	48.71	2.04	1.74	4.38	2.58	0.10	10.84
S44	0.53	0.008	0.020	0.165	0.002	0.005	7.06	2.38	38.17	0.09	0.030	0.015	48.48	0.11	0.23	0.05	0.10	0.02	0.50
S45	0.39	0.003	0.005	0.041	0.001	0.002	6.59	1.49	38.42	0.10	0.030	0.000	47.07	0.04	0.13	0.04	0.10	0.01	0.32
S46	0.62	0.002	0.001	0.032	0.001	0.003	5.33	2.93	41.66	0.16	0.028	0.030	50.81	0.20	0.39	0.04	0.10	0.04	0.77
S47	0.54	0.006	0.011	0.037	0.002	0.005	3.66	2.57	35.76	0.12	0.031	0.017	42.76	0.65	0.50	1.19	0.53	0.24	3.11
S48	0.55	0.005	0.009	0.039	0.005	0.007	3.86	2.68	35.76	0.19	0.035	0.029	43.17	1.91	1.30	2.69	1.81	0.27	7.97
S49	1.06	0.022	0.025	0.030	0.004	0.005	1.56	2.75	31.18	0.27	0.040	0.084	37.03	4.42	2.03	6.00	4.03	0.31	16.78
S50	0.37	0.005	0.017	0.025	0.002	0.007	3.06	1.69	31.22	0.10	0.032	0.000	36.53	2.26	0.69	4.06	1.88	0.19	9.08

CV(%)	49.1 0	78.99	68.18	55.76	41.48	65.05	36.12	28.64	13.63	49.74	12.96	122.35	15.62	99.04	73.88	94.5 0	112. 80	102.79	90.22
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1. Danshensu; 2. Protocatechuic acid; 3. Protocatechualdehyde; 4. Caffeic acid; 5. Ferulic acid; 6. Isferulic acid; 7. Rosmarinic acid; 8. Lithospermic acid; 9. Salvianolic acid B; 10. Salvianolic acid A; 11. Cinnamic acid; 12. Salvianolic acid C; 13. Dihydrotanshinone I; 14. Tanshinone I; 15. Cryptotanshinone; 16. Tanshinone IIA ; 17. Miltirone.

Table S2. Results of antioxidant capability in different places of *S. miltiorrhiza*

Sample code	Regression eq		R ²		IC ₅₀ (µg/mL)	
	DPPH	ABTS	DPPH	ABTS	DPPH	ABTS
S1	y = 1.739x + 1.0138	y = 2.566x + 0.8915	0.9997	0.9993	28.1692	19.1382
S2	y = 1.819x + 1.5661	y = 2.136x + 12.731	0.9994	0.9927	26.6267	17.4480
S3	y = 1.588x + 2.5685	y = 2.172x + 4.1808	0.9953	0.9955	29.8687	21.0954
S4	y = 1.889x + 4.1088	y = 2.715x - 4.2156	0.9913	0.991	24.2939	19.9689
S5	y = 0.808x + 1.0621	y = 1.248x + 1.5313	0.9991	0.9975	60.5667	38.8371
S6	y = 1.571x + 2.253	y = 2.124x + 0.8815	0.999	0.9967	30.3927	23.1255
S7	y = 1.289x + 1.4497	y = 1.587x - 1.4348	0.9965	0.9973	37.6651	32.4101
S8	y = 2.858x + 2.7148	y = 3.910x + 0.2379	0.9946	0.9995	16.5449	12.7269
S9	y = 1.580x + 0.1297	y = 2.269x + 3.2957	0.9973	0.9962	31.5635	20.5836
S10	y = 1.908x - 0.0794	y = 2.228x + 8.2593	0.9938	0.9965	26.2471	18.7346
S11	y = 0.565x + 1.8479	y = 0.832x + 2.5904	0.9965	0.9961	85.2250	56.9827
S12	y = 2.073x + 3.0204	y = 2.578x + 2.3079	0.9986	0.9932	22.6626	18.4997
S13	y = 1.894x + 1.288	y = 2.484x + 3.3326	0.9975	0.9976	25.7191	18.7872
S14	y = 1.557x + 1.621	y = 1.933x - 0.8819	0.9943	0.997	31.0719	26.3228
S15	y = 2.454x + 3.0832	y = 3.889x - 2.0765	0.9979	0.9975	19.1185	13.3907
S16	y = 2.642x - 2.182	y = 3.135x + 1.8245	0.9956	0.9957	19.7509	15.3670
S17	y = 1.914x + 0.4717	y = 2.689x + 2.1914	0.9976	0.9968	25.8769	17.7793
S18	y = 1.394x - 0.5783	y = 2.143x - 1.094	0.9997	0.9976	36.2829	23.8423
S19	y = 1.878x + 1.2885	y = 3.037x - 7.7037	0.999	0.9988	25.9380	19.0002
S20	y = 1.518x + 1.4355	y = 2.942x + 2.3213	0.9982	0.9966	31.9924	23.3490
S21	y = 1.586x + 2.6846	y = 1.994x + 3.2512	0.9987	0.9964	29.8332	23.4447
S22	y = 2.368x + 0.5635	y = 2.839x + 0.9522	0.9978	0.9965	20.8769	17.2764
S23	y = 1.839x - 1.8809	y = 2.400x - 1.7102	0.9962	0.9978	28.2115	21.5459
S24	y = 1.634x - 1.8429	y = 2.048x + 3.3345	0.9959	0.9975	31.7276	22.7859
S25	y = 2.277x + 1.3545	y = 2.972x + 0.7943	0.9985	0.9989	21.3639	16.5564
S26	y = 1.506x + 1.3545	y = 2.031x + 0.0105	0.9943	0.9956	33.8957	24.6132

S27	$y = 2.163x + 0.4673$	$y = 2.064x + 7.8243$	0.9997	0.9934	22.9000	16.1965
S28	$y = 1.896x + 3.4849$	$y = 2.954x + 0.3666$	0.9952	0.999	24.5333	16.8021
S29	$y = 1.900x + 2.8888$	$y = 2.554x + 3.1689$	0.9955	0.9985	24.7954	18.3364
S30	$y = 1.489x + 1.6804$	$y = 1.831x + 2.4852$	0.9977	0.997	32.4510	25.9502
S31	$y = 1.575x + 2.7806$	$y = 2.012x + 3.6016$	0.9998	0.9962	29.9806	23.0608
S32	$y = 1.891x + 3.8279$	$y = 2.344x + 5.1419$	0.9929	0.9908	24.4168	19.1374
S33	$y = 2.624x + 3.0601$	$y = 3.236x + 2.916$	0.9991	0.9997	17.8887	14.5501
S34	$y = 1.554x + 1.6607$	$y = 2.235x + 0.802$	0.9992	0.9996	31.1064	22.0125
S35	$y = 1.484x + 2.4322$	$y = 1.931x + 2.8026$	0.9953	0.9937	32.0538	24.4419
S36	$y = 2.042x + 0.9879$	$y = 2.584x + 3.7799$	0.9985	0.991	24.0020	17.8870
S37	$y = 1.807x + 0.303$	$y = 2.548x + 4.7965$	0.9992	0.994	27.5025	17.7408
S38	$y = 0.689x + 2.7603$	$y = 0.983x + 2.3965$	0.9969	0.9943	68.5627	48.4268
S39	$y = 1.569x + 4.6095$	$y = 2.517x + 1.1579$	0.9969	0.9999	28.9296	19.4049
S40	$y = 1.571x - 0.9355$	$y = 1.893x + 2.9754$	0.9922	0.9952	32.4223	24.8413
S41	$y = 1.581x - 1.8948$	$y = 1.992x + 0.7091$	0.9979	0.9991	32.8240	24.7444
S42	$y = 1.930x + 0.4095$	$y = 2.532x - 2.3259$	0.998	0.9951	25.6946	20.6658
S43	$y = 1.459x + 1.6408$	$y = 2.247x - 1.0428$	0.9975	0.9959	33.1454	22.7160
S44	$y = 1.500x + 1.932$	$y = 1.912x + 3.0423$	0.993	0.9957	32.0453	24.5595
S45	$y = 1.366x + 2.1022$	$y = 2.009x - 0.7853$	0.9953	0.9984	35.0643	25.2789
S46	$y = 1.843x + 2.3915$	$y = 2.512x + 2.5477$	0.9978	0.997	25.8321	18.8902
S47	$y = 1.164x + 2.2764$	$y = 1.590x + 4.2234$	0.9981	0.9922	40.9997	28.7903
S48	$y = 1.083x + 1.0093$	$y = 1.363x + 2.3316$	0.9998	0.9936	45.2361	34.9731
S49	$y = 0.931x + 2.5459$	$y = 1.595x + 0.2166$	0.9946	0.9988	50.9711	31.2122
S50	$y = 0.754x - 0.5189$	$y = 1.121x - 0.9335$	0.998	0.9953	67.0012	45.4358
Trolox	$y = 10.625x - 0.7075$	$y = 16.129x - 1.1556$	0.9974	0.9991	4.7725	3.1717
mean					32.2369	23.3933

Table S3. *S. miltiorrhiza* populations included in this study, their collection sites, habitat and geographical coordinates.

Sample code	Place of origin or Geographic region	Latitude(°N)	Longitude(°E)	Altitude (m)	Habitat
S1	Hanzhong, Shaanxi	33.75598	106.33001	517	Pine forest
S2	Guilin, Guangxi	25.285235	110.275236	154	Roadside
S3	Guilin, Guangxi	25.285825	110.276488	158	Park
S4	Shangluo, Shaanxi	33.271065	110.354161	462	Hillside
S5	Lingbao, Henan	34.195045	110.430931	703	Roadside
S6	Shiyan, Hubei	32.016233	110.566046	715	Field
S7	Shiyan, Hubei	32.016797	110.566581	689	Hillside
S8	Shiyan, Hubei	32.03189	110.568964	544	Mountain roads
S9	Zhangjiajie, Hunan	29.240994	110.724758	159	Hillside
S10	Zhangjiajie, Hunan	29.240094	110.724758	149	Hillside
S11	Nanyang, Henan	33.274778	111.533463	608	Grass
S12	Yuncheng, Shanxi	35.279606	111.884369	537	Hillside
S13	Changzhi, Shanxi	36.64011	112.318259	1217	Valley
S14	Hengyang, Hunan	27.281111	112.729685	390	Hill
S15	Hengyang, Hunan	27.281857	112.730637	353	Hill
S16	Jiaozuo, Henan	35.337025	113.252312	382	Grass
S17	Yangquan, Shanxi	38.205892	113.59612	1169	Field

S18	Tongcheng, Hubei	29.316633	113.670079	132	Behind a house
S19	Anyang, Henan	36.162731	113.718918	668	Roadside
S20	Anyang, Henan	36.163708	113.719491	670	Roadside
S21	Xingtai, Hebei	37.156893	113.94061	533	Chestnut forest
S22	Xingtai, Hebei	37.157747	113.943564	553	Woods
S23	Xingtai, Hebei	37.159808	113.943781	496	Side of a village
S24	Xinyang, Henan	31.502254	114.01514	238	Roadside
S25	Ji'an, Jiangxi	26.312302	114.114013	418	Woods
S26	Ji'an, Jiangxi	26.311784	114.114088	407	Grass
S27	Ji'an, Jiangxi	26.31209	114.11409	415	Grass
S28	Ji'an, Jiangxi	26.312522	114.114259	429	Brookside
S29	Ganzhou, Jiangxi	25.382957	114.180527	816	Bamboo forest
S30	Wuhan, Hubei	30.553826	114.414365	20	Park
S31	Baoding, Hebei	39.271298	115.305802	143	Hill
S32	Baoding, Hebei	39.269757	115.307681	152	Roadside
S33	Baoding, Hebei	39.268056	115.308162	148	Roadside
S34	Huanggang, Hubei	30.78971	115.367631	94	Hill
S35	Jiujiang, Jiangxi	29.538842	116.031751	354	Woods
S36	Jiujiang, Jiangxi	29.538866	116.031758	362	Temple nearby
S37	Nanfeng, Jiangxi	27.035884	116.230774	165	Valley
S38	Jinan, Shandong	36.32271	117.152962	452	Grass
S39	Linyi, Shandong	35.145267	117.331005	352	Hill
S40	Tangshan, Hebei	40.207318	117.665181	142	Pine forest
S41	Laiwu, Shandong	36.353555	117.813792	353	Hill

S42	Laiwu, Shandong	36.353827	117.813812	317	Field
S43	Laiwu, Shandong	36.351476	117.818788	387	Woods
S44	Xuancheng, Anhui	30.602898	118.696055	278	Roadside
S45	Hangzhou, Zhejiang	29.791199	118.97704	480	Hillside
S46	Linan, Zhejiang	29.361699	119.022079	350	Roadside
S47	Qinhuangdao, Hebei	39.817158	119.450445	90	Roadside
S48	Qinhuangdao, Hebei	39.819352	119.451303	65	Bushes
S49	Qingdao, Shandong	36.160122	120.302143	187	Pine trees
S50	Dalian, Liaoning	38.922769	121.502179	75	Highway side

Table S4. Intercorrelations between effective compounds of *S. miltiorrhiza*.

	Tanshinone I	Dihydrotanshinone I	Miltirone	Tanshinone IIA	Cryptotanshinone	Total tanshinones	Protocatechualdehyde	Cinnamic acid	Protocatechuic acid	Caffeic acid	Ferulic acid	Isferulic acid	Danshensu	Rosmarinic acid	Salvianolic acid C	Salvianolic acid A	Lithospermic acid	Salvianolic acid B	Total phenolics
Tanshinone I	1																		
Dihydrotanshinone I	0.635**	1																	
Miltirone	0.449**	0.449**	1																
Tanshinone IIA	0.732**	0.913**	0.530**	1															
Cryptotanshinone	0.634**	0.938**	0.620**	0.897**	1														
Total tanshinones	0.738**	0.965**	0.614**	0.962**	0.974**	1													
Protocatechualdehyde	0.286	0.297	0.134	0.314*	0.226	0.303	1												
Cinnamic acid	0.308	0.139	0.064	0.138	0.062	0.134	0.317*	1											
Protocatechuic acid	0.343*	0.326*	0.119	0.354*	0.315*	0.345*	0.652**	0.284	1										
Caffeic acid	-0.327*	-0.370*	-0.201	-0.310*	-0.378*	-0.372*	0.239	0.042	0.027	1									
Ferulic acid	0.256	0.249	0.043	0.252	0.219	0.247	0.305	0.255	0.412**	0.006	1								
Isferulic acid	0.243	0.142	0.128	0.179	0.185	0.189	0.428**	0.206	0.343**	0.134	0.162	1							
Danshensu	0.124	0.092	0.091	0.139	0.181	0.149	0.375*	0.203	0.700**	-0.011	0.199	0.316*	1						

Rosmarinic acid	-0.537**	-0.520**	-0.216	-0.432**	-0.465**	-0.501**	-0.139	-0.29	-0.438**	0.438**	-0.296	-0.087	-0.152	1					
Salvianolic acid C	0.107	0.013	-0.03	0.048	0.026	0.036	0.235	0.259	0.691**	0.020	0.245	0.189	0.691**	-0.232	1				
Salvianolic acid A	0.360*	0.261	0.16	0.334*	0.343*	0.337*	0.256	0.262	0.719**	-0.211	0.251	0.348*	0.832**	-0.445**	0.677**	1			
Lithospermic acid	-0.088	-0.053	-0.033	0.012	0.031	-0.01	-0.178	0.034	0.213	0.006	0.045	0.045	0.619**	0.22	0.615**	0.473**	1		
Salvianolic acid B	-0.331*	-0.309*	-0.016	-0.167	-0.168	-0.227	-0.181	-0.172	-0.177	0.235	-0.194	-0.01	0.316*	0.700**	0.008	0.082	0.580**	1	
Total phenolics	-0.383*	-0.363*	-0.07	-0.227	-0.233	-0.291	-0.155	-0.181	-0.17	0.292	-0.199	-0.01	0.318*	0.786**	0.062	0.046	0.622**	0.983**	1

* shows significance at the level as $p=0.05$; ** shows significance at the level as $p=0.01$