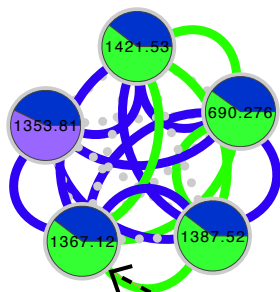


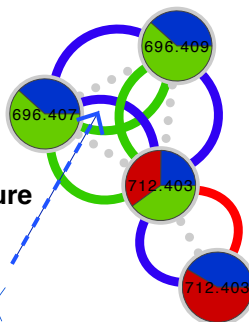
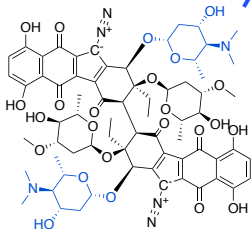
(a)



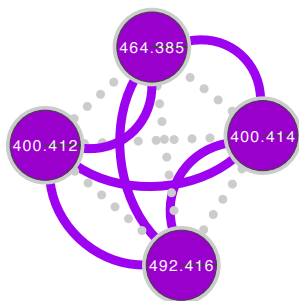
**[M+H]<sup>+</sup>  
GNPS library**

(b)

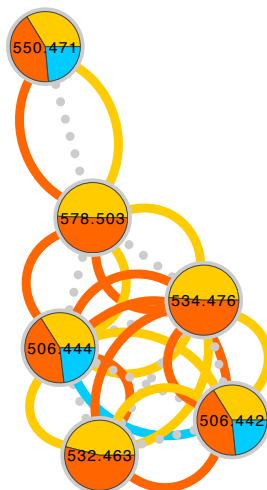
**MS2LDA  
substructure  
discovery**



(c)



(d)



- **M2M\_285**  
Aminosugar related
- **M2M\_283**
- **M2M\_183**
- **M2M\_276**
- **M2M\_66**
- **M2M\_35**  
Unknown fragment-based
- **M2M\_250**  
Unknown loss-based
- **M2M\_261**  
Unknown loss-based
- **M2M\_256**

● ● ● ● cosine