

# Mining Frequent Pattern

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## Mining Frequent Pattern on Liquid Chromatography-Mass Spectrometer Data of Rodent Tuber to Find The Association Rules of Compounds for Machine Learning

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**ABSTRACT.** *Liquid Chromatography-Mass Spectrometry (LC-MS) data contains a lot of measurement data, which contains rodent tuber plant measurement. This paper aims to obtain frequent patterns on LC-MS data utilizing the FP-Growth method, where frequent patterns will be used for interpretation and identification of chemical compound in a biological sample. For faster computation, it needed representative sampling data and Linear Systematic Sampling was utilized for this purpose. In conclusion, FP-Growth can be applied successfully on Rodent Tuber's sample LC-MS data and generate an association rule of chemical compound formula. The result showed that C49H79O13P was the dominant compound in the LC-MS data with the highest support value of 41.67%. But it depends on the other, namely [C43H49O23]+. It can be said that when [C43H49O23]+ appears, there is possibility that C49H79O13P will also appear. Also, there is a perfect rule that [C43H49O23]+ implies C49H79O13P but not conversely. These results can be utilized for rule-based machine learning.*

**Keywords:** LC-MS, Frequent Pattern Growth, Rodent Tuber, Data Mining, Linear Systematic Sampling, Machine Learning

<sup>3</sup>  
**1. Introduction.** Raw data of Liquid Chromatography-Mass Spectrometry (LC-MS) contains millions of data points, there are hundreds to thousands of chromatographic peaks, after integration and peak extraction [1]. This raw data provide highly complex biological samples [2]. Meanwhile, LC-MS is widely used, especially in the interpretation or identification of the content of chemical compounds in a biological sample [2]–[6]. It consists of hundreds of thousands of mass per charge (m/z), retention time, and intensity [7]. Likewise, the LC-MS data of Rodent Tuber from the studies of Sianipar et. al [8]–[12] which is used in this paper.

It is not trivial to processing this data to be useful information. Many techniques are used to process these data. It is challenging to extract the information contained in the LC-MS data. One of them is finding certain patterns in the data with Association Rule. This pattern can be used to find and recognize certain chemical compounds contained in other LC-MS data. Further, the association rule can be used in machine learning.

Association Rule is a standardized and well-researched technique for finding interesting relationships between variables [13], finding causalities [14] between variables, finding the frequent patterns [15], [16] in large databases, and feature selection for classification [17].

The Association Rule is obtained by searching the frequent itemset of all frequent itemsets in the database. The discovery of frequent itemset is an important step in obtain Association Rule [18]. Two algorithms are popular in this field, namely Apriori and FP-Growth which are mining frequent patterns from a set of transactions in horizontal data format [19], although utilize only one minimum support threshold [20].

In this paper, FP-Growth was chosen because of its popularity [16], among the best ones to extract association patterns of the frequent item sets [21], and advantages such as more efficient than Apriori and adopting divide and conquer strategy as discussed in [13], [15], [22]–[24].

This paper describes pattern mining on Rodent Tuber's LC-MS data to obtain Association Rules to determine the relationships and/or casualties between chemical compounds. The results of this study will help biological or pharmaceutical scientists to 1) analyze and identify the possible presence of other compounds, 2) finding interesting relationships and/or casualties between compounds, 3) finding the frequent patterns, and 4) can be used for further processing in machine learning.

This paper categorized as follow: section 2 describes the problem statement and preliminaries process for further processing. Section 3 describes the research method. Section 4 describes the result and discussion. Section 5 focuses on conclusions and future work.

**2. Problem Statement and Preliminaries.** LC-MS data contain a huge number of compounds. It is possible to identify compounds that frequently occurs and their association with other compounds. It can be established as a pattern for other purposes.

There are more than 700,000 records in each of LC-MS data of Rodent Tuber from studies of Sianipar et. al [8]–[12]. Their studies resulted in 10 datasets. We have calculated, to get one compound name manually, will take about 20 seconds at the fastest time. By a simple calculation, if about 700,000 records will take 20 x 700,000 seconds. That means 5 months to complete the labeling for each dataset.

Using large native data like this case would be expensive. Therefore data sampling will be carried out. This LC-MS data of Rodent Tuber is time-series data, so required sampling per period to obtain a representative sample that represents the actual dataset. Linear systematic sampling is chosen because it is simple and can represent the actual dataset.

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#### Algorithm 1: LSS

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**Result:** Sample File in type .xlsx

```
df = pd.read_excel(file)
listDF = df.values.tolist()
pivotDF = pd.pivot_table(df,index=["Retention Time"])
arrRT = pivotDF.index.array.to_numpy()
```

```
arrSample = []
arrTempRT = []
arrTempI = []
totalRec = 0
k = len(listDF)/18000
for n in range(len(arrRT)):
    arrTemp=[]
```

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```

arrTempInt=[]
for i in range(len(listDF)):
    if listDF[i][2] == arrRT[n]:
        arrTemp.append(listDF[i][0])
        arrTempInt.append(listDF[i][1])
indexes = np.arrange(random.randint(0,k),
                    len(arrTemp), step=k)

for i in indexes:
    arrSample.append(arrTemp[i])
    arrTempRT.append(arrRT[n])
    arrTempInt.append(arrTempInt[i])
df1.to_excel('sampleFile.xlsx', index=False)

```

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Figure 1. Algorithm of Linear Systematic Sampling

9

To obtain a systematic sample, given that  $N$  is the number of population of elements, while  $n$  is the number of samples desired, so if  $N/n$  is an integer, then  $k = N/n$ ; otherwise, let  $k$  be the next integer after  $N/n$ .

After that, find a random integer  $R$  between 1 and  $k$ , defining the sample as the unit numbered  $R, R + k, R + 2k$ , and so on. The initial unit  $R$  selected is called “random start” and  $k$  is called “sampling interval” [25], [26].

Based on that, we develop Algorithm 1 as shown in Figure 1 and implemented in Python. It applied to one of ten of the LC-MS dataset of Rodent Tuber which we have and the result will be used in this paper.

**3. Research Method.** Our research method consists of several stages as shown in Figure 2. Preliminaries above are the first stage of this method as preparation and initial stage by implementing Algorithm 1 as shown in Figure 1 utilizing Linear Systematic Sampling. This preliminary generate a representative sample of the whole dataset. It generates 18,271 records out of 985,924 records.

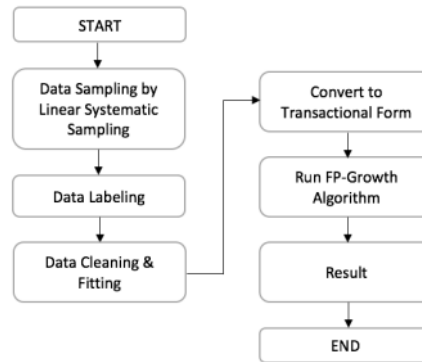


Figure 2. Diagram of research method

FP-Growth is commonly used for market basket analysis which usually has data label. The LCMS data to be analyzed does not have label, so it needs to be labeled. Labeling in this

study is giving name of chemical compounds based on their mass per charge ( $m/z$ ) in the data. After labeling, the LCMS data will be converted into a kind of transactional data like a market basket transaction. It is labeled with another previously developed tool in stage “Data Labeling”.

5.022	139408	54.743965	0.00	-	-
5.022	314416	82.195709	82.0531	C4H6N2	2-Methylimidazole
5.022	49996	105.536	0.00	-	-
5.022	140672	130.6474	0.00	-	-
5.022	164000	157.34009	157.16901	C7H11NO3	Acetylproline
5.022	83488	180.99664	181.00198	C8H7N5	2-(Methylsulfonyl)-1,3-benzothiazole
5.022	208448	204.9698	205.03751	C10H7NO4	Xanthurenic acid
5.022	114944	232.29471	232.2847	C13H16N2O2	3-Dimethylaminoacetyl-5-methoxyindole
5.022	78616	255.88803	256.00415	C10H8O6	4-Methylumbelliferyl sulfate
5.022	70692	278.78558	0.00	-	-
5.022	53868	299.59576	299.3786	C20H17N3	Komarovicine
5.022	29919	322.55652	322.41049	C20H22N2O2	Haplamidine
5.022	20764	341.15289	341.14749	C16H23NO7	Monocrotaline N-oxide
5.022	31190	368.1618	368.12598	C21H20O6	Curcumin
5.022	25493	395.4238	395.3399	C24H45NO3	N-Oleoyl-isoleucine
5.022	14206	427.999	428.01309	C15H19C13N2O4S	PR2_M429
5.022	14206	427.99902	428.01309	C15H19C13N2O4S	Scutellarin-7-glucuronide
5.022	20871	462.0291	462.0798	C21H18O12	10-Deacetyl baccatin III
5.022	20871	462.02905	462.0798	C21H18O12	Erythromycin
5.022	27615	494.98376	0.00	-	-
5.022	4040	544.44751	544.59698	C29H36O10	4'-O-(2'-E-Feruloyl GluA(1-2)GluA) Apigenin (NMR)
5.022	12046	597.95947	0.00	-	-
5.022	9886	693.66699	0.00	-	-
5.022	36472	733.38379	733.46124	C37H67NO13	PG 42.9
5.022	17375	798.15466	798.16431	C37H67NO13	PG 40.7
5.022	191	821.24194	821.08801	C46H77O10P	PG 42.9
5.022	191	844.89856	845.10999	C48H77O10P	PG 42.9
5.022	191	878.80212	0.00000	-	-

Figure 3A. Snippet unclean data

5.022	314416	82.19571	82.0531	C4H6N2	2-Methylimidazole
5.022	164000	157.3401	157.16901	C7H11NO3	Acetylproline
5.022	83488	180.9966	181.00198	C8H7N5	2-(Methylsulfonyl)-1,3-benzothiazole
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5.022	4040	544.4475	544.59698	C29H36O10	10-Deacetyl baccatin III
5.022	36472	733.3838	733.46124	C37H67NO13	Erythromycin
5.022	17375	798.1547	798.16431	C37H67NO13	4'-O-(2'-E-Feruloyl GluA(1-2)GluA) Apigenin (NMR)
5.022	191	821.2419	821.08801	C46H77O10P	PG 40.7
5.022	191	844.8986	845.10999	C48H77O10P	PG 42.9
5.022	191	914.5399	914.58844	C48H77O13P	Phosphatidylinositol 18:0-22:4
5.022	191	958.7537	958.51367	C48H77O19	3-Glc-Gal-GlcUA Soyasapogenol B
5.022	265	1029.344	1029.18005	C51H80O21	Soyasapogenol B + dHex + Hex + HexA + malonyl
5.022	191	1103.097	1103.25903	C54H86O23	Soyasapogenol B base + O-dHex, O-HexA-HexA-dHex
10.045	12949	163.2226	163.24001	C6H13NO25	(3R)-3-amino-5-methylsulfonylpentanoic acid, R-3-A...
10.045	8657	191.1804	191.186	C10H9NO3	5-Hydroxyindole-3-acetate, 5-HIAA, 5-Oxyindoleace...
10.045	71648	216.7978	217.00612	C9H9C12NO	Proanil

Figure 3B. Snippet cleaning and fitting result

The result of labeling is an unclean dataset as shown in Figure 3A, because there are several missing names of chemical compounds, in this case, we write it with characters “-“. Therefore, “Data Cleaning and Fitting” were carried out. Data cleaning and fitting is intended to dispose empty data or has no label. It generate dataset as shown in Figure 3B.

After the dataset is clean and fit according to what we want, it needs to be processed again to adjust the use of the FP-Growth algorithm. We called it “Convert to Transactional Form”.

ID	Items
1	{Bread, Milk}
2	{Bread, Diapers, Beer, Eggs}
3	{Milk, Diapers, Beer, Cola}
4	{Bread, Milk, Diapers, Beer}
5	{Bread, Milk, Diapers, Cola}
...	...

market basket transactions

{Diapers, Beer} Example of a frequent itemset  
{Diapers} → {Beer} Example of an association rule

Figure 4A. Illustration of Market Basket Transactions [27]

C4H6N2	C7H11NO3	C8H7N5	C10H7NO4	C13H16N2O2	C10H8O6	C20H17N3
C6H13NO25	C6H13NO25	C10H9NO3	C10H9NO3	C10H9NO3	C9H9C12NO	{C15H11O6}+
C4H7NO2	C7H6O2	C5H6O5	C7H3C12N	C10H13NO3	C16H35N	C16H35N
C5H5N	C3H7NO6	C8H7NO4S	C6H13O8P	C18H34O2	C18H34O2	C18H34O2
C4H8N2O	C3H8O3S	C7H5NO5	C10H8O4	C14H17NO	C15H11NO2	C16H34O2
C4H4O3S	C4H4O3S	C4H4O3S	C4H4O3S	C6H12N2O	C4H6N4O3	C6H12N2O
C5H4N4O	C8H7NO3	C6H3C12NO2	C9H9C12NO	C6H12N2O4S2	C15H18O4	C6H8C13O4S2
C3H9NO	C3H9NO	C3H9NO	C3H9NO	C3H4O5	C7H5NO5	C11H19NO5
C5H5N	C3H6O2S	C10H16	C10H16	C9H8O3	C8H8N2O3S	C9H10C12N2O
C3H4N4O2	C3H7O7P	C14H31N	C20H36O2	C15H17C12N3O2	C14H17N2O2	C22H23N5O3
C5H5NO	C4H6O5	C4H5NO4S	C9H10C1NO3	C12H18N2O3	C6H15O9P	C14H24N2O4
C3H7NO3	C8H5NO2	C7H8N4O2	C7H8N4O2	C7H8N4O2	C7H5NO3S2	C14H16N2O2
C3H7NO	C4H6O5	C8H18N2O	C13H22O	C13H22O	C12H15NO3	C9H16N2O6
C4H7NO2	C4H7NO2	C5H6O5	C9H21N3O	C8H6C12O3	C10H9C12N3O	C19H28O2
C2H5NO3	C2H5NO3	C2H5NO3	C2H5NO3	C4H6O5	C6H6O3S	C10H10O6
C4H4N2	C4H4N2	C4H4N2	C4H4N2	C6H5NO2	C7H4C12O2	C7H4C12O2
C3H4O5	C6H11NO4	C6H11NO4	C6H11NO4	C5H2C13NO	C12H11NO2S	C8H4C13NO3

Figure 4B. Snippet data

This process convert the dataset to the transactional form as a market basket transaction as illustrated in Figure 4A and the snippet of real result dataset of this conversion is shown in Figure 4B. In this case, Transaction ID (TID) is Retention Time and the item set is compound formula. It is done by Algorithm 2 as seen in Figure 5. Retention Time is a TID because it has many duplicates with different  $m/z$ , as in actual case, a grocery receipt consisting of many shopping items with one TID which actually it can be interpreted that there are many duplicates of TID because it is attached to one item which is then summarized into one.

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**Algorithm 2** ConvertToMarketBasketTransaction

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- 1: Get data from the dataset that has been made into an excel file and convert it to an actual data list, namely listDF[].
  - 2: Create a list that contains “Retention Time” column without duplication with the pivot feature, namely arrRT[].
  - 3: rows, cols = (len(arrRT), len(listDF))  
arr=[]
  - 4: for i in range(rows):  
    row = []  
    for j in range(cols):  
        if listDF[j][4] == arrRT[i]:   ⇒ check same Retention Time  
            row.append(listDF[j][1])   ⇒ append Formula to new list as row  
    arr.append(row)                   ⇒ appen list ROW in list ARR
  - 5: Write arr[] list into an excel file.   ⇒ result is 2D list
- 

Figure 5. Algorithm Conversion to Market Basket Transaction

The next step is “Run FP-Growth Algorithm” which is processing the transactional form as a market basket transaction into FP-Growth algorithm. This aims to find the frequent pattern of item. This algorithm is implemented in the python library namely `mlxtend.frequent_patterns` [28]. We just used it without adjustment anything.

**4. Result and Discussion.** Linear Systematic Sampling successfully builds a sample of LC-MS data which at first contains 985,924 records to 18,271 records done by Algorithm 1. Using a smaller number of data sample but representing the entire dataset, labeling work is faster. Labeling was done by web scraping technique [29]–[31]. The next steps are cleaning and fitting, converting, and processed to FP-Growth algorithm. All processes implemented in python programming and `fp-growth` library.

The results of FP-Growth processing with minimum support of 35% is shown in Figure 6A and the association rule with a minimum threshold of 35% is shown in Figure 6B.

	support	itemsets
0	0.416667	(C49H79O13P)
1	0.361111	(C50H86NO8P)
2	0.361111	(C48H76O18)
3	0.361111	[(C43H49O23)+]
4	0.361111	(C48H78O18)
5	0.361111	[(C43H49O23)+, C49H79O13P]

Figure 6A. Result of FP-Growth

As seen in Figure 6A, the highest support is 0.416667 and it is a single item, which is C49H79O13P, namely Phosphatidylinositol 20:4-20:4 with exact mass is 906.52582; it means this item appears most frequently (41.6%) in the data. It is dominant than others.

In Figure 6B, the highest confidence value is 1.00, this can be interpreted that if there is [C43H49O23]+, then absolutey C49H79O13P exists, but if conversely, the confidence value is smaller (86.67%) which is still a good value because of more than 50%. This result have



an association with Lift value which is more than 1. They are dependent on each other as can be seen in the Leverage value which is more than 0.

	antecedents	consequents	antecedent support	consequent support	support	confidence	lift	leverage	conviction
0	[(C43H49O23)+]	(C49H79O13P)	0.361111	0.416667	0.361111	1.000000	2.4	0.210648	inf
1	(C49H79O13P)	[(C43H49O23)+]	0.416667	0.361111	0.361111	0.866667	2.4	0.210648	4.791667

Figure 6B. Result of Association Rule

The conviction will be infinity ( $\infty$ ) if a perfect rule and has a value of 1 if it is a completely uncorrelated rule [32]. [C43H49O23]+ implies C49H79O13P has conviction infinity which means that this is a perfect rule of the antecedent ([C43H49O23]+) to the consequent (C49H79O13P) but not conversely.

**5.Conclusion.** The FP-Growth algorithm using python library namely `mlxtend.frequent_patterns` can be applied well to the sample of LC-MS data of Rodent Tuber. Sampling was done by the Linear Systematic Sampling method. It serves to simplify a huge dataset but still reflects the actual dataset.

There is a huge number of compounds in LC-MS data of Rodent Tuber when closely observed. However, by processing the dataset with FP-Growth, it can be seen which compounds are more dominant than others. As seen from Figure 6A, the highest support value is 41.67% which is C49H79O13P. It can be interpreted that C49H79O13P is the dominant compound in this LC-MS data. But this compound depends on other compounds, namely [C43H49O23]+ which can be seen in Figure 6B with an infinity conviction value. It can also be said that when [C43H49O23]+ appears, absolutely C49H79O13P will also appear. These association rule can be utilized for processing with rule-based machine learning.

For future works, this study will be applied to other datasets from the existing LC-MS data of Rodent Tuber so that more comprehensive results are obtained.

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