http://www.scirp.org/journal/ns Natural Science, 2017, Vol. 9, (No. 12), pp: 412-420

The Monte Carlo Simulation and Non-Parametric Tests Application on Chemical Data

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Keywords: Kruskal-Wall, Monte Carlo Calculations
Received: November 1, 2017 **Accepted:** December 26, 2017 **Published:** December 29, 2017

ABSTRACT

This work addressed the application of Monte-Carlo (MC) simulation on obtained chemical data previous published in one of authors' paper. The chemical data were subjected into MC simulation. Also, Kruskal-Wall test was performed to enhance our hypothesis of difference among the reported data. Moreover, Nonparametric Runs Test was calculated to get bigger vision of the hypothesis. The chemical data tested in this study showed significant difference when using MC simulation.

1. INTRODUCTION

Monte Carlo simulation (MC) was named after the gambling city of Monte Carlo in Monaco. During the simulation steps to generating variables and random distribution, this is so-called MC. MC is very powerful tools in radiation physics owing to it has great chance to resolve very complex physical models [1].

The difference between MC and real experiment is that MC carries out random sampling and performs a large number of computed experiments. The statistical measurements of the computed model are observed and then concluded. Every computed run is generated with accordance to its distribution [2].

The steps of MC are summarized in **Figure 1**. In first step, MC generates random variables which are distributed between 0 to 1. The significance of this distribution is that they can be formed into actual values which shape distribution of the purpose. The second step is to estimate the performance. The last step

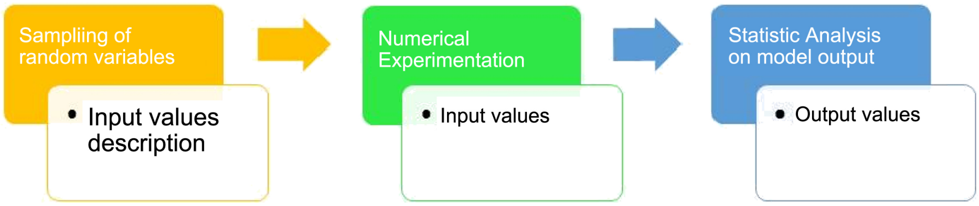

Figure 1. Flowchart of MC file.

is carried out to characterize the output values.

Statistical evaluation is vital method in which to determine the validity of measurements. It also provides meaning of reported numbers and grants scientists senses to draw discussion and conclusion from their obtained numbers and variables. Luckily, most of articles dealing with applied sciences pay more attention to statistical methods to enhance statistical validity as proven evidence of their theory. Nowadays, advanced statistical software opens the appetite for more movement towards statistical techniques. Nevertheless, inappropriate understanding of these statistical packages can lead to misinterpretation of the reported data [5].

Statistical methods developed to carry out statistical analysis can be broken into two categorizes: the first is so-called parametric method and the second one is non-parametric. The parametric methods are based on one assumption which is normal (homogeneous and independent) distribution of the reported data. However, most of scientific data are violated this assumption [3].

Mood's test is rarely used in literature for chemical data but is mostly clinical studies. Many non-parametric tests depend on Mood's test [4]. The median test is very important quantification of studying distribution owing to normal skewness. For instance, if variables are shared in their median then their medians can be comparable.

Using Mood's Median Test, the obtained results listed in **Table 1** except Fe and Mn were not included in the Mood's test, one can end-up with precise conclusion. Thus, the chemical data calculations were performed to answer whether MC is applicable with other non-parametric tests e.g. Kruskal-Wallis. The MC results are discussed with more emphasized on matching between these performed tests.

2. RESULTS

In **Table 2**, the mood's test of the chemical data are listed. Almost half of the test was above the median and the other half was less than the median. All the median values of elements were located within upper and lower confidence intervals. For instance, for chromium the upper median was 28.11 ppm whereas the lower median was 18.4 ppm. The median for chromium was 22.11 ppm. Another example, for major element, e.g. iron, not reported here, the median was away from the upper and lower confidence intervals, thus, it was decided to removed from the list because only trace levels were part of this investigation.

In Kruskal-Wallis Test each group of elements was treated as independent unit. It should be noted that the Kruskal-Wallis test merely informs us that the groups differ in some way. In this case, the degree of freedom was above 5, thus we cannot use critical values of Kruskal-Wallis table. It was at 0.05 significance level. We can only use Chi tables. We are going to inspect each group medians to decide precisely how they differ rather giving two examples and later visualizing them in one figure. In **Table 3**, it showed the performance of Kruskal-Wallis Test for the study materials. The lowest score given by Kruskal-Wallis Test was for cadmium with z-values of −3.5 while the highest score was given to vanadium with z-value of 4.8. Thus, the data obviously have big different and the population medians of the chemical data were not all equal. The observations of median values of the study materials can easily recognize the median of easy element located between the lower and upper intervals. For example, let's take zinc element, the lower limit of median was 19 ppm whereas the upper limit of median was 23.7 ppm. Fortunately, all the both-side tailings were near to zero which indicated the distributions were con dent. The test statistic for the Kruskal Wallis test is denoted H_0. The calculated H_0 (as Chi-Square) was 162 and medians for all reported elements were more than H_0 indicating the original data can be tested as non-parametric. So, we can conclude that there is a difference of original data

The Nonparametric Runs Test was performed for the chemical data as listed in **Table 4** as supportive for MC results. The run test can be helpful in testing the null hypothesis of the equality of the distributions. Now, let's look at one method in which the distribution functions could be unequal. One possibility is that one of the distribution functions is at least as great as the other distribution function at all data. Nonparametric Runs can do the same job as Kruskal-Wallis Test. Therefore, the test was carried out to

Table 1. **Elemental analysis and statistical evaluation for chemical data of the study materials.**

Sample code	Cr 52	Mn 55	Fe 57	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Ba 138	Pb 208	Bi 209	U 238
A10117	3.24	30.58	2866	9.60	5.35	4.10	12.97	0.23	1.11	27.46	0.12	1.76	3.47	1.50	0.02	0.21
A01120	29.95	65.36	2967	0.31	1.29	3.81	14.69	7.81	1.34	4.25	0.24	0.14	57.40	6.23	0.05	1.40
A01122	11.38	367.12	10122	9.96	6.70	1.86	3.29	1.05	2.90	198.19	0.91	0.16	15.38	1.01	0.01	0.51
A01123	0.67	7.10	2996	7.47	3.28	3.23	2.19	0.15	1.02	46.74	0.05	0.18	1.96	0.28	0.00	0.05
A01124	0.50	2.40	117	0.08	0.15	0.29	0.09	0.03	0.00	0.11	0.00	0.00	0.07	0.00	0.00	0.00
A01125	46.81	13.88	1129	1.32	4.63	6.25	88.63	8.70	1.59	11.36	0.27	0.20	90.86	5.87	1.36	0.37
A01126	3.96	58.16	4227	9.78	7.09	6.11	3.41	0.61	1.71	101.84	0.05	0.17	4.48	0.60	0.03	0.13
A01127	22.24	134.42	5233	0.28	1.35	9.96	33.61	11.13	2.21	5.70	0.23	0.10	73.28	3.33	0.03	0.74
A01135	1.31	10.21	3089	8.84	3.22	6.56	2.07	0.19	1.17	39.74	0.10	0.12	1.35	0.24	0.41	0.07
A01137	0.87	6.17	3190	9.64	3.79	19.27	2.28	0.13	1.31	34.78	0.03	0.12	0.99	0.24	0.01	0.12
A01041	7.28	6.16	2032	6.23	3.73	1.61	3.78	0.43	0.91	48.01	0.30	0.09	4.09	0.39	0.01	1.00
B01036	0.99	30.88	3264	9.06	3.20	2.08	1.96	0.36	1.46	43.28	0.12	0.09	3.64	0.41	0.00	0.05
B01037	14.39	136.95	9245	12.03	43.16	4.05	8.47	9.91	1.10	223.84	0.12	0.06	72.63	0.45	0.00	0.02
B01039	1.65	183.57	6913	8.07	4.31	5.23	23.86	0.30	1.24	147.87	0.21	0.13	2.31	2.24	0.01	0.21
B01045	2.42	27.45	2449	5.45	5.57	1.69	1.98	0.23	1.35	51.24	0.16	0.10	1.50	0.35	0.09	0.21
B01046-KSU-7	1.18	9.36	3350	9.67	3.70	1.00	1.41	0.22	1.32	144.58	0.16	0.09	1.74	0.25	0.01	0.17
B01046-KSU-8	6.05	1307.76	9321	10.10	8.31	3.11	5.67	1.54	4.91	70.76	0.36	0.33	12.36	2.64	2.49	0.16
B01049	34.26	79.78	2821	0.76	1.53	4.20	12.24	16.48	1.09	77.50	0.22	0.10	290.64	6.53	1.66	0.71
B01051	45.65	181.86	13275	5.13	16.97	14.43	16.65	11.82	1.19	34.56	0.20	0.13	136.50	7.59	1.80	1.68
B01052	65.99	340.95	13800	6.86	18.51	11.92	21.23	10.81	1.16	60.96	0.08	0.11	135.95	3.76	0.06	0.48
B01053	1.45	19.05	2051	6.07	2.71	4.09	1.97	0.33	1.57	54.88	0.57	0.09	2.82	0.49	0.01	1.01
B01055	0.76	39.42	2697	8.10	2.81	1.19	2.18	0.42	1.12	41.10	0.24	0.08	3.08	0.54	0.01	0.07
C0530	1.87	30.55	2721	8.12	4.39	1.84	3.60	0.56	1.10	28.13	0.29	0.12	3.67	0.55	3.59	0.08
C0532-KSU-4	2.35	22.20	2027	6.97	4.00	9.55	2.79	0.37	1.18	36.31	0.14	0.14	2.83	1.47	1.56	0.22
C0532-KSU-6	2.49	996.92	4070	7.53	3.29	1.14	2.04	1.03	1.96	37.85	0.22	0.18	29.84	0.28	0.89	0.09
C0537	1.91	28.93	1758	6.30	2.60	2.86	1.60	0.13	1.26	132.00	0.18	0.10	1.64	0.35	0.43	0.07
C0539	9.88	113.98	1988	0.26	0.62	1.10	6.06	6.82	0.71	27.82	0.07	0.04	176.43	3.20	0.29	0.71
C0541	1.01	3.52	1024	5.72	1.52	1.11	1.33	0.14	1.09	26.03	0.01	0.08	0.95	1.04	0.01	0.14
C0542-KSU-1	32.87	344.94	13295	6.66	12.45	11.70	13.69	6.82	1.45	9.54	0.55	0.08	85.19	4.45	0.03	0.62
C0542-KSU-2	40.54	296.89	3664	1.38	2.47	3.86	8.50	4.94	0.94	20.66	0.18	0.22	101.77	4.77	0.06	0.42
C0544	39.43	220.73	3542	1.49	2.76	10.59	11.31	4.49	1.49	15.98	0.12	0.18	85.18	3.51	0.05	0.44
C0546	0.52	4.95	1111	6.08	1.58	0.89	1.05	0.11	0.66	12.90	0.03	0.05	0.84	0.09	0.01	0.04
C0550	4.11	3.15	1069	3.14	1.56	1.00	1.04	0.26	1.07	39.36	0.01	0.06	4.50	0.41	0.01	0.16
C0551	1.93	9.00	1211	6.62	2.50	1.85	1.79	0.22	0.73	30.87	0.17	0.08	1.75	0.31	1.08	0.38
C0553	0.88	15.34	940.60	5.51	1.92	0.83	0.93	0.32	0.63	49.78	0.03	0.08	4.98	0.09	0.08	0.24
Count	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35
Mean	12.65	147.13	4159	6.02	5.51	4.70	9.15	3.12	1.34	55.31	0.19	0.16	40.46	1.87	0.46	0.37
Stdev	17.56	276.08	3722	3.40	7.72	4.51	15.83	4.51	0.79	53.44	0.18	0.28	65.06	2.19	0.85	0.40
Range	65.49	1305.35	13683	11.95	43.02	18.98	88.54	16.46	4.91	223.73	0.91	1.76	290.57	7.59	3.59	1.68
Minimum	0.50	2.40	117	0.08	0.15	0.29	0.09	0.03	0.00	0.11	0.00	0.00	0.07	0.00	0.00	0.00

Continued

25th Percentile (Q1)	1.18	9.36	1988	3.14	1.92	1.19	1.96	0.22	1.07	26.03	0.07	0.08	1.75	0.31	0.01	0.08
50th Percentile (Median)	2.49	30.58	2967	6.62	3.28	3.23	3.29	0.42	1.18	39.36	0.16	0.10	4.09	0.55	0.03	0.21
75th Percentile (Q3)	22.24	181.86	4227	8.84	5.35	6.25	12.24	6.82	1.46	60.96	0.24	0.16	73.28	3.33	0.43	0.51
Maximum	65.99	1307.76	13800	12.03	43.16	19.27	88.63	16.48	4.91	223.84	0.91	1.76	290.64	7.59	3.59	1.68
95.0% CI Mean	6.62 to 18.652.2 to 2,412,880 to 5438 4.8 to 7.2 2.86 to 8.163.15 to 6.23.72 to 14.591.5 to 4.661.07 to 1.6136.9 to 73.70.13 to 0.250.07 to 0.2618.1 to 62.8 1.1 to 2.60.17 to 0.750.23 to 0.51															
95.0% CI Sigma	14.2 to 23.0223 to 3,613,010 to 48,772.75 to 4.466.24 to 10.123.64 to 5.912.8 to 20.7 3.6 to 5.90.63 to 1.0343.3 to 70.020.15 to 0.240.23 to 0.3752.62 to 85.21.76 to 2.80.68 to 1.110.32 to 0.53															
Anderson-Darling Normality Test	4.26	5.44	3.190	1.08	5.22	2.26	5.02	4.58	3.04	2.79	1.90	8.10	4.37	3.11	5.59	2.34
P-Value (A-D Test)	**0.00**	**0.00**	**0.0000**	**0.01**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
Skewness	1.52	3.20	1.574	−0.48	3.83	1.56	4.05	1.43	2.94	1.81	2.23	5.52	2.19	1.26	2.24	1.72
P-Value (Skewness)	**0.00**	**0.00**	**0.0007**	0.21	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
Kurtosis	1.36	10.90	1.499	−0.82	17.07	2.17	19.30	1.02	12.37	2.91	6.60	31.73	5.53	0.43	5.03	2.84
P-Value (Kurtosis)	0.11	**0.00**	0.0933	0.18	**0.00**	**0.04**	**0.00**	0.19	**0.00**	**0.01**	**0.00**	**0.00**	**0.00**	0.45	**0.00**	**0.02**

Table 2. Mood's median test for the study materials.

Mood's Median-Monte Carlo: U 238

Test Information

H_0: Median 1 = Median 2 = … = Median k

Ha: At least one pair Median *i* Median *j*

Results:	V 51	Cr 52	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Te 130	Ba 138	Tl 205	Pb 208	Bi 209	U 238
Count (N ≤ Overall Median)	0	1	10	1	0	0	8	0	0	11	11	11	0	11	11	8	11
Count (N > Overall Median)	11	10	1	10	11	11	3	11	11	0	0	0	11	0	0	3	0
Median	69.07	22.10	5.71	14.80	37.57	19.10	8.59	27.56	60.17	5.29	1.04	0.04	45.46	0.04	4.25	0.30	1.60
UC Median (2-sided, 95% approx.)	82.16	28.11	8.13	17.79	51.68	23.76	9.89	37.24	187.31	7.04	1.51	0.06	59.41	0.06	5.46	37.01	1.82
LC Median (2-sided, 95% approx.)	55.71	18.38	4.80	12.29	29.78	15.40	6.97	18.56	35.92	3.77	0.65	0.04	30.55	0.04	3.95	0.16	1.24
Overall Median	9.849																
Chi-Square	158.64																
DF	16																
Monte Carlo P-Value (2-sided)	0.0000																
Monte Carlo P-Value 99% CI Upper	0.0000																
Monte Carlo P-Value 99% CI Lower	0.0000																

Table 3. Kruskal-wallis test for the study materials.

Test Information

H0: Median 1 = Median 2 = … = Median k

Ha: At least one pair Median *i* Median *j*

Results:	V 51	Cr 52	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Te 130	Ba 138	Tl 205	Pb 208	Bi 209	U 238
Count (N)	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00	11.00
Median	69.07	22.10	5.71	14.80	37.57	19.10	8.59	27.56	60.17	5.29	1.04	0.04	45.46	0.04	4.25	0.30	1.60
UC Median (2-sided, 95%)	82.16	28.11	8.13	17.79	51.68	23.76	9.89	37.24	187.31	7.04	1.51	0.06	59.41	0.06	5.46	37.01	1.82
LC Median (2-sided, 95%)	55.71	18.38	4.80	12.29	29.78	15.40	6.97	18.56	35.92	3.77	0.65	0.04	30.55	0.04	3.95	0.16	1.24
Z	4.83	1.89	−1.18	0.61	3.66	1.85	−0.29	2.50	4.46	−1.49	−3.51	−5.22	3.92	−5.18	−1.86	−1.84	−3.14
Kruskal-Wallis Statistic (H)	162.37																
DF	16.00																
P-Value (2-sided, adjusted for ties)	0.00																

Table 4. **Nonparametric runs test for the study materials.**

Nonparametric Runs Test																	
Test Information	V 51	Cr 52	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Te 130	Ba 138	Tl 205	Pb 208	Bi 209	U 238
Number of Runs about Median:	5.00	6.00	5.00	2.00	6.00	6.00	6.00	9.00	4.00	4.00	4.00	6.00	6.00	8.00	8.00	4.00	5.00
Expected Number of Runs about Median:	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45	6.45
Number of Points above Median:	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Number of Points equal to or below Median:	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
P-Value for Clustering:	0.18	0.39	0.18	0.00	0.39	0.39	0.39	0.95	0.06	0.06	0.06	0.39	0.39	0.84	0.84	0.06	0.18
P-Value for Mixtures:	0.82	0.61	0.82	1.00	0.61	0.61	0.61	0.05	0.94	0.94	0.94	0.61	0.61	0.16	0.16	0.94	0.82
P-Value for Lack of Randomness (2-Sided):	0.35	0.77	0.35	0.00	0.77	0.77	0.77	0.10	0.12	0.12	0.12	0.77	0.77	0.32	0.32	0.12	0.35
Number of Runs Up or Down:	5.00	5.00	6.00	6.00	8.00	5.00	5.00	8.00	5.00	8.00	7.00	7.00	7.00	8.00	7.00	5.00	4.00
Expected Number of Runs Up or Down:	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00	7.00
P-Value for Trends:	0.06	0.06	0.22	0.22	0.78	0.06	0.06	0.78	0.06	0.78	0.50	0.50	0.50	0.78	0.50	0.06	0.01
P-Value for Oscillation:	0.94	0.94	0.78	0.78	0.22	0.94	0.94	0.22	0.94	0.22	0.50	0.50	0.50	0.22	0.50	0.94	0.99

support our hypothesis of difference between the variables.

Matrix correlations were studied for the study chemical using Pearson Methods as listed in **Table 5**. Arsenic was almost correlated with all elements.

3. CONCLUSION

As seen in result section, Monte Carlo simulation showed clear difference at significant level of 95% among the study data. The difference of the reported data makes the non-parametric test valid. The **Figure 2**, log scale, illustrated the significant difference in the reported data. To support the Monte Carlo simulation, Kruskal-Wall test in **Figure 3** showed the significant difference among median variables. At 95%

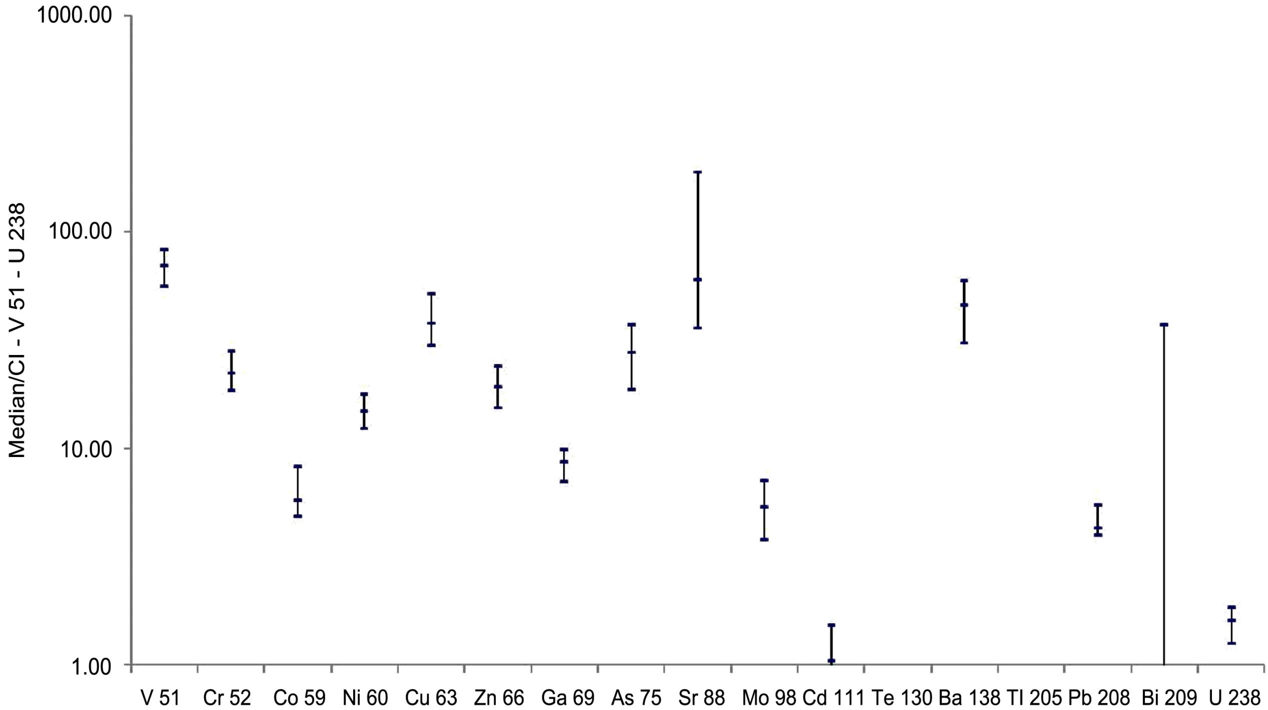

Figure 2. **Medians (log scale) of the study materials for mood's median test.**

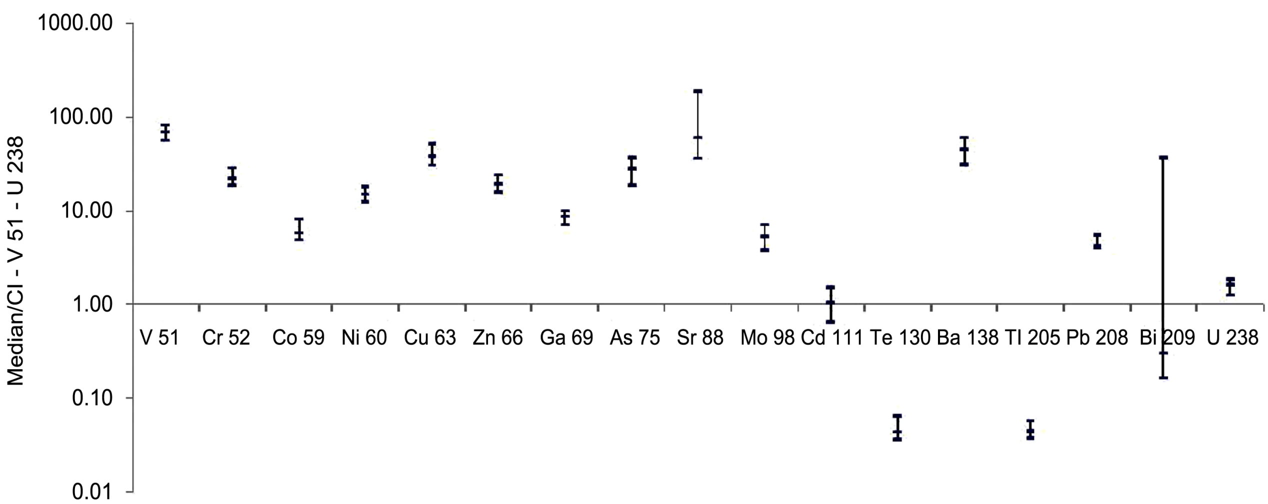

Figure 3. **Kruskal-wall test for of study materials.**

Table 5. **Correlation calculations between chemical and radiation measurements using pearson methods for adhesive materials.**

Pearson Correlations	V 51	Cr 52	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Ba 138	Pb 208	U 238
V 51	1	**0.8760**	**0.7750**	**0.8310**	0.5657	0.5150	0.5226	0.7542	−0.3594	0.1520	0.2643	0.2938	0.3885	0.6338
Cr 52		1	**0.8497**	**0.9131**	**0.7277**	0.6793	**0.7778**	**0.8411**	−0.2014	0.2396	0.3863	0.5029	0.4371	0.4608
Co 59			1	**0.6871**	0.5913	0.4029	**0.7719**	**0.7406**	0.1103	−0.0366	0.0353	0.3864	0.2491	0.3372
Ni 60				1	**0.7296**	0.6306	0.6703	**0.8673**	−0.3837	0.3910	0.5516	0.4769	0.3896	0.3355
Cu 63					1	0.5413	**0.9020**	**0.9206**	0.1427	**0.7565**	**0.7535**	0.5898	0.5024	−0.0918
Zn 66						1	0.6165	0.4656	0.0334	0.4472	0.6353	**0.8333**	0.8842	0.3295
Ga 69							1	**0.8363**	0.3635	0.5006	0.5395	**0.7060**	0.5255	−0.0540
As 75								1	−0.0479	0.5283	0.5985	0.5103	0.3535	0.1042
Sr 88									1	0.0759	−0.0212	0.3956	0.2847	−0.4002
Mo 98										1	**0.9293**	0.4730	0.5549	−0.3364
Cd 111											1	0.6580	0.6371	−0.1757
Ba 138												1	**0.7936**	−0.0433
Pb 208													1	0.2459
U 238														1

Pearson Probabilities	V 51	Cr 52	Co 59	Ni 60	Cu 63	Zn 66	Ga 69	As 75	Sr 88	Mo 98	Cd 111	Ba 138	Pb 208	U 238
V 51		0.0004	0.0051	**0.0015**	0.0697	0.1050	0.0991	0.0073	0.2777	0.6555	0.4322	0.3806	0.2377	0.0363
Cr 52			**0.0009**	**0.0001**	**0.0111**	0.0215	**0.0048**	**0.0012**	0.5526	0.4780	0.2406	0.1148	0.1789	0.1538
Co 59				0.0195	0.0554	0.2192	0.0054	**0.0091**	0.7468	0.9149	0.9179	0.2405	0.4600	0.3105
Ni 60					0.0108	0.0375	0.0240	**0.0005**	0.2441	0.2345	0.0786	0.1381	0.2362	0.3131
Cu 63						0.0855	**0.0001**	**0.0001**	0.6755	**0.0070**	0.0074	**0.0561**	0.1153	0.7884
Zn 66							0.0434	0.1490	0.9223	0.1678	0.0357	**0.0014**	**0.0003**	0.3225
Ga 69								**0.0013**	0.2719	0.1168	0.0867	**0.0152**	0.0969	0.8748
As 75									0.8888	0.0948	0.0517	0.1087	0.2863	0.7605
Sr 88										0.8246	0.9508	0.2285	0.3961	0.2227
Mo 98											0.0000	0.1417	0.0764	0.3118
Cd 111												0.0277	0.0350	0.6054
Ba 138													**0.0035**	0.8995
Pb 208														0.4662
U 238														

significance level, we conclude that the study data were non-identical populations.

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