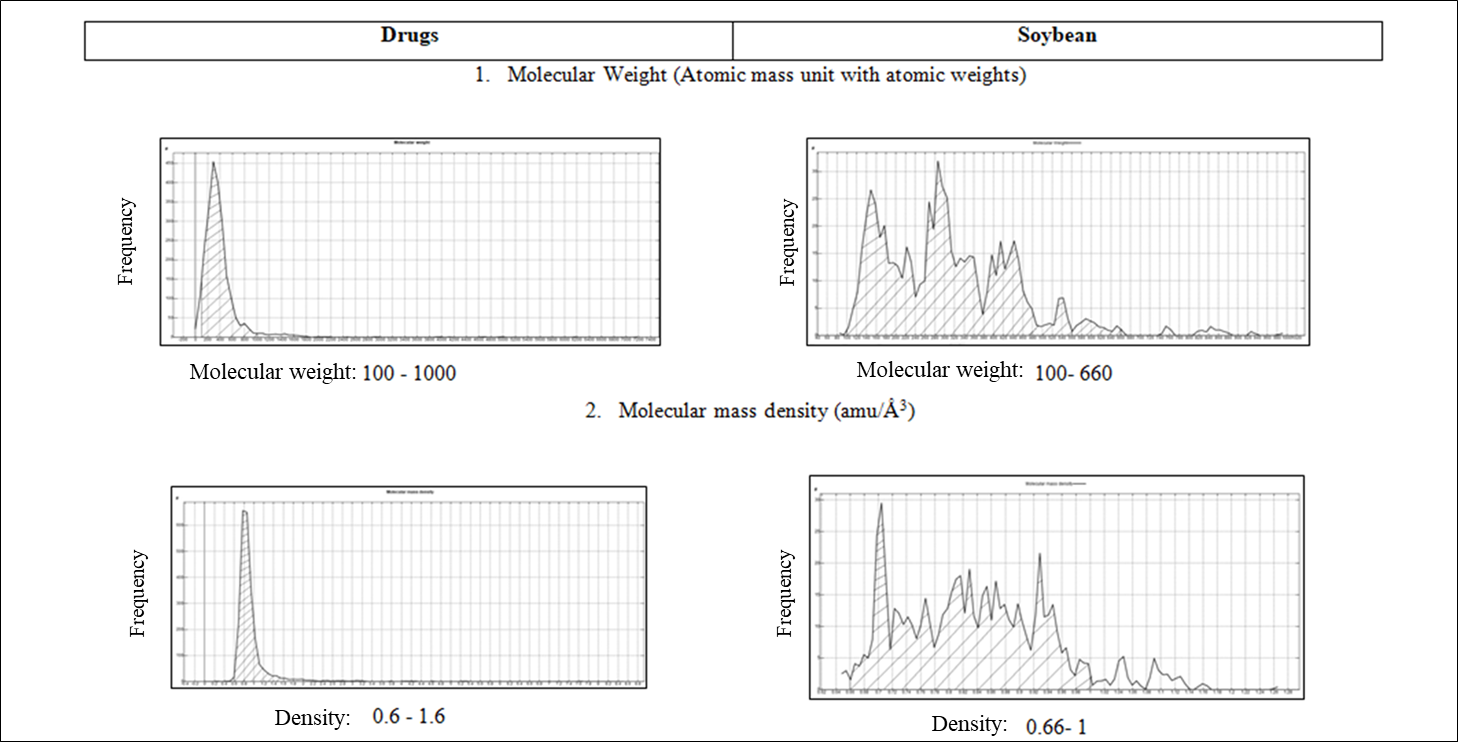
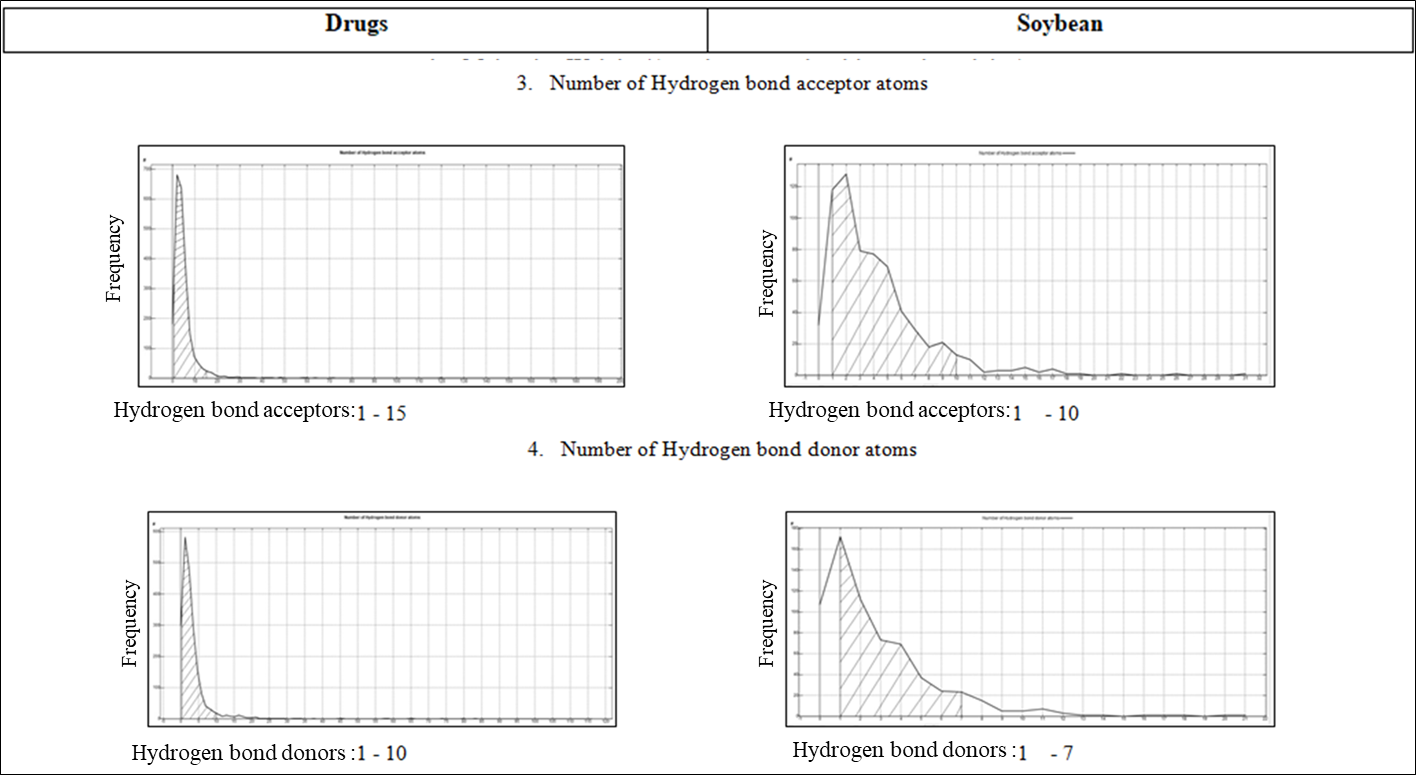
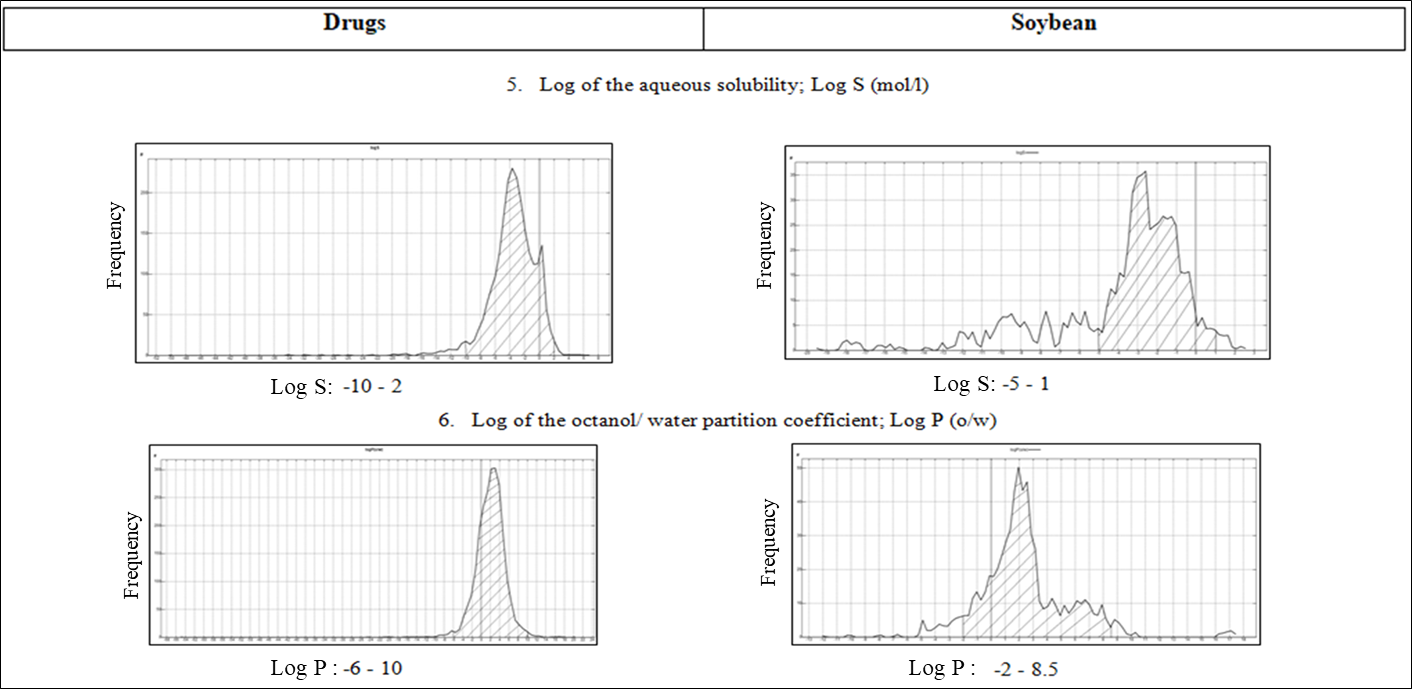
Bridging *In-Silico* and Experimental: Chemoinformatics Analysis of Mass Spectrometry-Based Metabolomics Study of Soybean

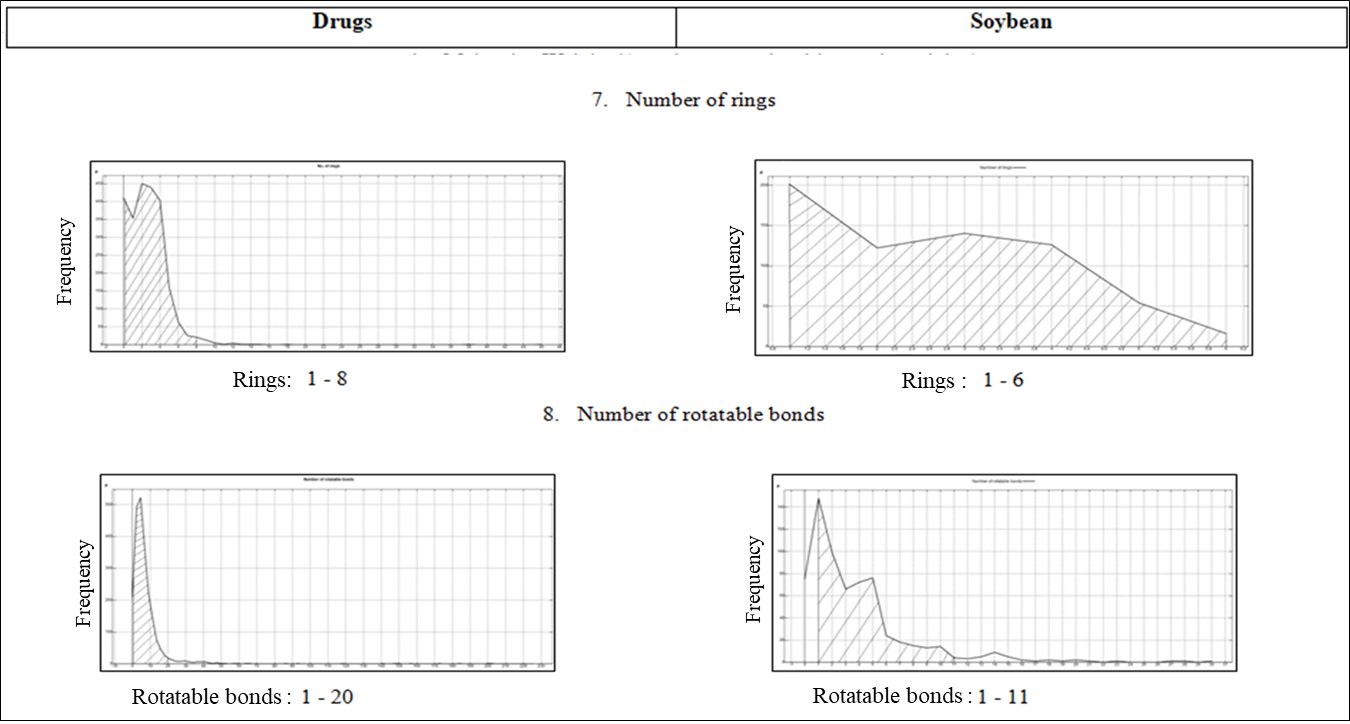
Divya Karade1,2, Swapnil Mundhe3,Narendra Kadoo2,3, Milind Ratnaparkhe4, Renu Vyas5, Muthukumarasamy Karthikeyan\*,1,2

1. Chemical Engineering and Process Development (CEPD) Division, CSIR-National Chemical Laboratory, Pune – 411008, India
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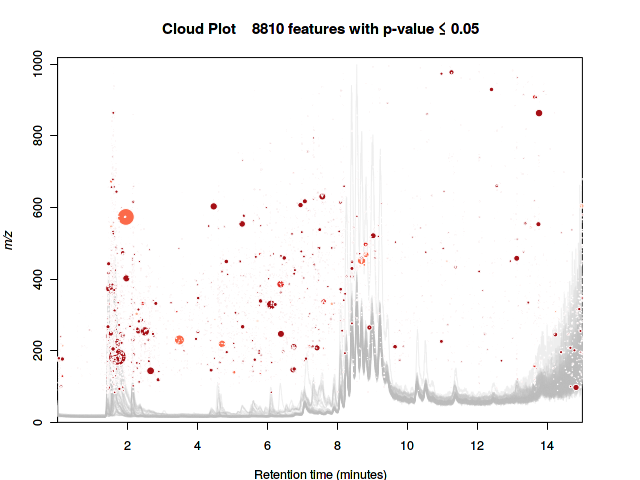
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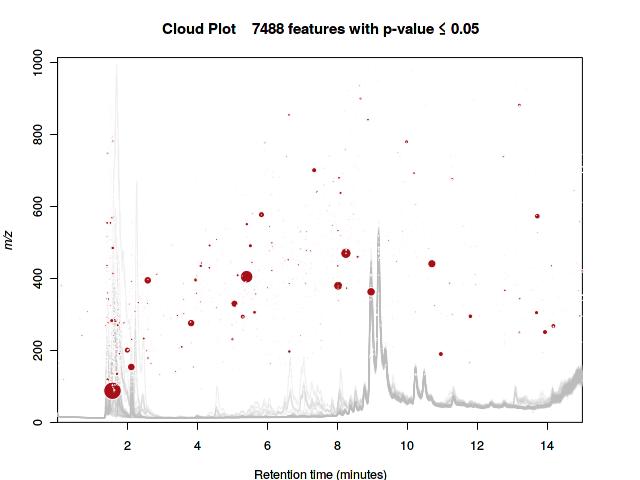
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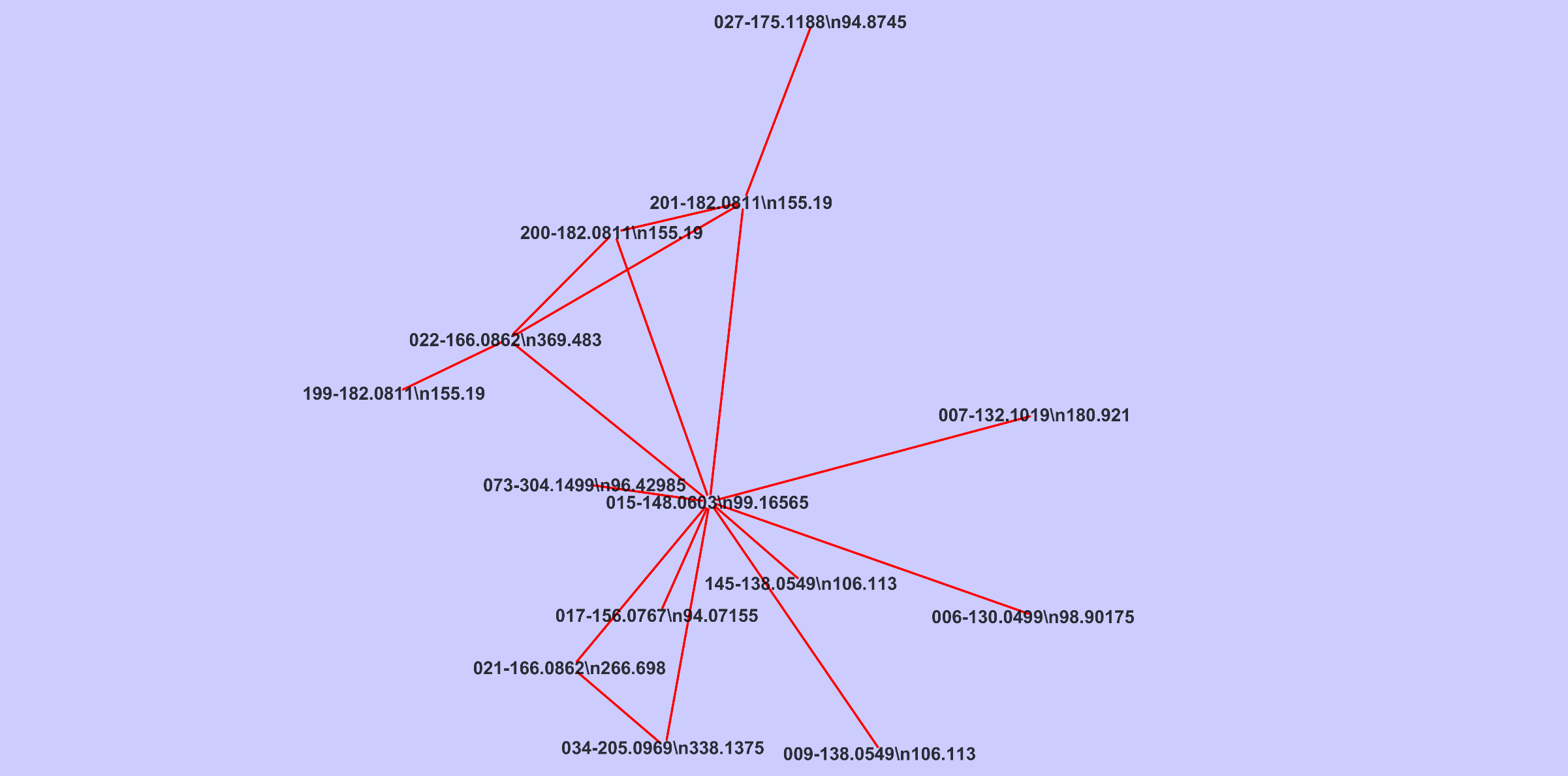
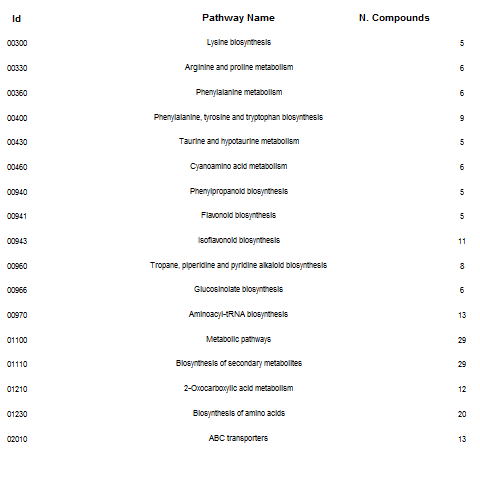
**Supplementary** **Fig. 1**: Histograms depicting descriptor ranges of soybean small molecules and approved drugs



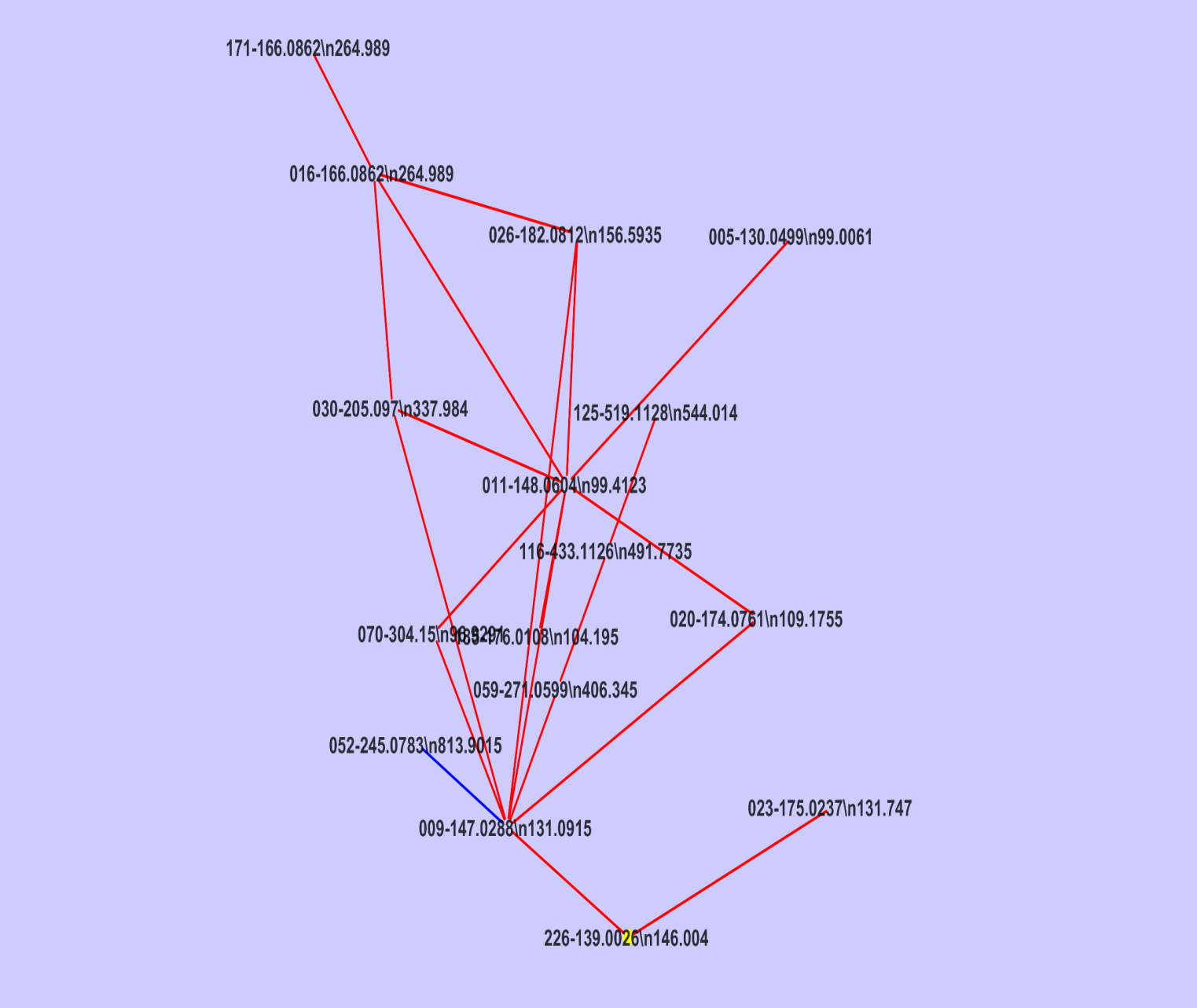
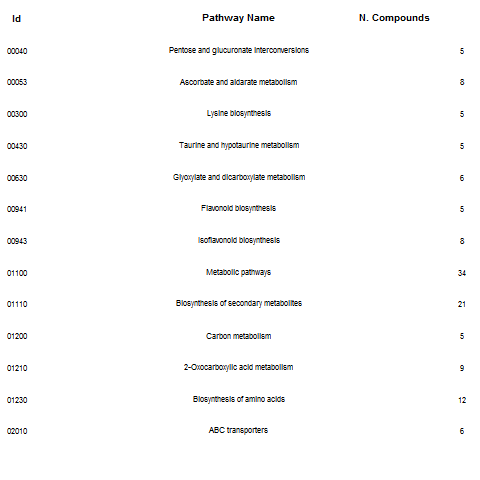
**Supplementary** **Fig. 2**: Cloud plot generated by XCMS for positive ion mode



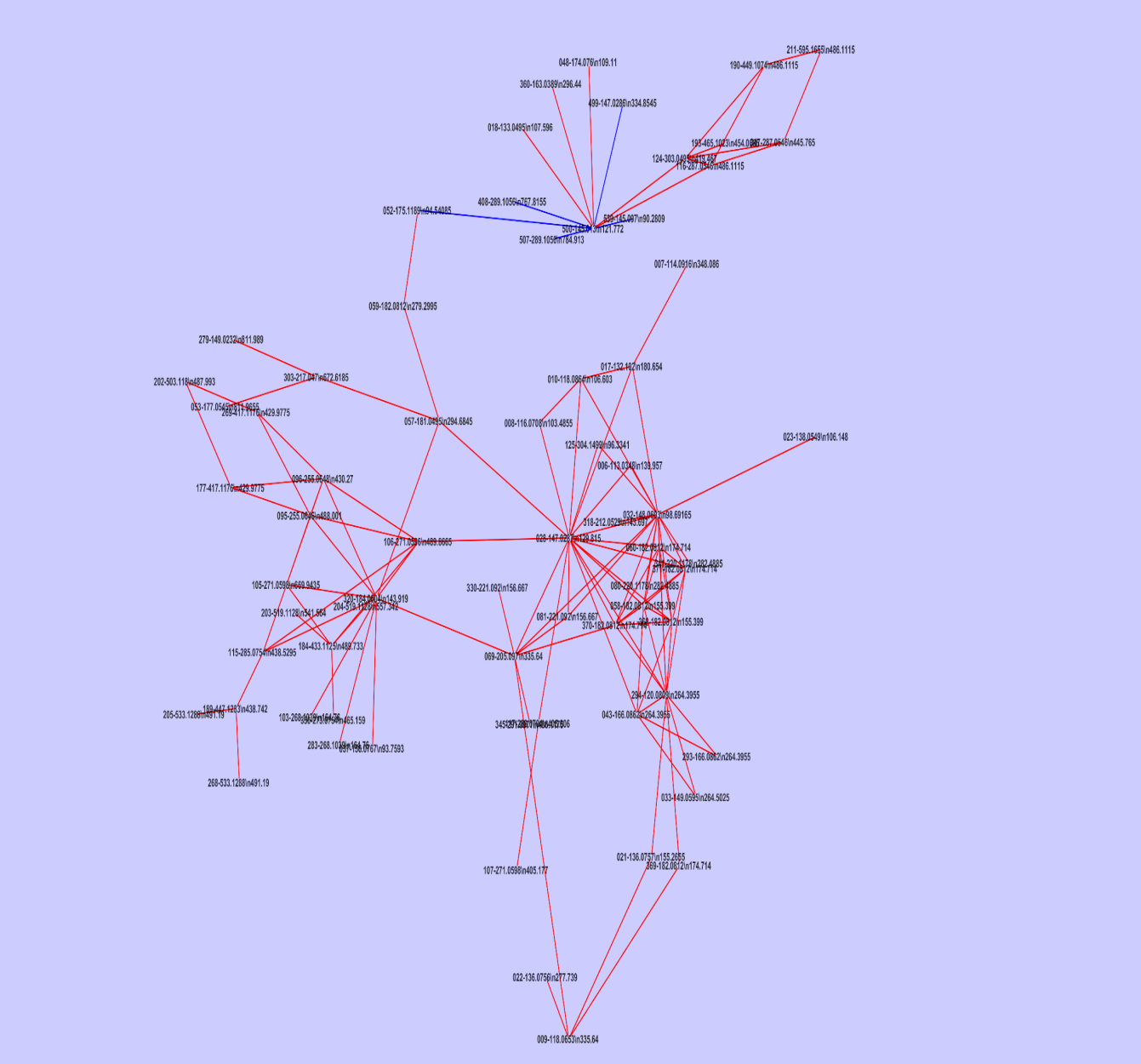
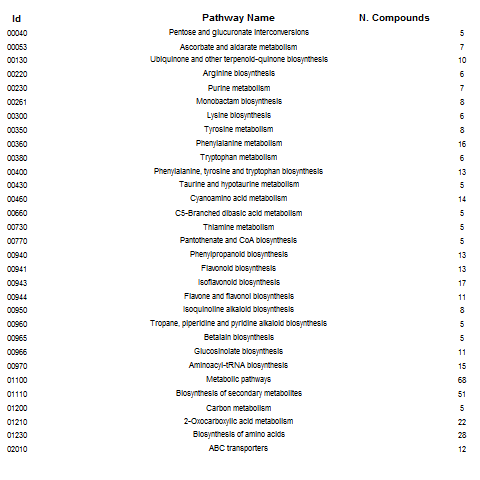
**Supplementary** **Fig. 3**: Cloud plot generated by XCMS for negative ion mode

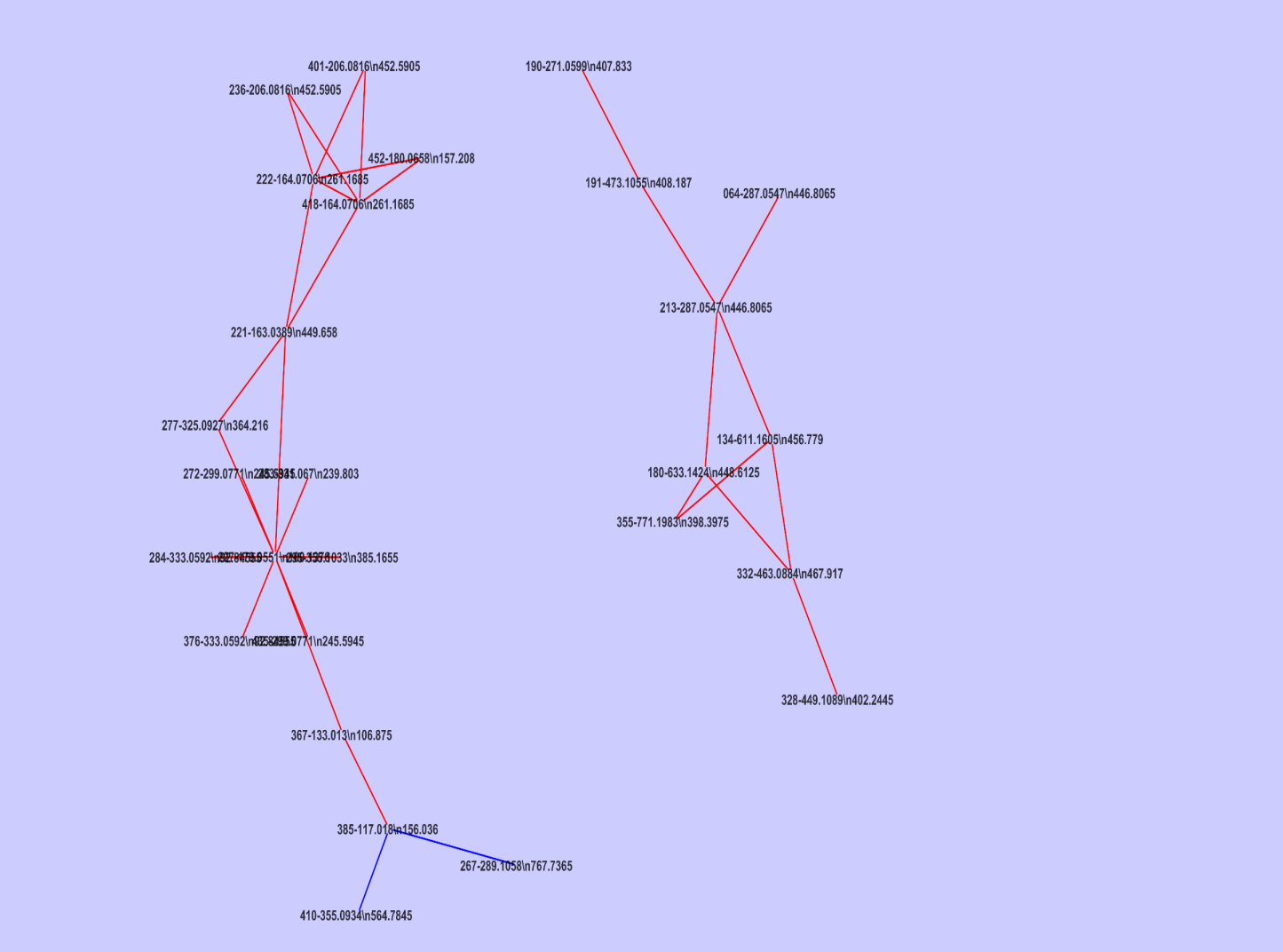
1. **Variety 1 - NRC119**

** **

1. **Variety 2 - JS335**

** **

1. **Variety 3 - JS7105**

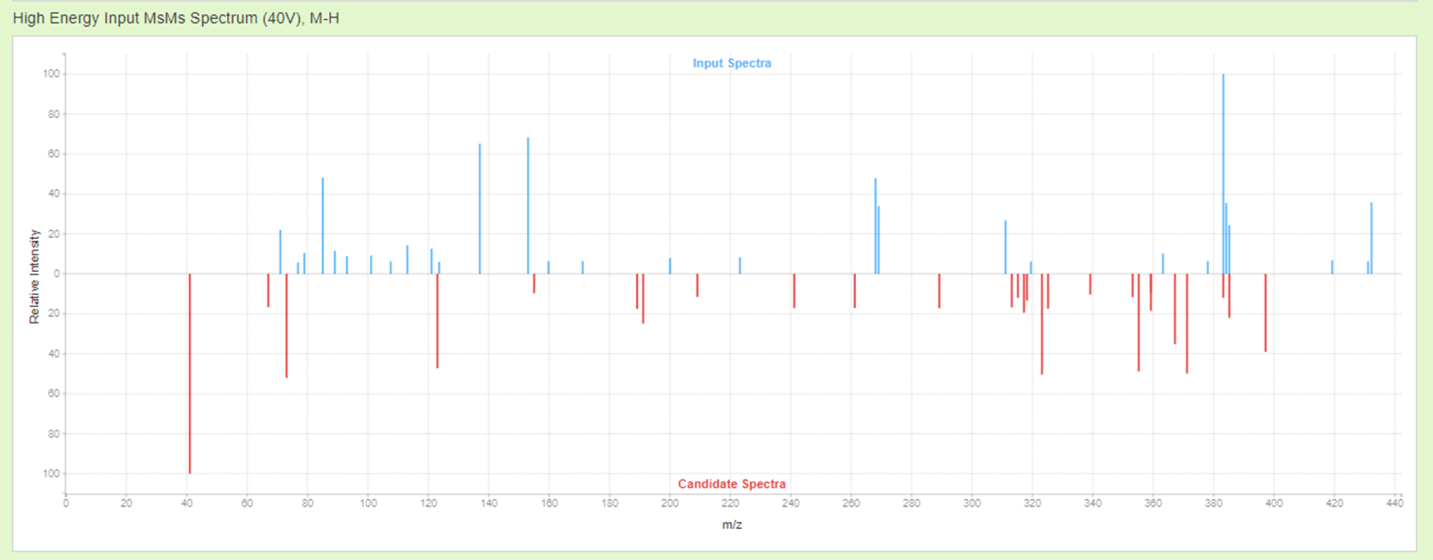
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1. **Variety 4 - JS9305**

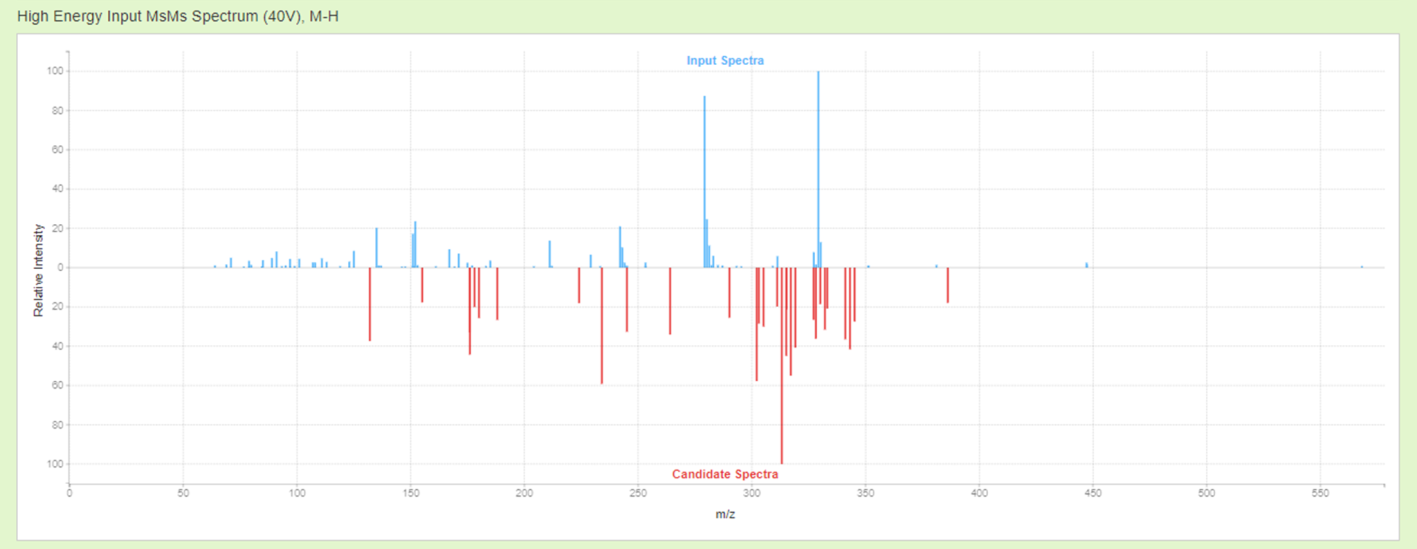
**Supplementary** **Fig. 4**: Metabolic pathway network with the list of pathway names and the number of molecules involved for four varieties of soybean (Retrieved from KEGG soybean pathways).



1. 1-Acetoxypinoresinol



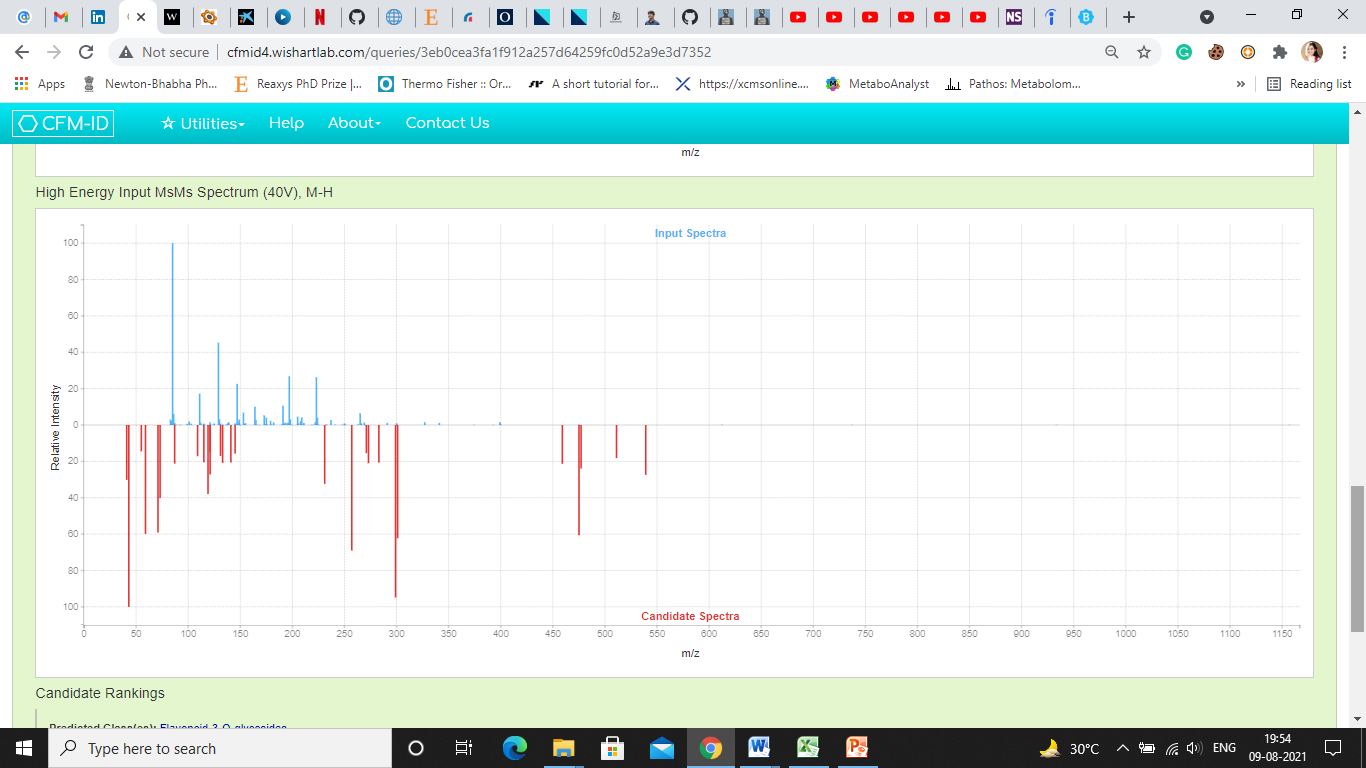
1. Cinegalline



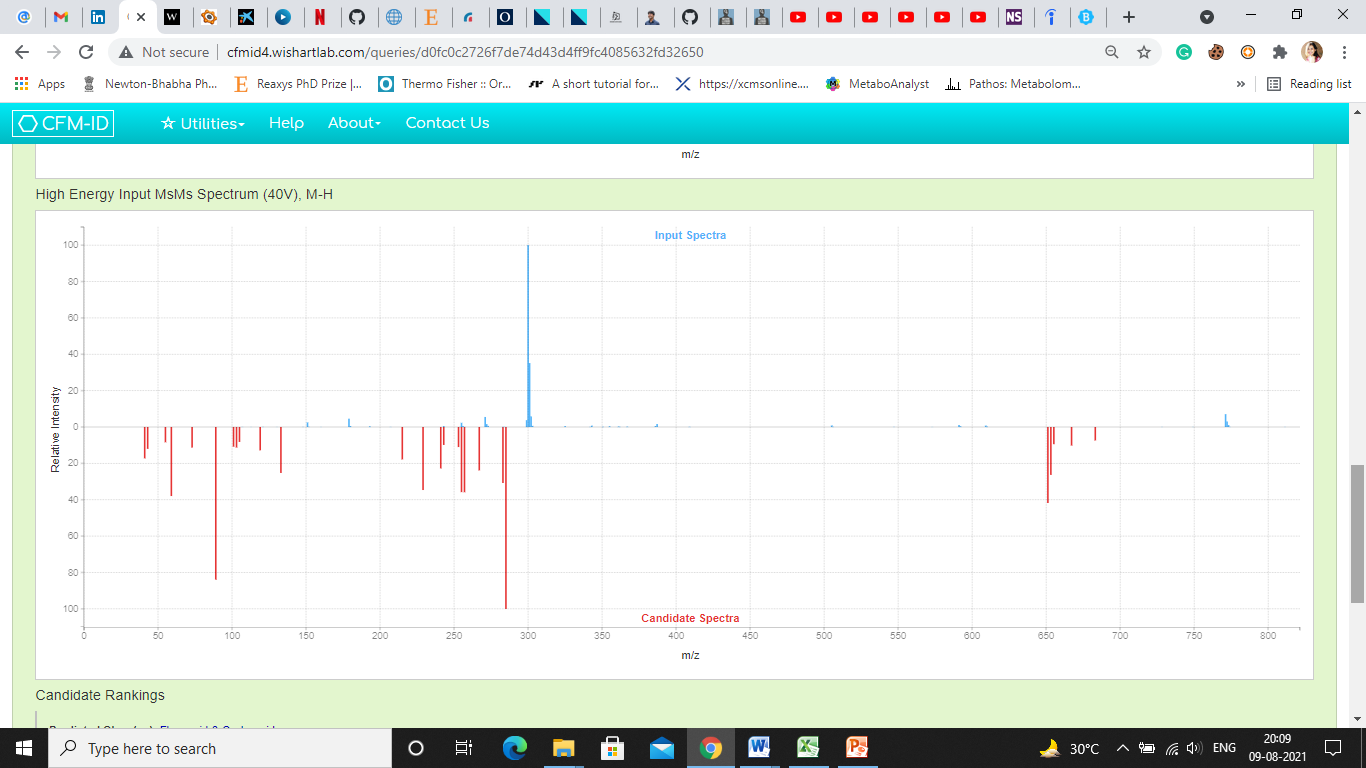
1. Lonchocarpenin



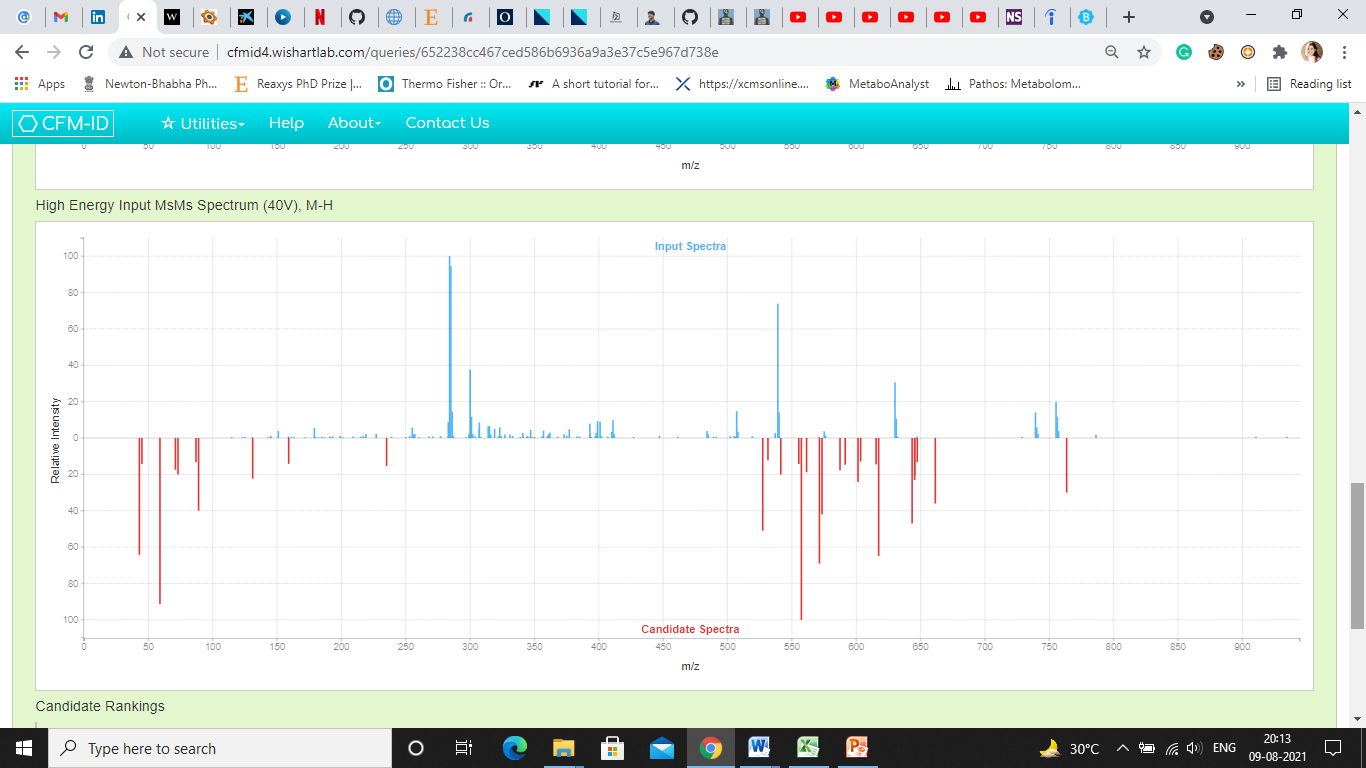
1. Decuroside III



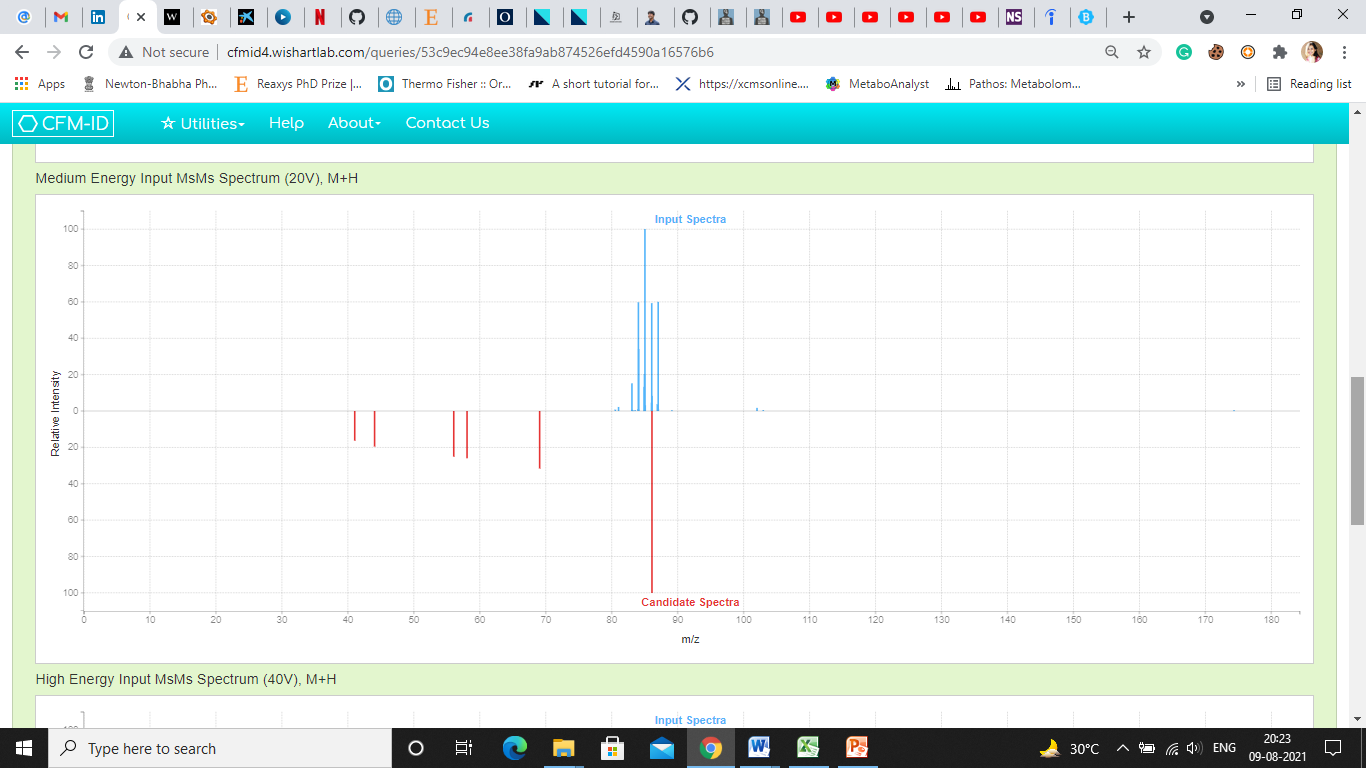
1. Quercetin 3-O-[beta-D-xylosyl-(1->2)-beta-D-glucoside]



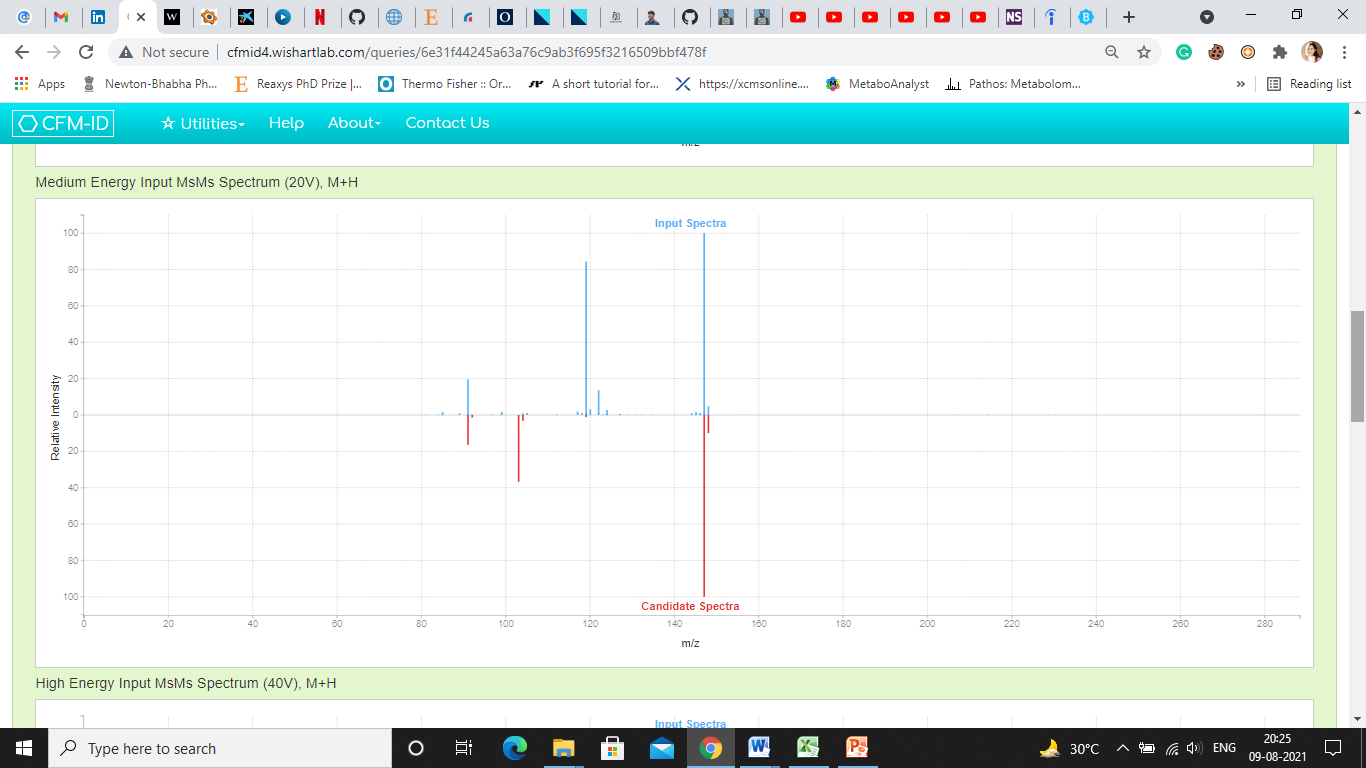
1. Kaempferol 3-sophorotrioside



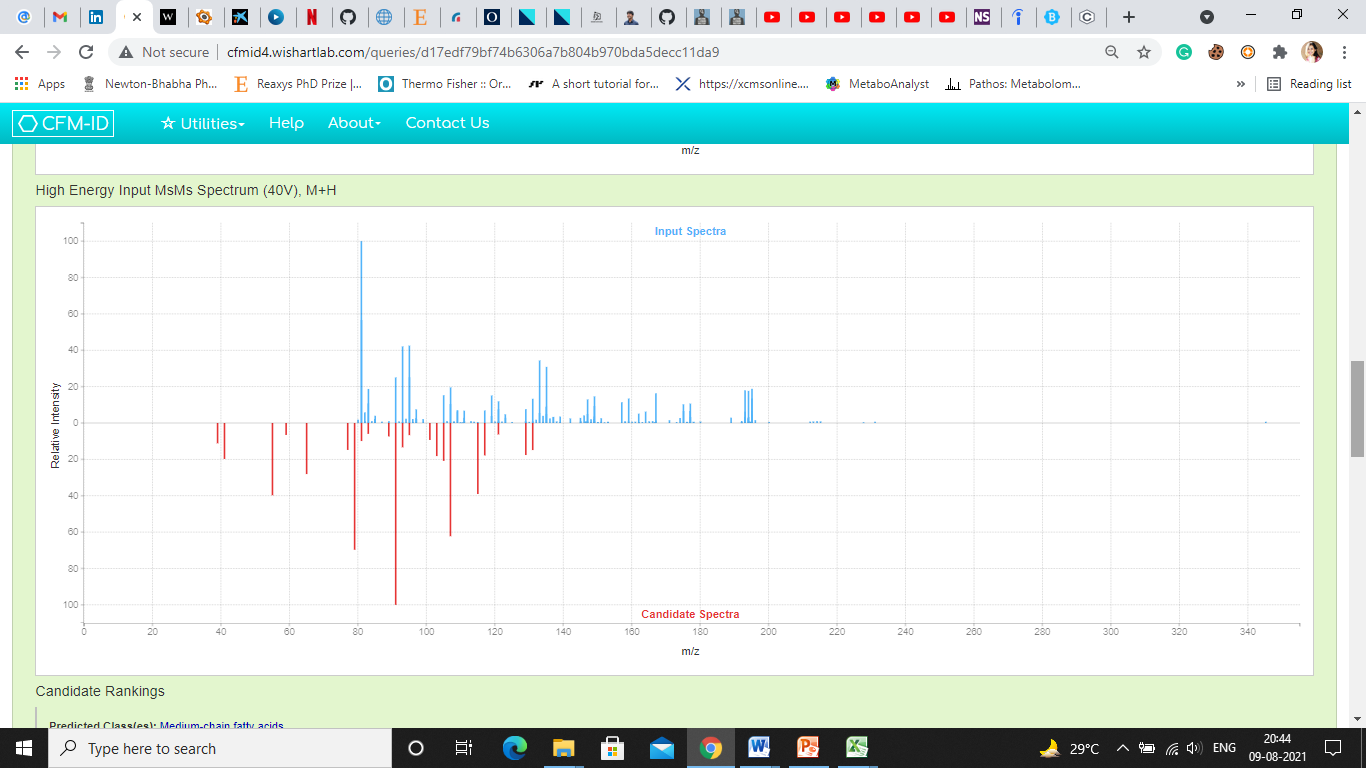
1. Yiamoloside B



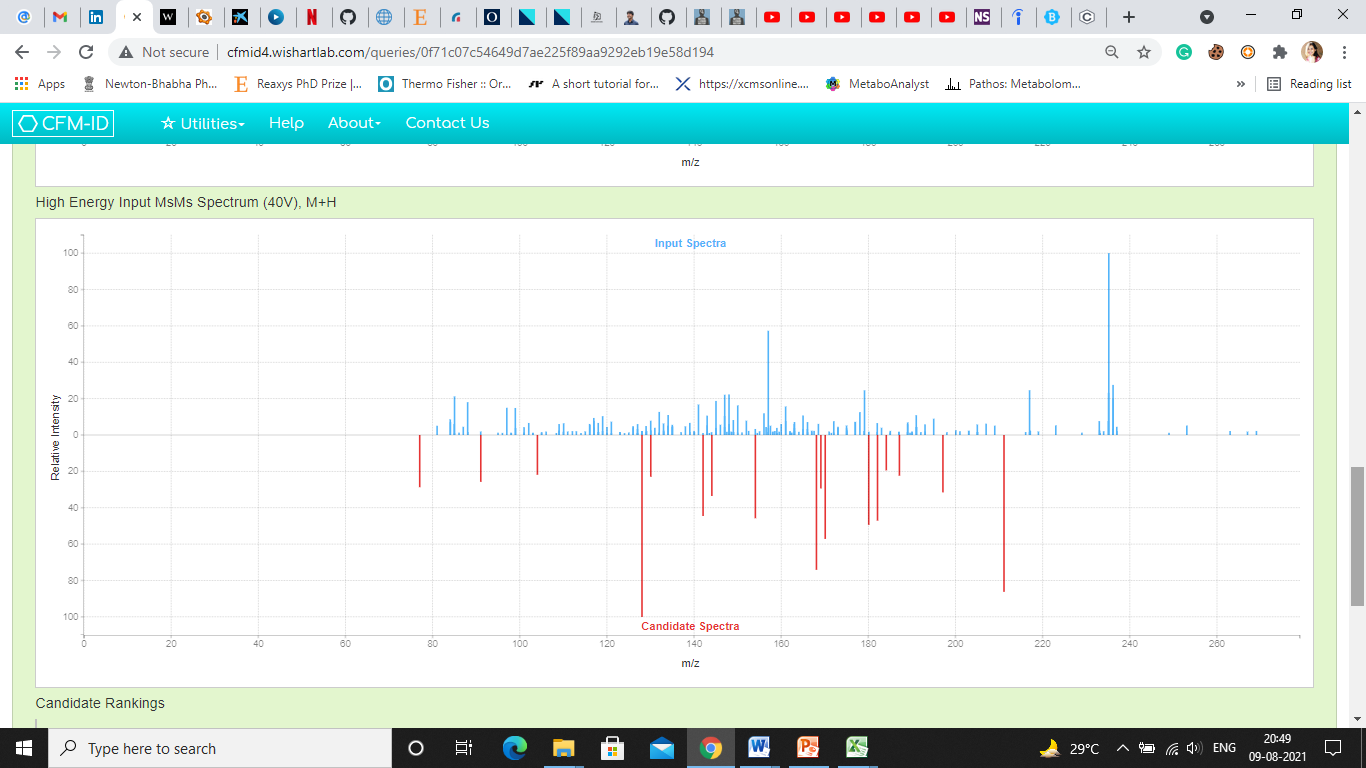
1. Piperidine



1. Coumarin



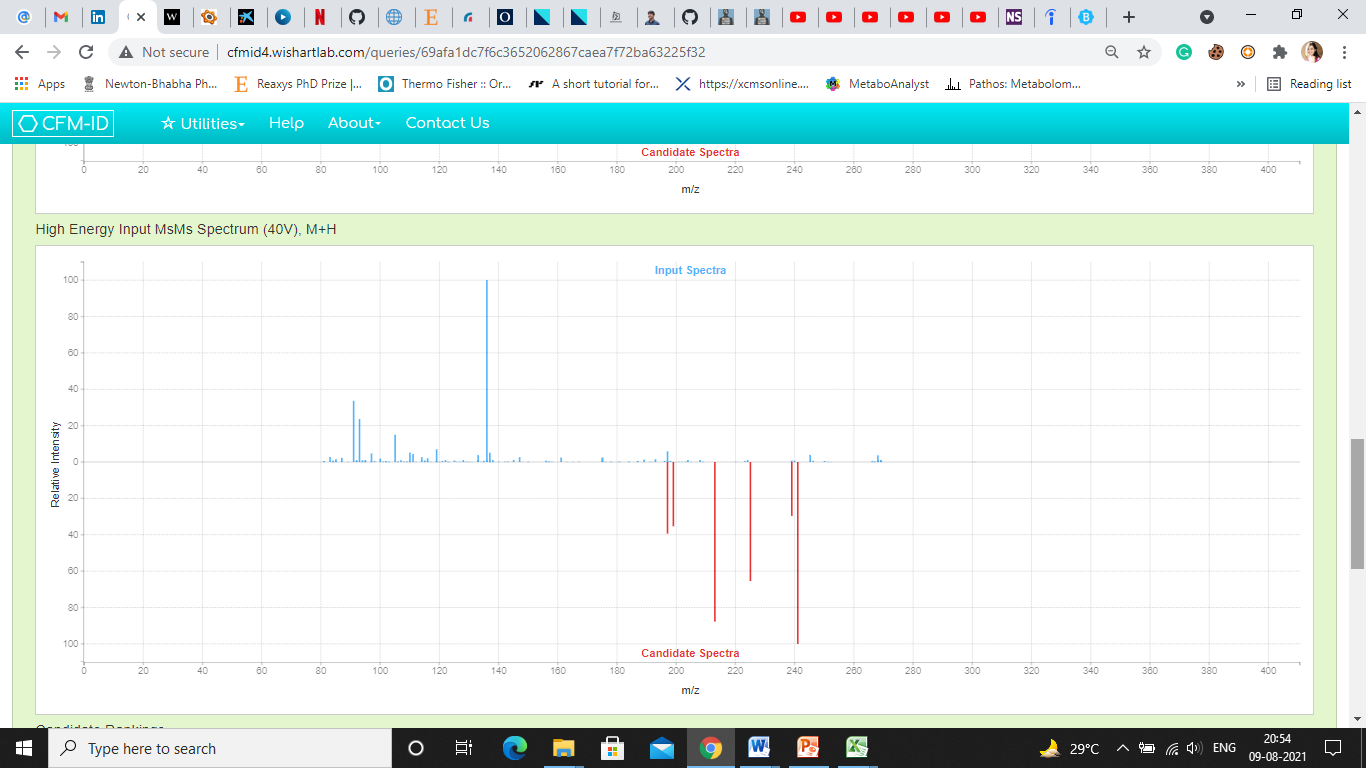
1. Zingerone



1. Lophophorine



1. Halfordinol



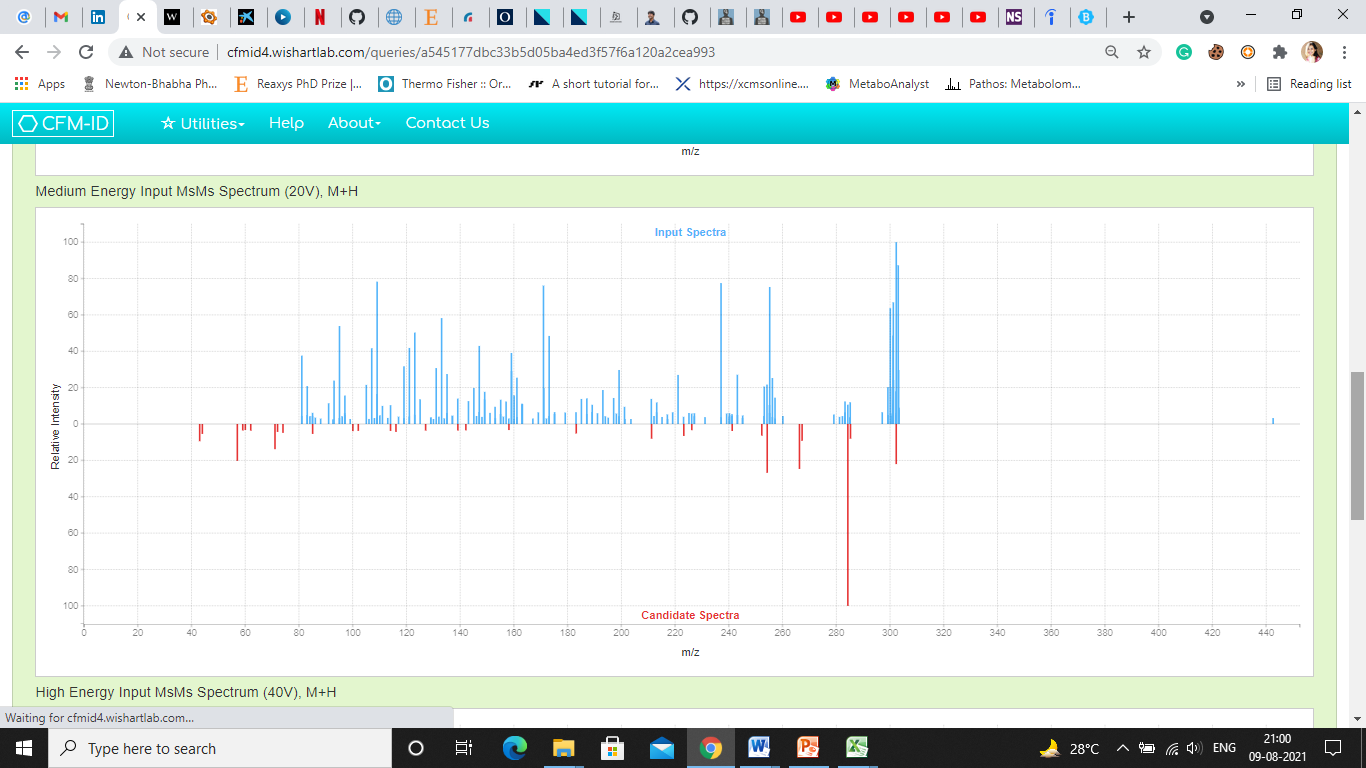
1. Coumestrol



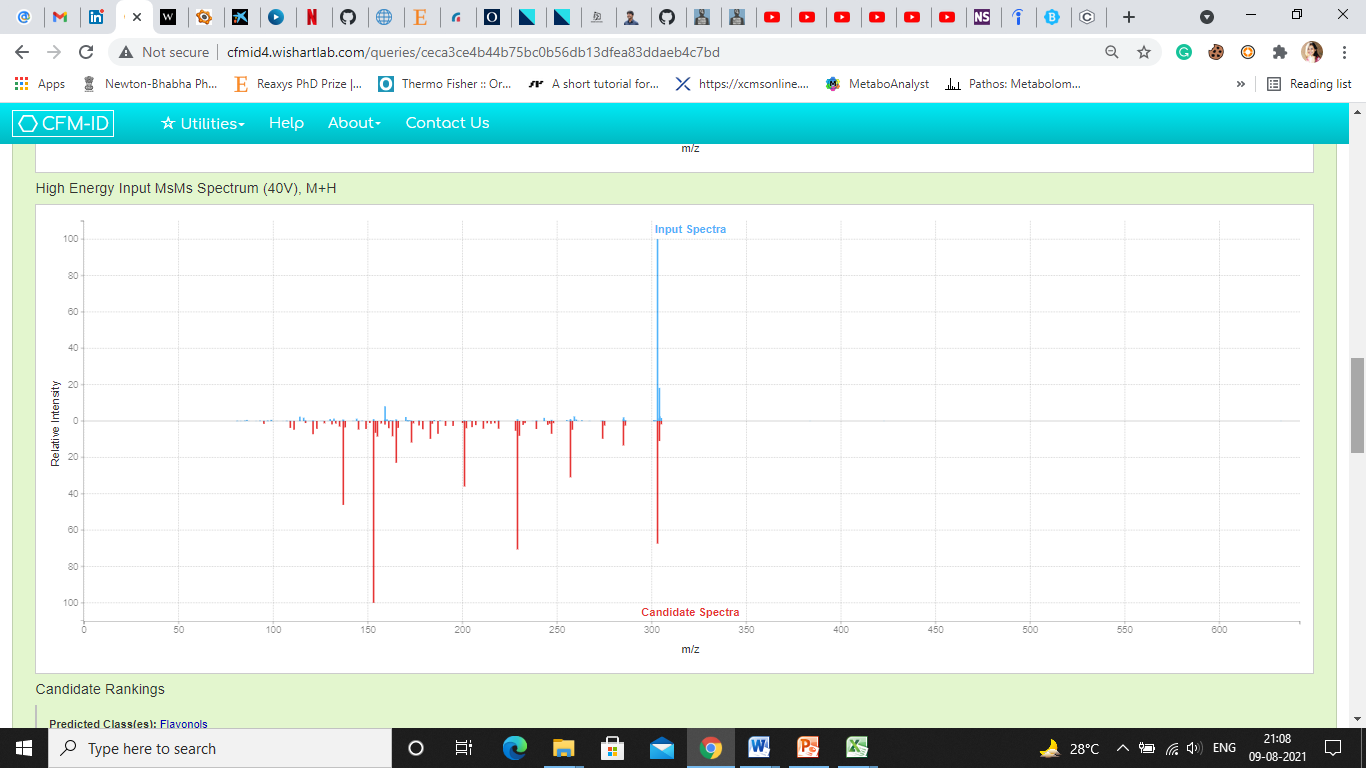
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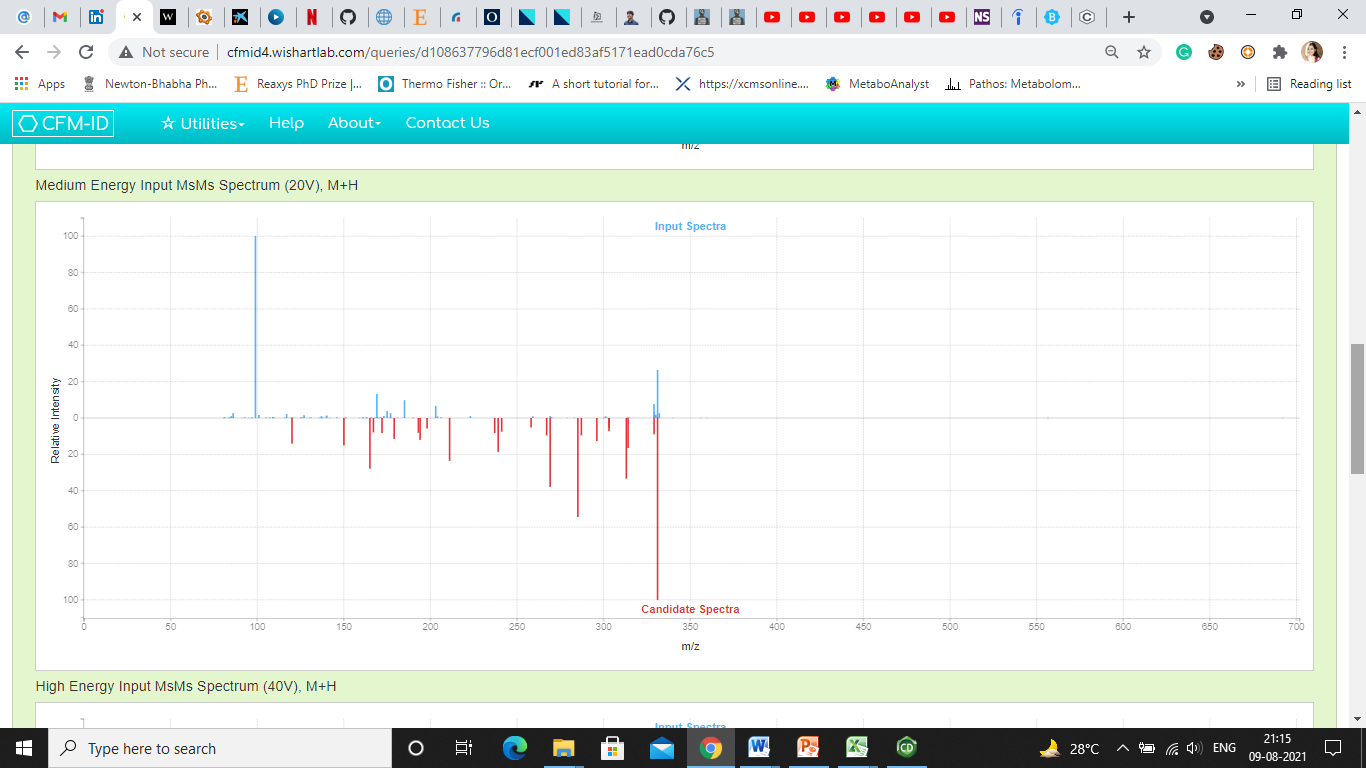
1. Aurantinidin



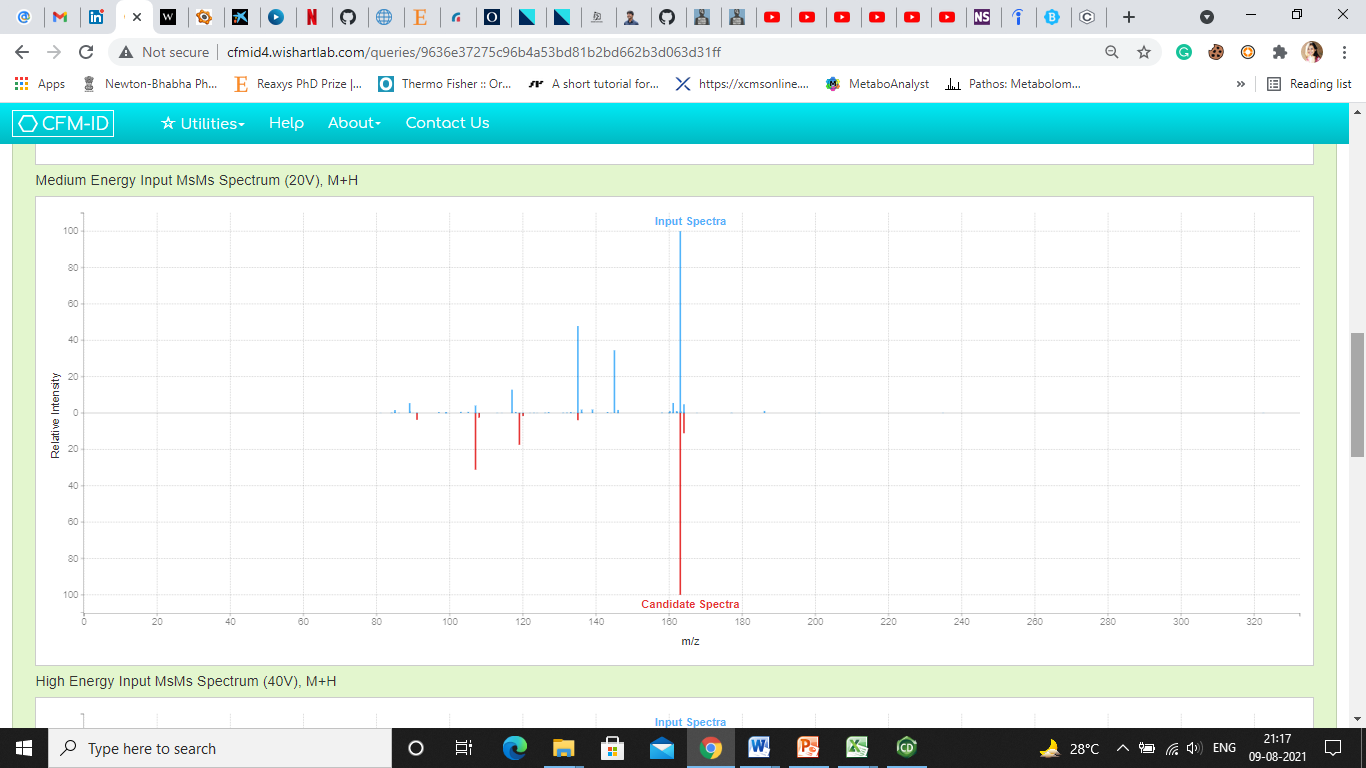
1. Sphinganine



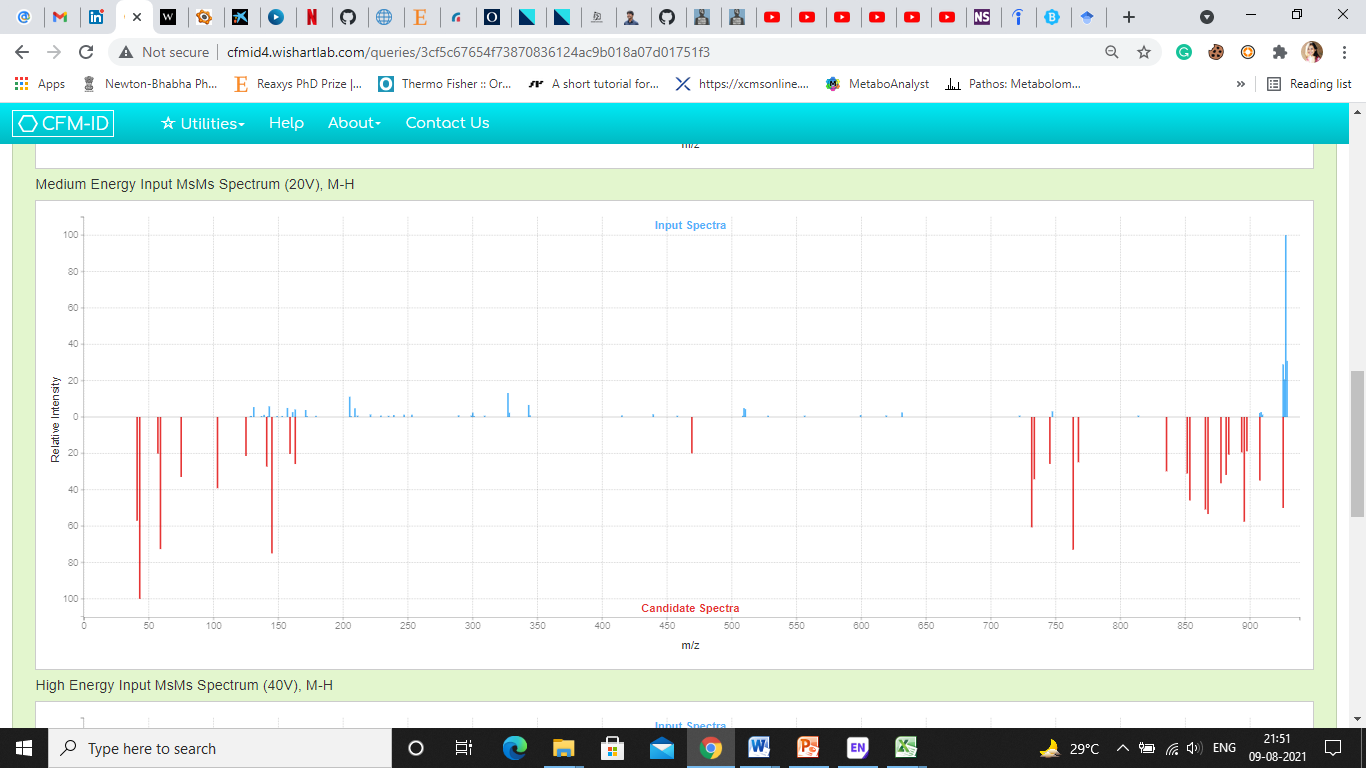
1. Quercetin



1. Miraxanthin-III



1. Umbelliferone



1. Saikosaponin BK1

**Supplementary** **Fig. 5**: MS/MS spectral similarities of 20 molecules compared to the *in-silico* spectra from CFM-ID webserver