A. Main MS2LDAvis screen

Type the motif number and press enter: 58   Previous Motif   Next Motif   Reset   Show labels

degree ≥ 0

Show Graph

Mass2Motif log(degree) vs. h-index

log(degree)

58

h-index

Overall frequencies

Within-motif frequencies

1. saliency(feature w) = freq(w) * [sum_t p(t | w) * log(p(t | w)/p(t))] for motif t. This measures how much information a feature conveys about the motifs. See Chuang et. al (2012) for more info.
2. Within each motif t, each feature w is ranked based on the conditional probability p(w|t)

Mass2Motif 58, degree=42, h-index=7
Ethylphenol substructure (e.g. resulting from Tyramine - MzCloud)

Mass2Motif 58 peak 24/42 (pid=25075 m/z=314.1589 RT=851.554)

91.0543 (C7H7)
121.0651 (C8H9O,loss_C7H15O5N)
53.0390 (C4H5)
93.0698 (C7H9)
103.0548 (C8H7)
152.1076 (C9H14ON,loss_C6H10O5)
314.1589 (C11H30ON3P2S)

Parent peak
Fragment peaks
M2M fragment
M2M loss

relative intensity

m/z

Show MS1 in new window   Prev MS1   Next MS1

Mass2Motif Feature Frequencies

fragment_121.06489
fragment_103.05448
fragment_93.06981
fragment_53.03888
fragment_91.05413
fragment_152.10755
loss_68.02601
fragment_T38.05067
fragment_166.12292
fragment_95.04936

Global Feature Frequencies

fragment_121.06489
fragment_103.05448
fragment_53.03888
fragment_91.05413
fragment_152.10755
loss_68.02601
fragment_T38.05067
fragment_166.12292
fragment_95.04936

B. Pop-up Network Graph

motif_290
motif_102
motif_221
motif_176
motif_195
motif_2
motif_262
motif_174
motif_260
motif_58
motif_275
motif_19
motif_156
motif_131
motif_129