

Plotting the complicated mass spectrometry data as a Circos plot makes the data analysis easy and less complicated

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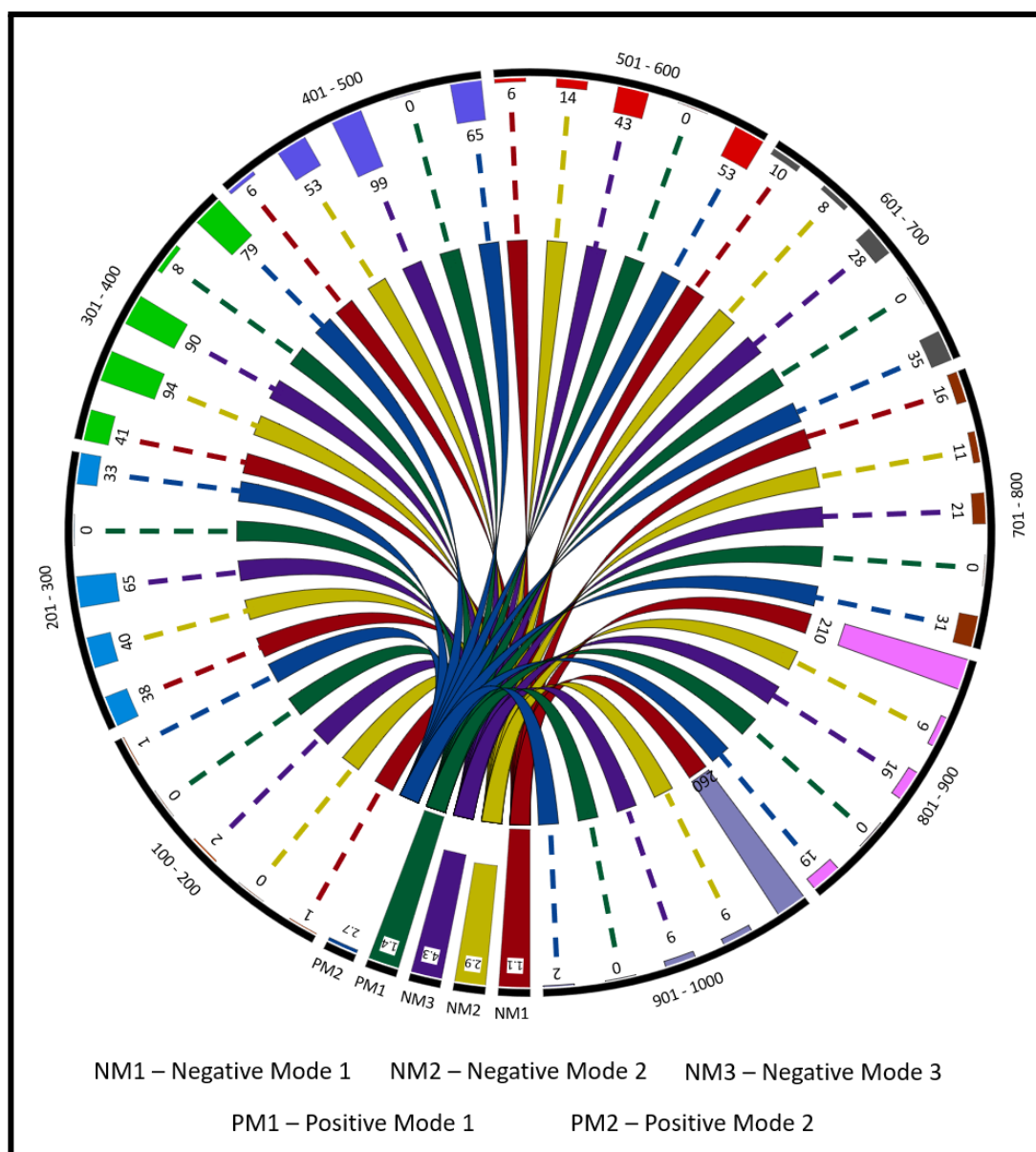


Figure 1. Circos plot showing the m/z peaks from mass spectrometry data.

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Conventionally Circos plots [1] have been used in genome analysis to connect the structural genomics with the functional genomics i.e., the multiomics analysis [2]; Genome-wide association studies to identify and annotate species with desirable traits [3]; microRNA-mediated genomic regulation network analysis [4]; identification of biomarkers for disease diagnosis [5]; antibiotic-resistance in bacteria and their ability in the biofilm formation [6], etc. Previously we have published hand drawn circular plots not only to connect the coronavirus mRNA stability with the viral replication and receptor binding capabilities [7, 8] but also to connect proton NMR spectral details of CYP450's role in paracetamol metabolism [9]. Interestingly, the Government of India has adapted the Circos plot to publish the national level researcher identification and network [10].

Microbiome analysis of humans primarily depends on the proteomics and metabolomics that are performed using mass spectrometry (MS) technique. The two-dimensional MS spectra are often complicated and messy in microbiome analysis. Understanding the m/z peaks and their overlaps are critical in order to avoid any false positives and hence the resolution of the m/z peaks is very important. However, depending on the number of proteins/metabolites present in the samples, the resolution can often be messy with too many overlaps. In such cases, converting the conventional 2D MS spectrum into a Circos plot can make analysis easier. Plotting the high intensity peaks is not complicated as they stand out but the low intensity peaks that are above the background noise may pose a challenge with overlaps. Here we made an attempt to convert all the m/z peaks taken from a typical MS spectrum into a Circos plot [Figure 1]. In this attempt, we succeeded in plotting the number of peaks that are present at various ranges of mass values. For example, 100-200, 200-300...900-1000 were taken as sectors in the Circos plot to clearly identify the number of peaks in each sector for clear understanding. All the positive mode and negative mode data collections were clubbed together and plotted separately in the Circos plot using different color codes for clarity. We were unable to include the peak intensities in the present plot which will be added in the future.

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Author contributions: M.V. performed spectral analysis and plotted the Circos plot. R.S.Y. is the principal investigator, trained M.V., provided the laboratory space and facilities needed, wrote the draft of the manuscript, edited and finalized.

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