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METABOLOMIC ANALYSIS USING MAVEN

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WHAT IS PREECLAMPSIA?

Preeclampsia is a pregnancy complication characterised by way of means of elevated maternal blood pressure and proteinuria after about 20 weeks of gestation. This pregnancy disorder affects as much as 8% of pregnancies international and might bring about extreme or deadly headaches for both the mom and foetus because of dangers related to excessive blood strain and decreased blood float.

WHAT IS MAVEN?

Due to the need for automatic evaluation strategies for LC-MS and GC-MS records, a couple of records evaluation software program systems have been developed, which include open-source software program like MAVEN.

El-MAVEN is an open-source, vendor-neutral software program platform that allows interactive, fast, efficient, and dependable evaluation of LC-MS, GC-MS, and LC-MS/MS datasets in only three-four steps from loading records to exporting results.

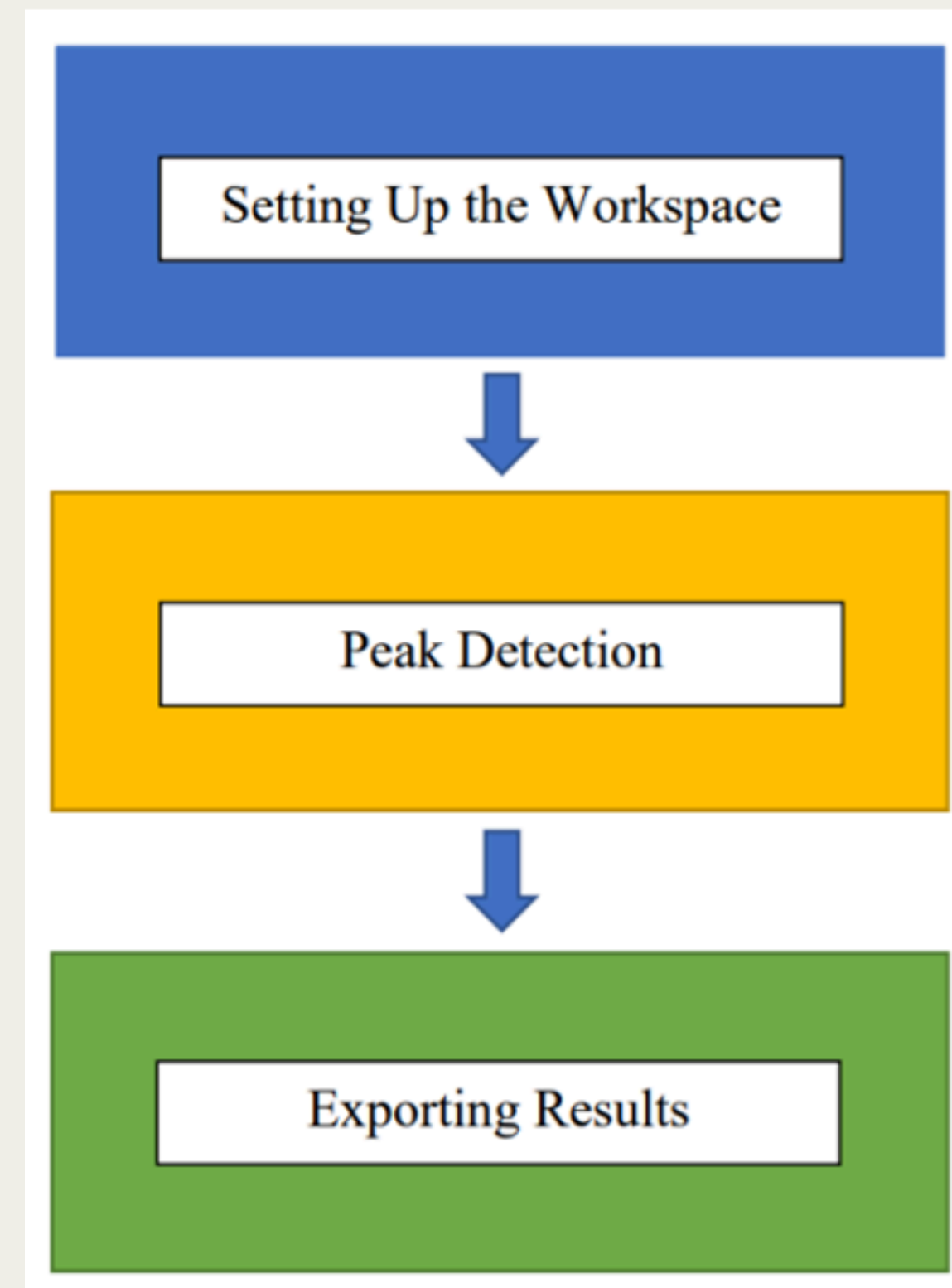
EL-MAVEN WORKFLOW

1) Setting Up the Workspace

- Launch El-MAVEN
- Adjust Global Settings
- Load Data
- Select Reference Compound Database

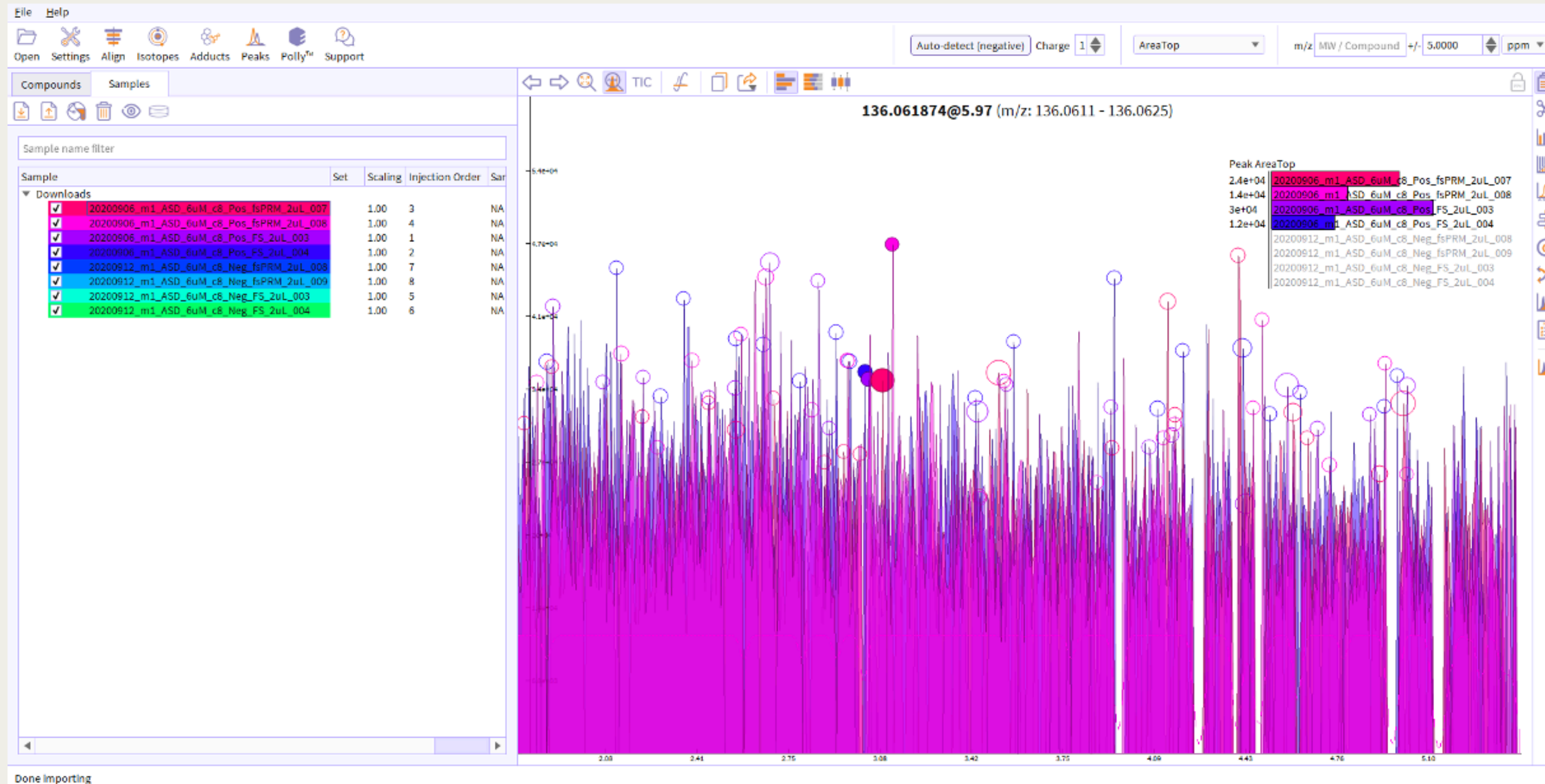
2. Peak Detection

3. Exporting Results



PROCEDURE AND RESULTS

1) Importing samples (Main page view) :-

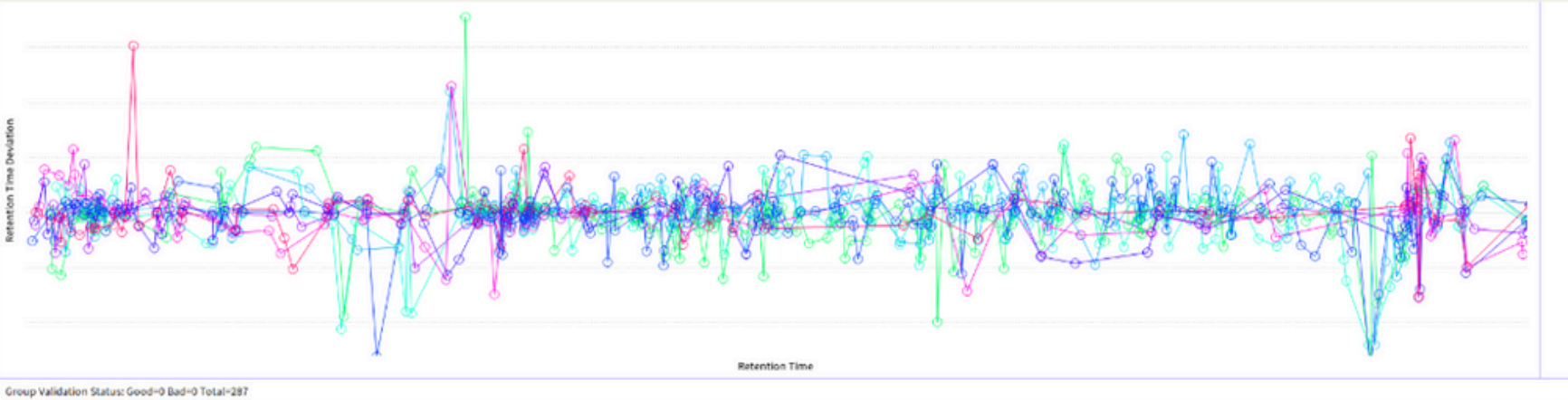


PROCEDURE AND RESULTS

2) Compounds list used and peak alignment visualisation :-

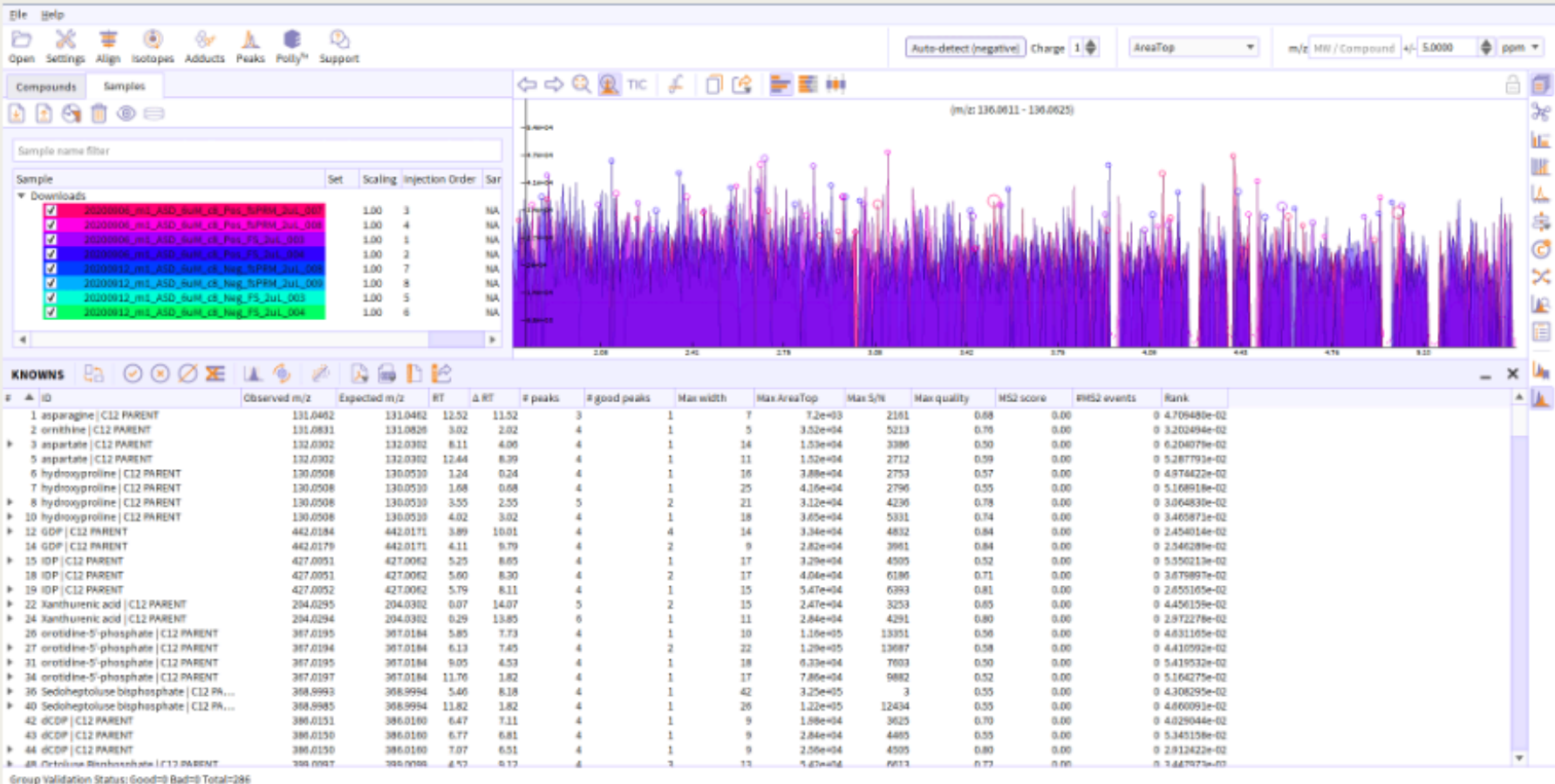
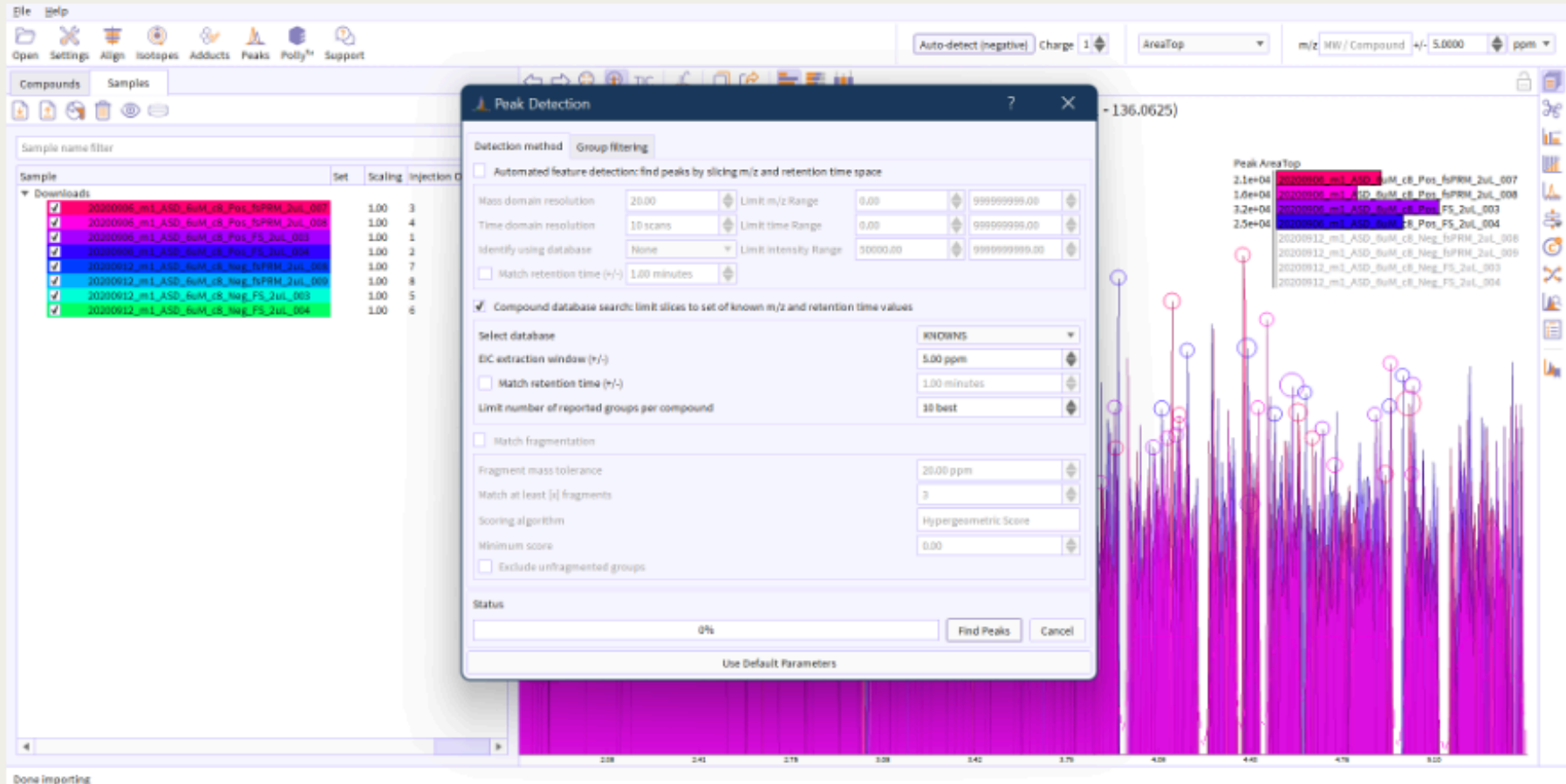
Compound name filter

Name	Formula	m/z	RT	Category
▶ 1-Methyl-Histidine	C7H11N3O2	170.092407	2.00	
▶ 1-Methyladenosine	C11H15N5O4	282.119690	3.00	
▶ 1_3-diphosphateglycerate	C3H8O10P2	266.966553		
▶ 2-Aminooctanoic acid	C8H17NO2	160.133209		
▶ 2-Hydroxy-2-methylbutanedioic acid	C5H8O5	149.044449	12.06	
▶ 2-Isopropylmalic acid	C7H12O5	177.075745	13.87	
▶ 2-dehydro-D-gluconate	C6H10O7	195.049927	5.00	
▶ 2-keto-isovalerate	C5H8O3	117.054619	13.06	
▶ 2-oxo-4-methylthiobutanoate	C5H8O3S	149.026688	13.75	
▶ 2-oxobutanoate	C4H6O3	103.038971	10.95	
▶ 2_3-Diphosphoglyceric acid	C3H8O10P2	266.966553	14.68	
▶ 2_3-dihydroxybenzoic acid	C7H6O4	155.033890	13.58	
▶ 3-S-methylthiopropionate	C4H8O2S	121.031776	11.92	
▶ 3-hydroxy-3-methylglutaryl-CoA-nega	C27H44N7O20P3S	912.164734	15.72	
▶ 3-hydroxybutyryl-CoA	C25H42N7O18P3S	854.159302	15.20	
▶ 3-methylphenylacetic acid	C9H10O2	151.075363	15.41	
▶ 3-phospho-serine	C3H8NO6P	186.016205	8.20	
▶ 3-phosphoglycerate	C3H7O7P	187.000214	13.58	
▶ 4-Pyridoxic acid	C8H9NO4	184.060440	14.14	
▶ 4-aminobutyrate	C4H9NO2	104.070602	4.00	
▶ 5-methoxytryptophan	C12H14N2O3	235.107727		
▶ 5-methyl-THF	C20H25N7O6	460.193909	14.10	
▶ 5-phosphoribosyl-1-pyrophosphate	C5H13O14P3	390.959106	14.94	
▶ 6-phospho-D-gluconate	C6H13O10P	277.031921	13.38	
▶ 7-methylguanosine	C11H16N5O5	299.122437	12.00	
▶ 7_8-dihydrofolate	C19H21N7O6	444.162598		
▶ ADP	C10H15N5O10P2	428.036713	13.80	
▶ ADP-D-glucose	C16H25N5O15P2	590.089539	14.14	
▶ AMP	C10H14N5O7P	348.070374	11.30	
▶ ATP	C10H16N5O13P3	508.003021	14.94	nucleic acids
▶ Acetylcarnitine	C9H18NO4	205.130859	2.40	
▶ Acetyllysine	C8H16N2O3	189.123367	1.10	
▶ Amino adipic acid	C6H11NO4	162.076080	3.22	
▶ Ascorbic acid	C6H8O6	177.039368	6.59	
▶ Atrolactic acid	C9H10O3	167.070267		
▶ CDP	C9H15N3O11P2	404.025452	13.53	
▶ CDP-choline	C14H27N4O11P2	490.122437	6.33	
▶ CDP-ethanolamine	C11H20N4O11P2	447.067657	6.38	



PROCEDURE AND RESULTS

3) Peak detection and metabolites found :-

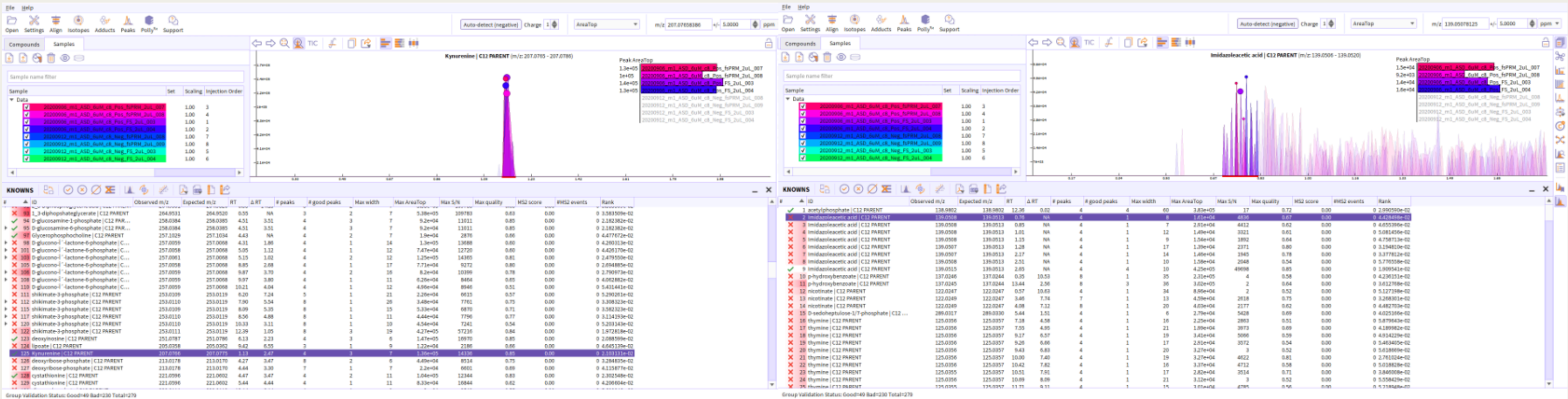


PROCEDURE AND RESULTS

4) Peak marking :-

Good peak

Bad peak



- All the peaks are linear (in a line)
- The detected peak collection is clean
- The peaks are non-linear (not in a line)
- The detected peak collection is scattered and can be considered to be noisy

CONCLUSION

This study represents crucial research on compounds measured in human placenta samples. It helped classify the metabolites into good (preferable for further work) and bad peaks (not preferred).

This result can be used in softwares like MetaboAnalyst and machine learning techniques to then perform exemplary metabolomic analysis and study.

Findings from this study lay the foundation for similar evaluation to better apprehend the chemical and organic interactions underlying preeclampsia.

FUTURE WORK

While open-source software program structures facilitate mass spectrometry data analysis, there are properly-documented troubles with these types of equipment. Efforts are being made to improve the practicality and efficiency of such software programs.

With the enhancements made in El-MAVEN, large omics datasets containing information from over a hundred samples are loaded in a matter of seconds (~4× development as compared to MAVEN), and analyses which include top detection and isotope detection have been finished within seconds.

Such advancements and improvements are driving the future work taking place to make the application better, and the overall experience as smooth and simple for the user as possible.

THANK YOU