enter your report title here

deltaProtein peptideNet report

Wed Apr 04 16:44:07 UTC 2018 by potf
inspected deltaMass range: 0.0 - 2000.0 [Dalton]
number of pairs in deltaMassBase:1279

deltaMasses PTM fingerprint section

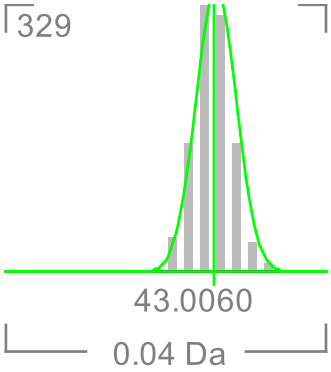
Gaussian fits to deltaMass pairs				
deltaMass	pairs	height	sigma	base
43.005964	1052	350.7	0.0024	0.5
99.066288	56	21.3	0.0021	-0.0

Origin of the deltaMasses PTM fingerprint: All detected deltaMasses in deltaMassBase were binned at bin width 0.01 Dalton. For bins with a count of more than 50, a Gaussian curve was fitted to another binned histogram of width 0.04 Dalton consisting of 20 bins i.e. with a bin width of 0.002 Dalton. The resulting parameters are deltaMass, height, base, and sigma. The number of pairs is derived from the curve under the fitted Gaussians.If there are more than 25 signals, the 25 most intense are reported.

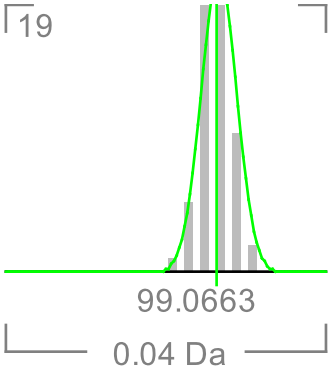
This approach is similar to the Mass Distance Fingerprint, see PUB-MED-ID : 17513179 (Click)

The following records have been used for this deltaProtein report:
C:\Users\potf\Downloads\example\example.mgf
That are 1 records in total.

experimental deltaMass:		43.005964 [Da]
sigma:0.0024 height:350.73 base:0.52 pairs: 1052		
modification	exact deltaMass [Da]	deviation [Da]
Carbamyl H C N O	43.005813665	+0.000151



experimental deltaMass:		99.066288 [Da]
sigma:0.0021 height:21.28 base:-0.01 pairs: 56		
modification	exact deltaMass [Da]	deviation [Da]
Amino V null	99.06841	-0.002122
NIPCAM H(9) C(5) N O	99.068413945	-0.002126



Protein identification by peptideNet analysis

The peptideNets on the following pages are colored according to this scheme:

peptideNet color table			
elemental composition	deltaMass	name	color
H O3 P	79.966331	phosphorylation	yellow
O	15.994915	oxidation	blue
H2 C	14.01565	methylation	green
H3 C2 N O	57.021464	carbamidomethylation	red
H C N O	43.005814	carbamylation	cyan
C2 H4	28.031300	Dimethylation	orange
weak delta signal	---	---	black

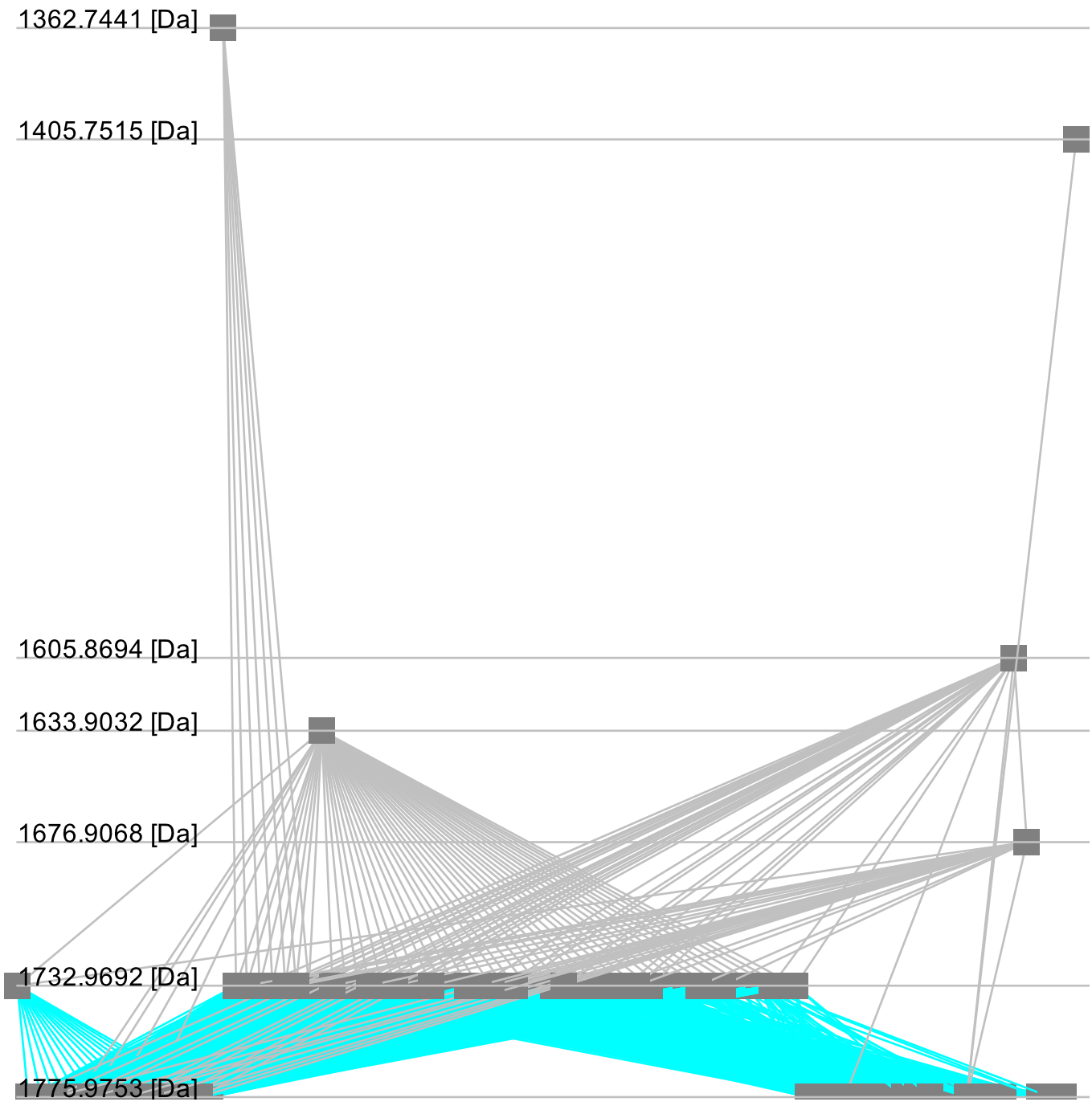
The peptideNets are orderd by the number of spectra they contain. At most 1000 nets are reported. In the graphical representation of a peptideNet, the y-axis corresponds to the weight of the peptide with mass decreasing upwards; the heaviest peptide is at the bottom of the plot. On te y-axis, the peptides are ordered by their spectrum id. If a spectrum has been annotated with an identification, it is marked with a circular symbol. The concept of peptideNets was first published in Journal of Chromatography B Volume 817, Issue 2, 25 March 2005, pages 225-230

http://dx.doi.org/10.1016/j.jchromb.2004.12.009 (Click)

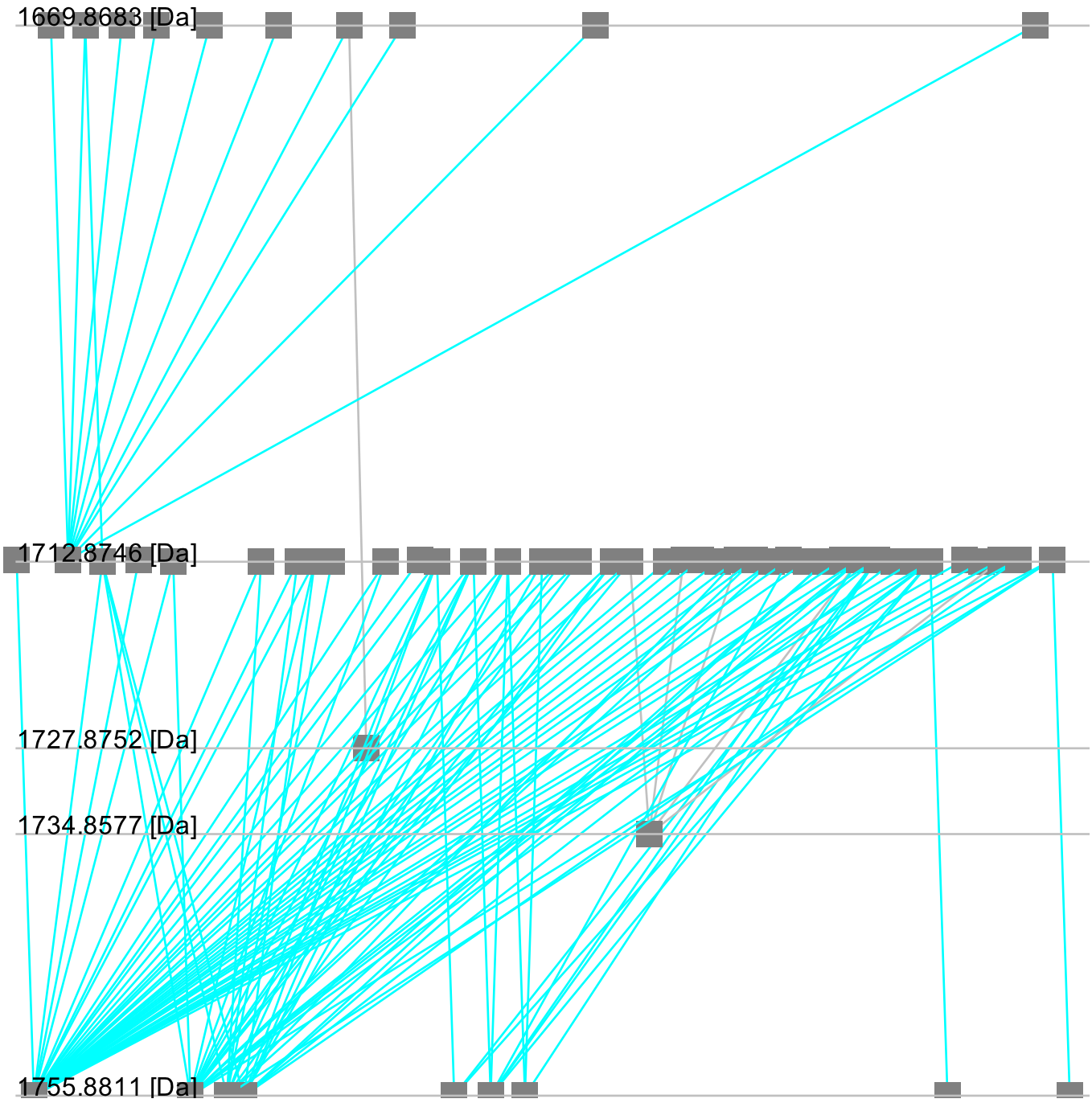
A more elaborate paper on peptideNets has recently been published: N. Bandeira, D. Tsur, A. Frank, and P.A. Pevzner: Protein identification by spectral network analysis. PNAS, 10 April 2007, vol. 104, no. 15, pages 6140-6145.

http://www.pnas.org/cgi/content/abstract/104/15/6140 (Click)

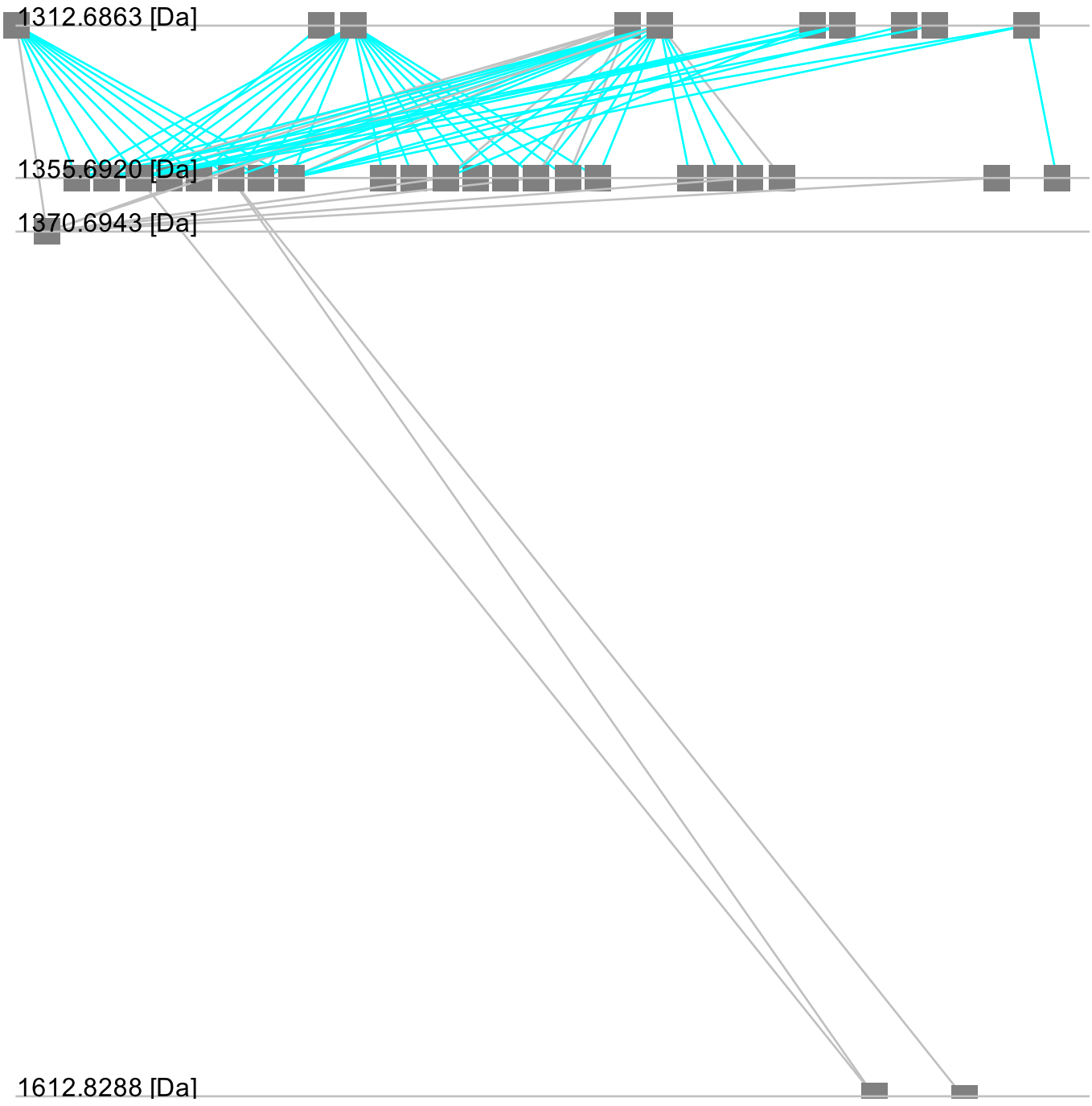
peptideNet ID : 27	
spectra in net : 88	pairs in net : 1008
mass width of peptideNet : 413.2352 [Da]	
minimal mass : 1362.7441 [Da]	maximal mass : 1775.9793 [Da]



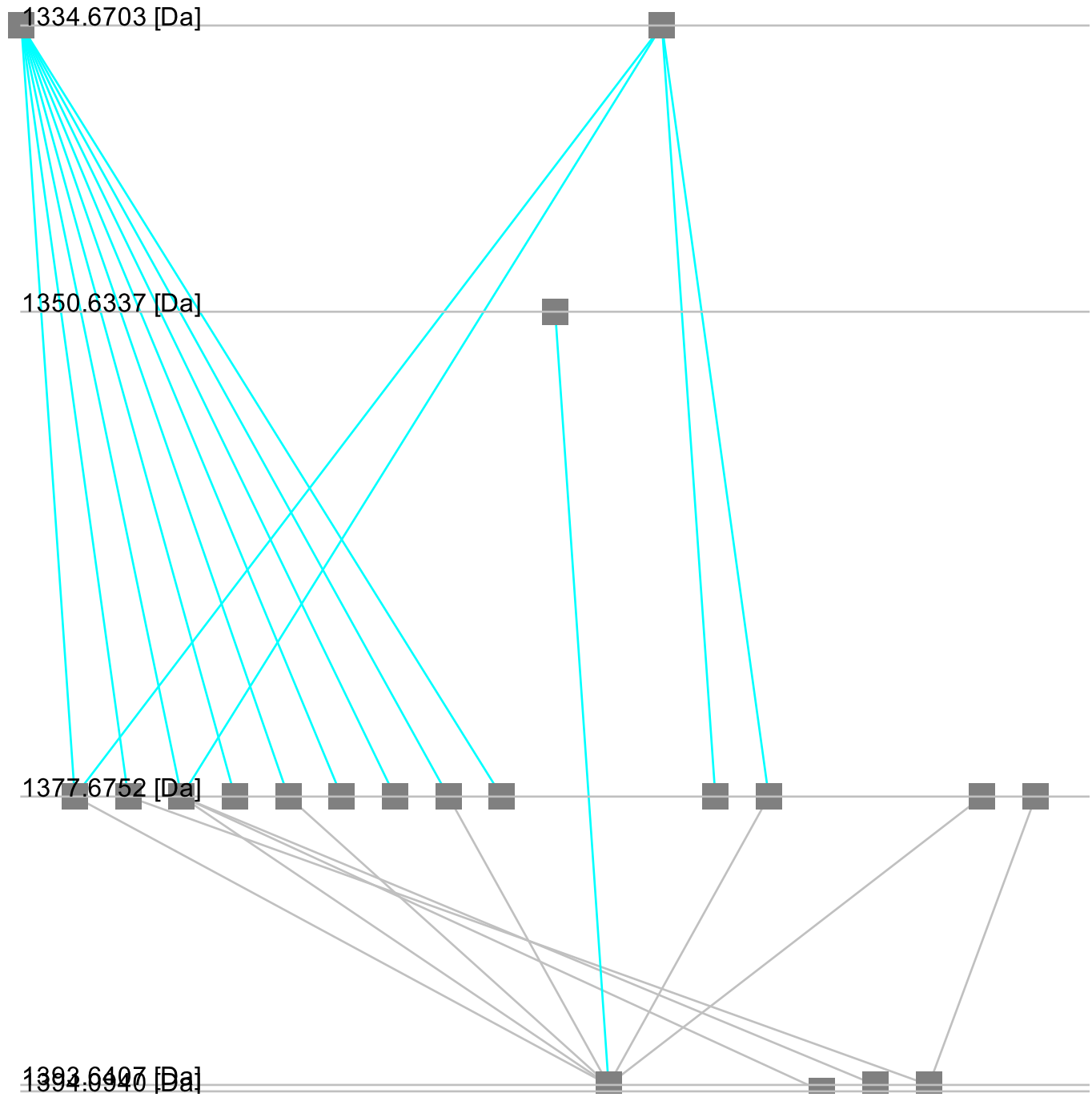
peptideNet ID : 24	
spectra in net : 61	pairs in net : 105
mass width of peptideNet : 86.0173 [Da]	
minimal mass : 1669.8656 [Da]	maximal mass : 1755.8830 [Da]



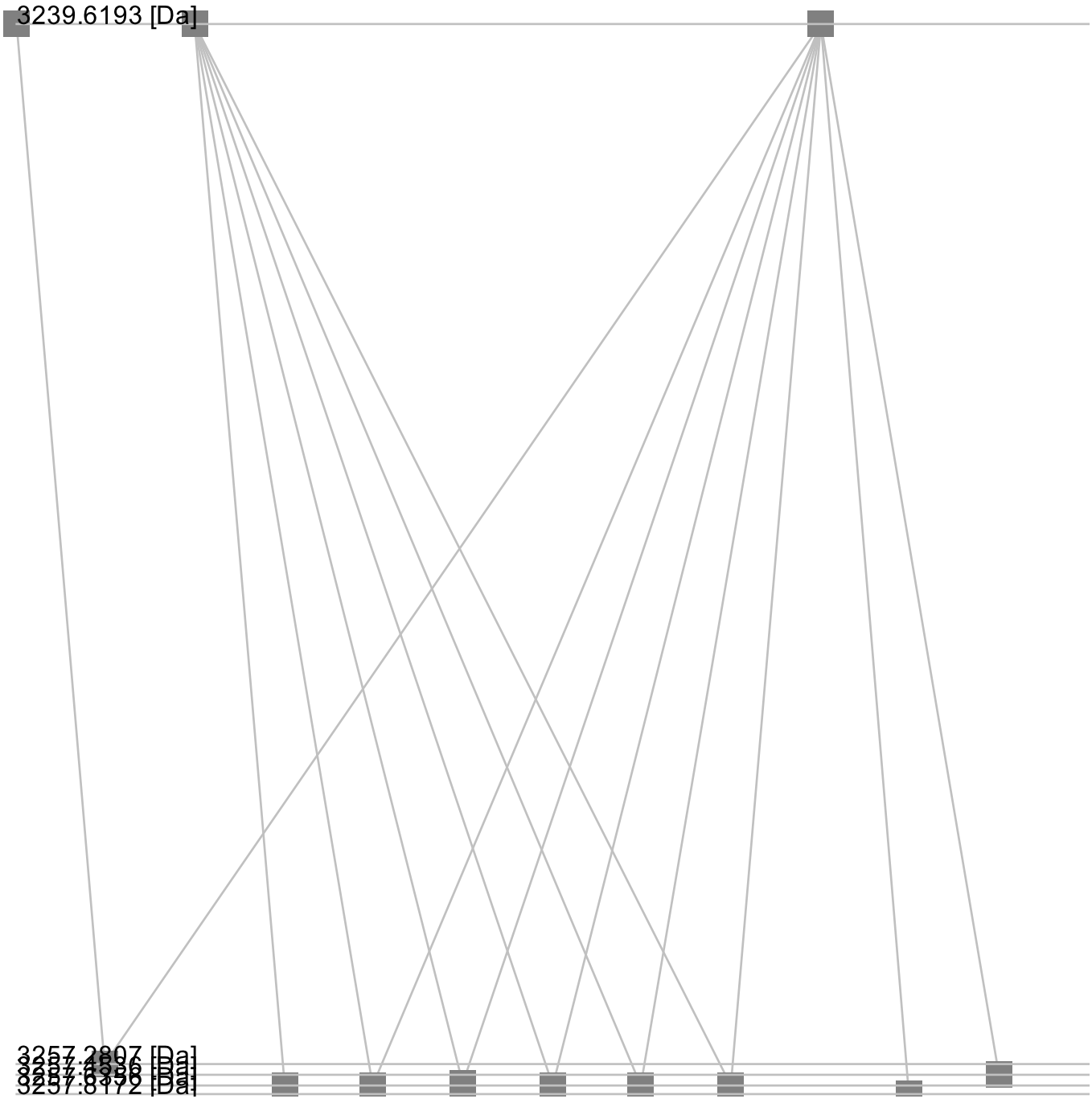
peptideNet ID : 6	
spectra in net : 35	pairs in net : 70
mass width of peptideNet : 300.1449 [Da]	
minimal mass : 1312.6841 [Da]	maximal mass : 1612.8290 [Da]



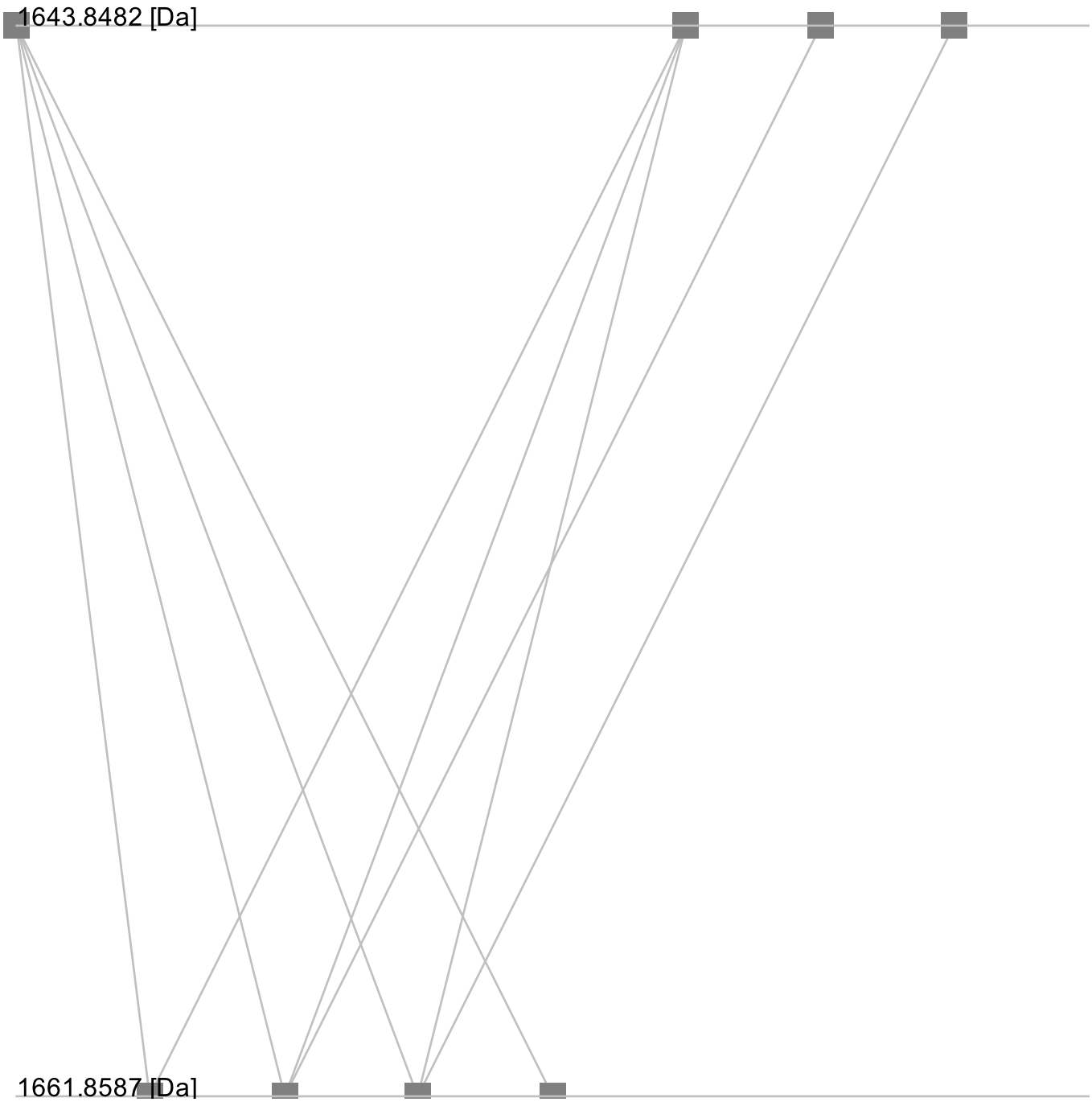
peptideNet ID : 4	
spectra in net : 20	pairs in net : 24
mass width of peptideNet : 59.4237 [Da]	
minimal mass : 1334.6703 [Da]	maximal mass : 1394.0940 [Da]



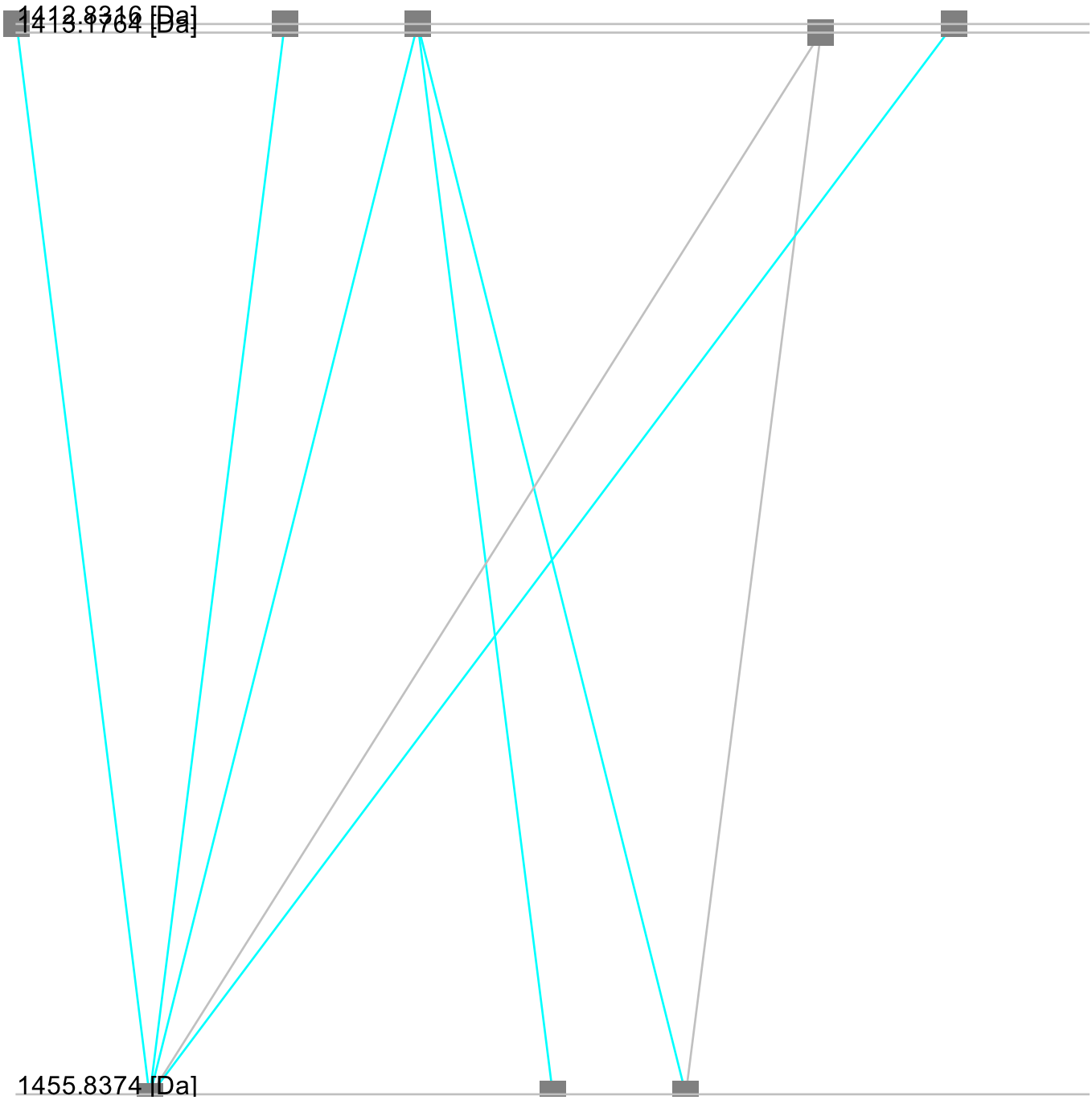
peptideNet ID : 23	
spectra in net : 12	pairs in net : 15
mass width of peptideNet : 18.1992 [Da]	
minimal mass : 3239.6180 [Da]	maximal mass : 3257.8172 [Da]



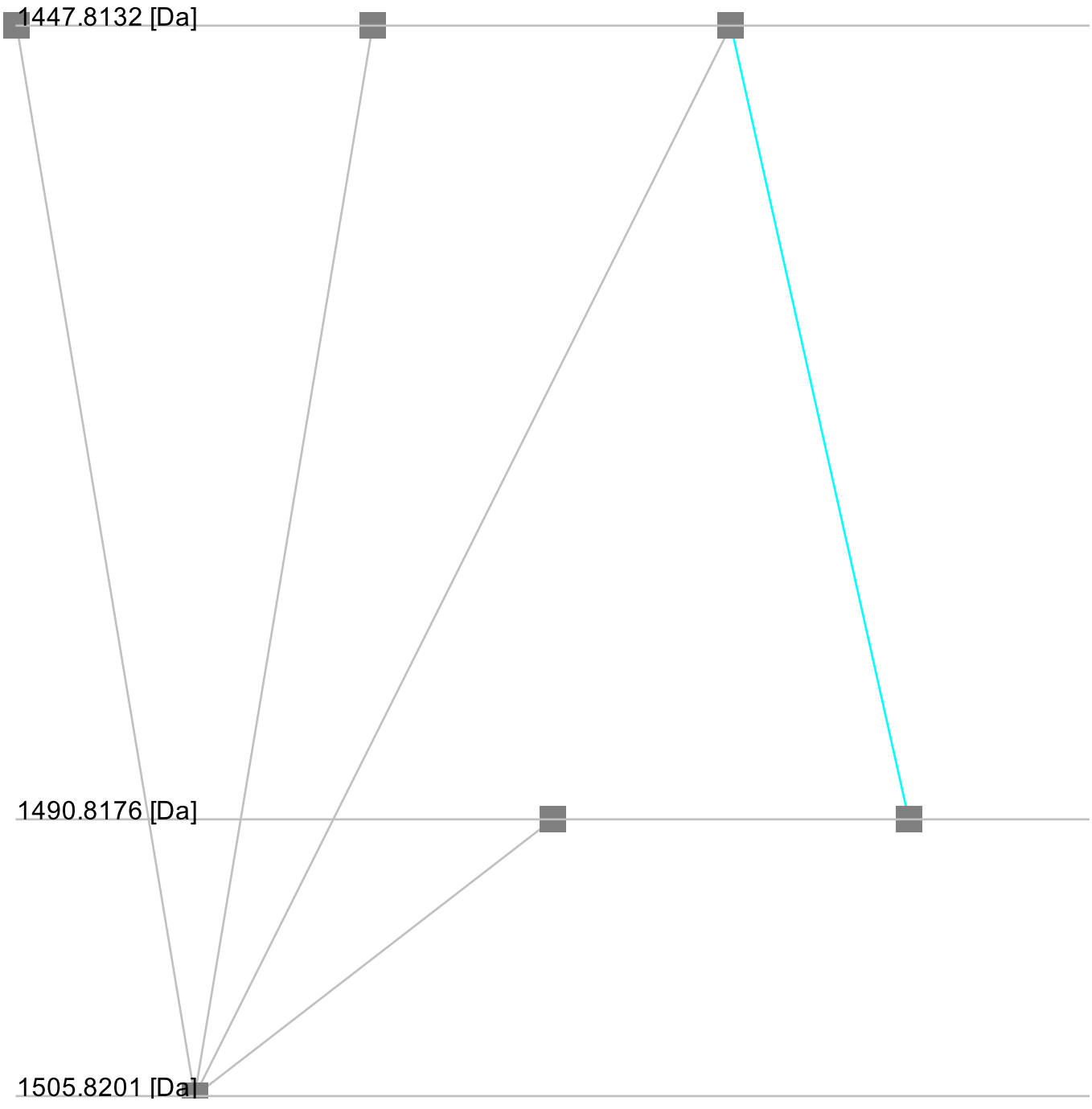
peptideNet ID : 12	
spectra in net : 8	pairs in net : 9
mass width of peptideNet : 18.0160 [Da]	
minimal mass : 1643.8438 [Da]	maximal mass : 1661.8598 [Da]



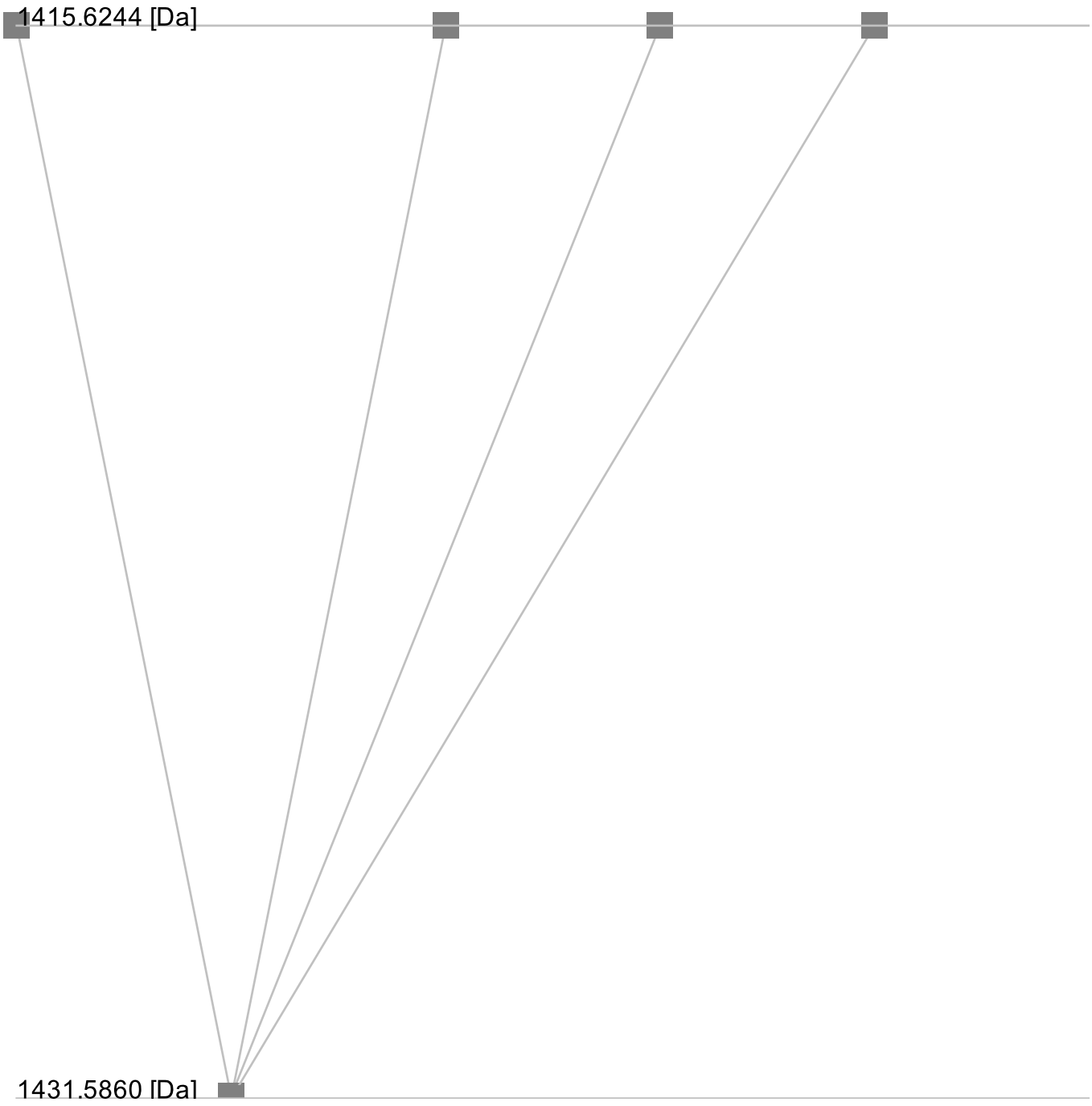
peptideNet ID : 19	
spectra in net : 8	pairs in net : 8
mass width of peptideNet : 43.0068 [Da]	
minimal mass : 1412.8306 [Da]	maximal mass : 1455.8374 [Da]



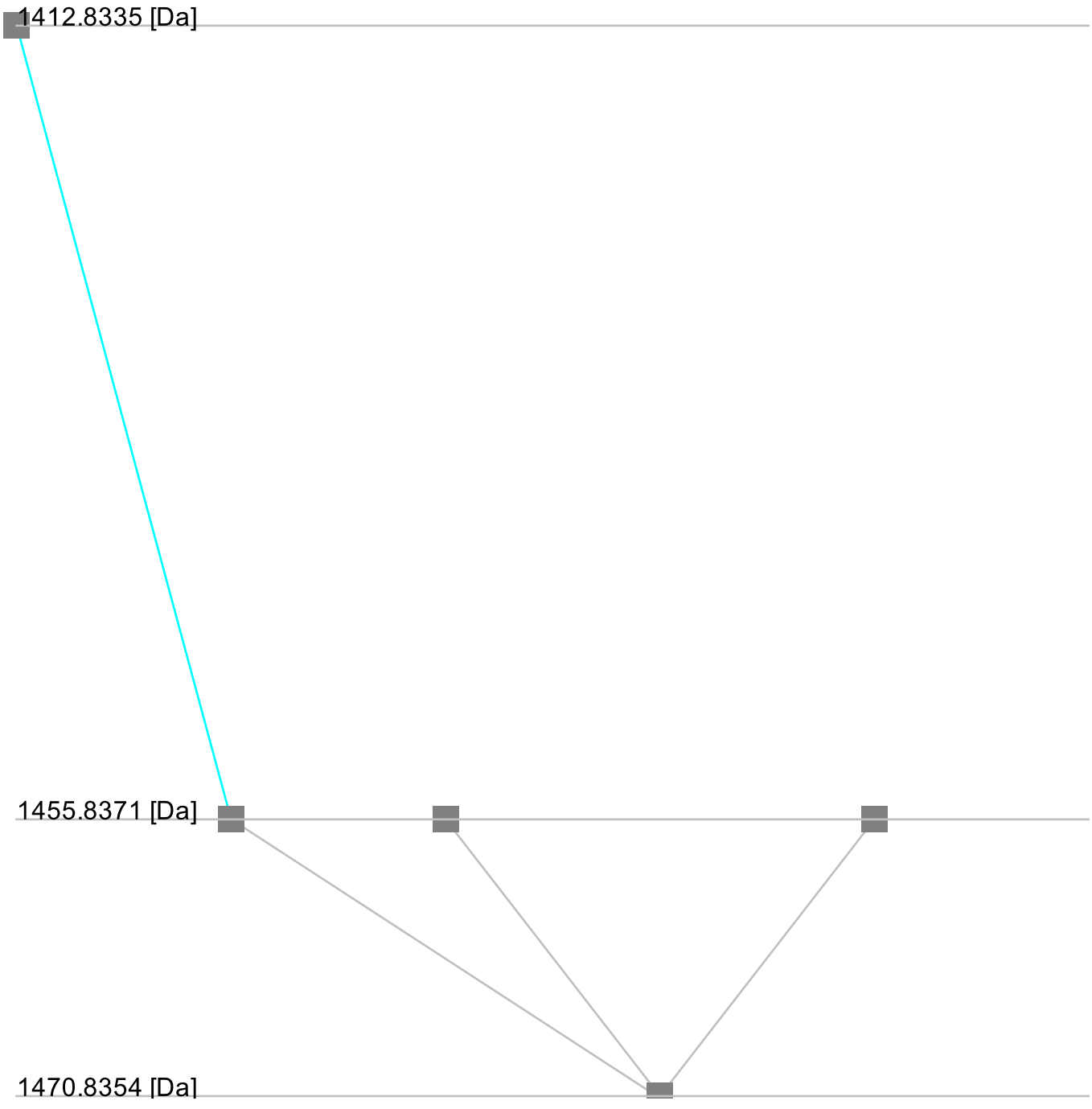
peptideNet ID : 14	
spectra in net : 6	pairs in net : 5
mass width of peptideNet : 58.0077 [Da]	
minimal mass : 1447.8124 [Da]	maximal mass : 1505.8201 [Da]



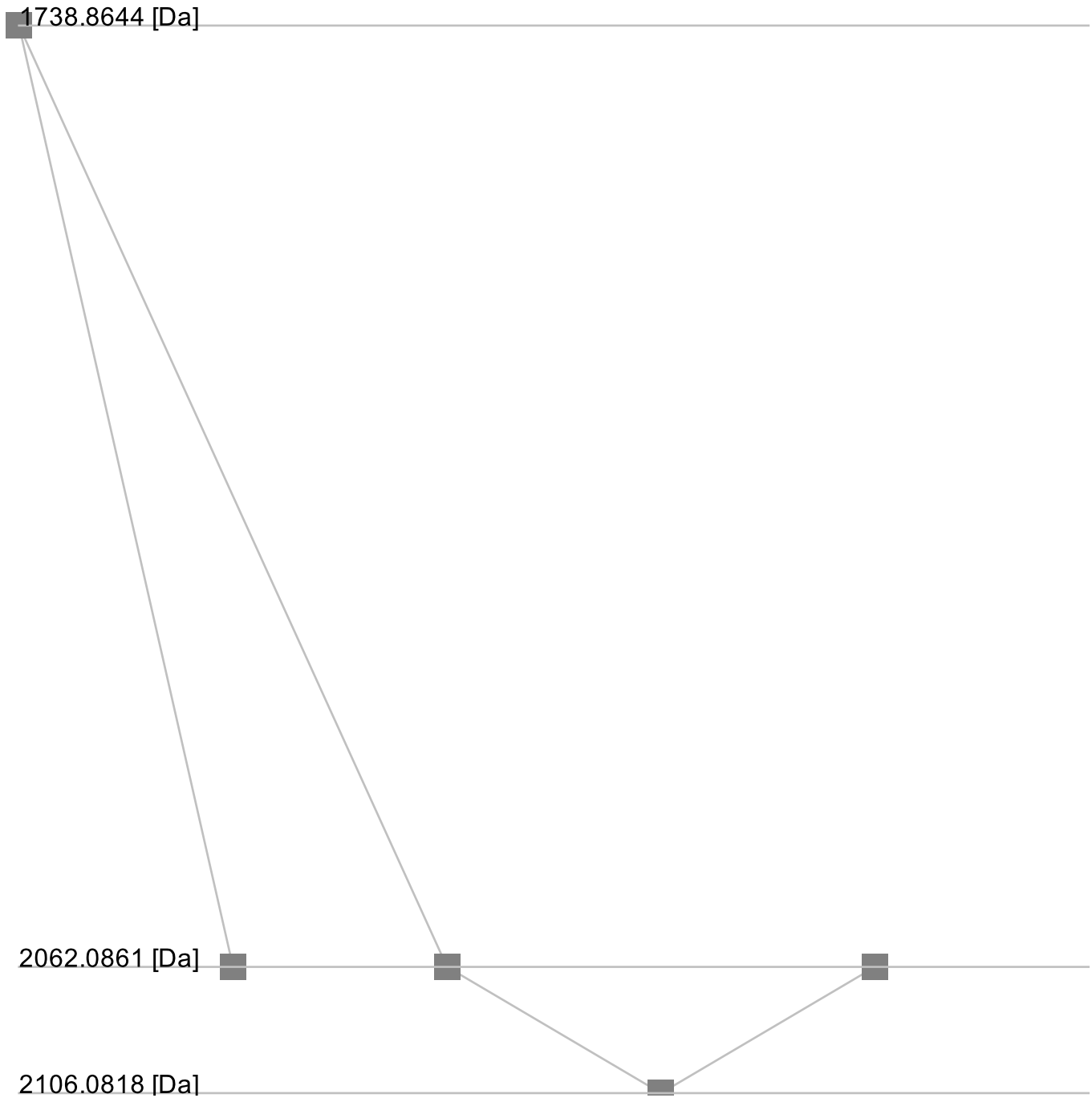
peptideNet ID : 8	
spectra in net : 5	pairs in net : 4
mass width of peptideNet : 15.9623 [Da]	
minimal mass : 1415.6237 [Da]	maximal mass : 1431.5860 [Da]



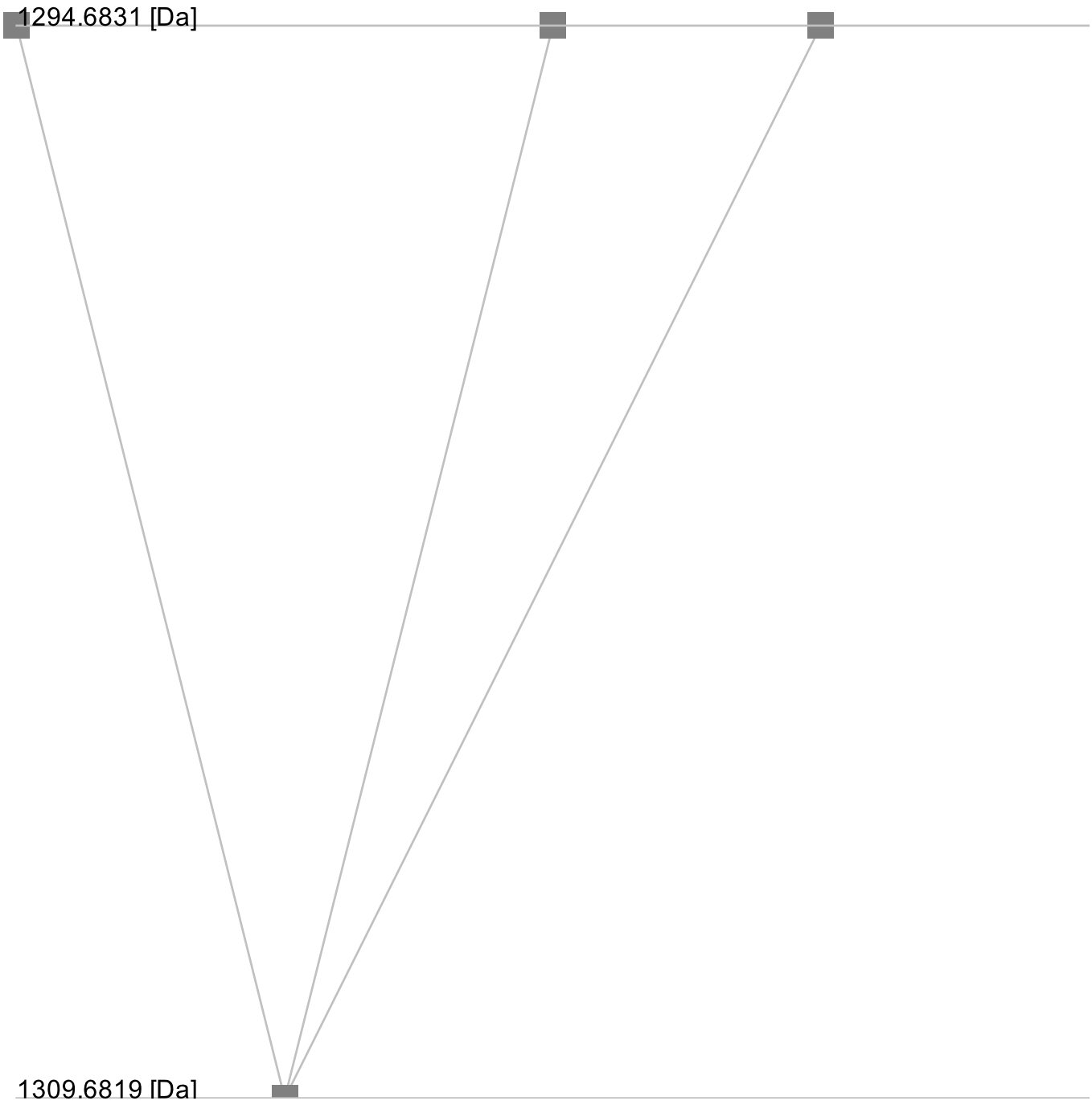
peptideNet ID : 17	
spectra in net : 5	pairs in net : 4
mass width of peptideNet : 58.0018 [Da]	
minimal mass : 1412.8335 [Da]	maximal mass : 1470.8354 [Da]



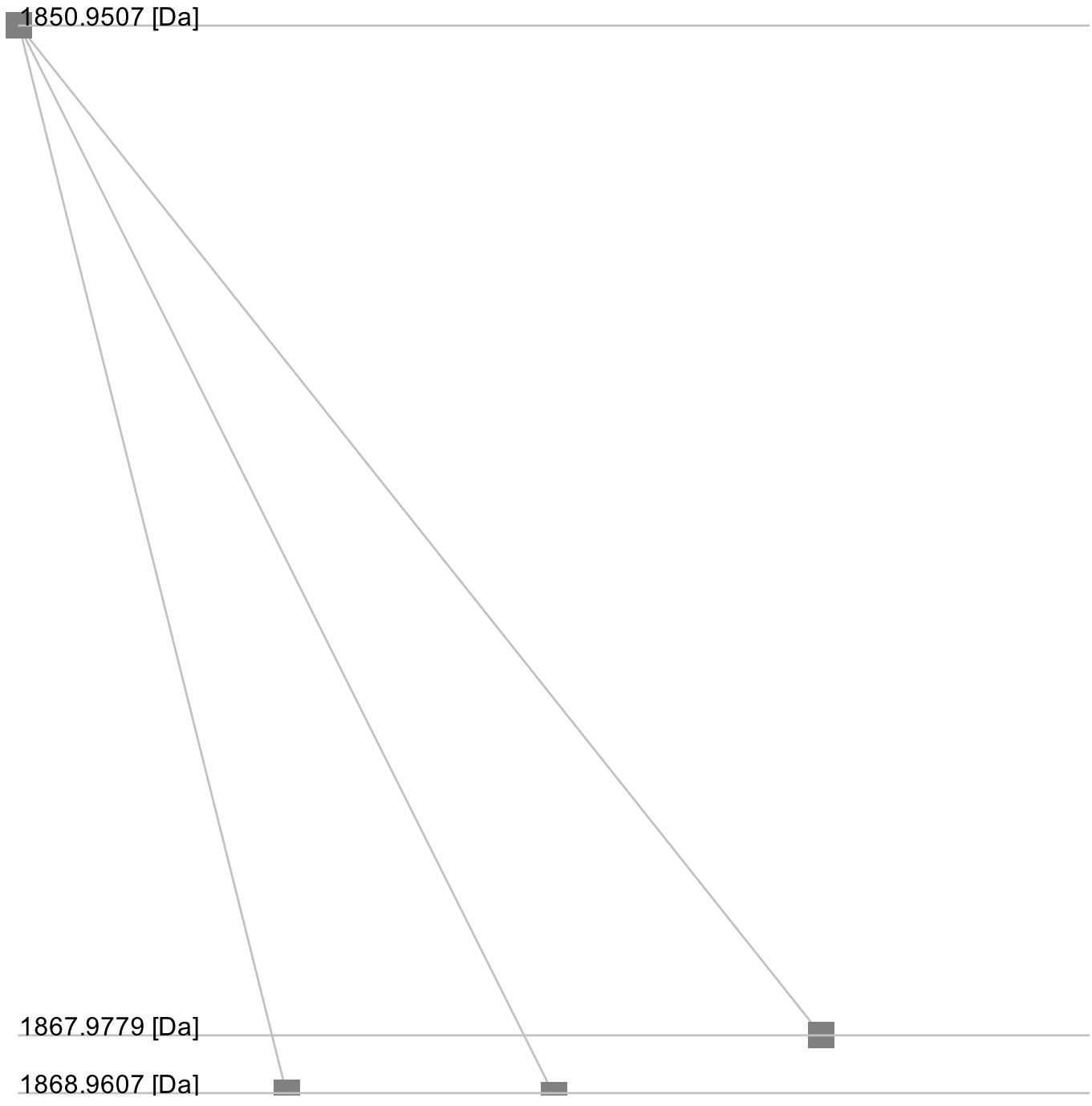
peptideNet ID : 18	
spectra in net : 5	pairs in net : 4
mass width of peptideNet : 367.2174 [Da]	
minimal mass : 1738.8644 [Da]	maximal mass : 2106.0818 [Da]



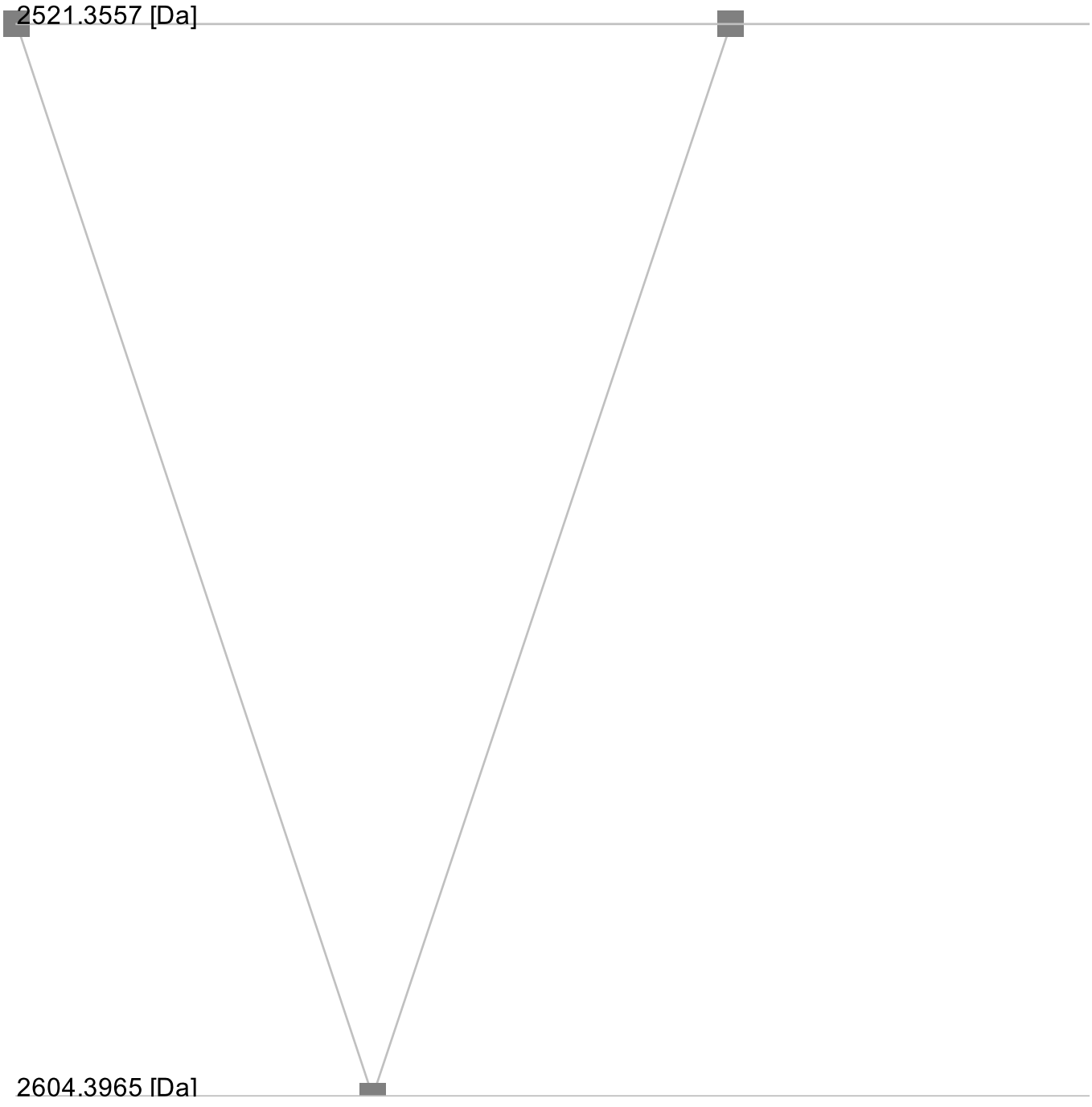
peptideNet ID : 16	
spectra in net : 4	pairs in net : 3
mass width of peptideNet : 14.9998 [Da]	
minimal mass : 1294.6822 [Da]	maximal mass : 1309.6819 [Da]



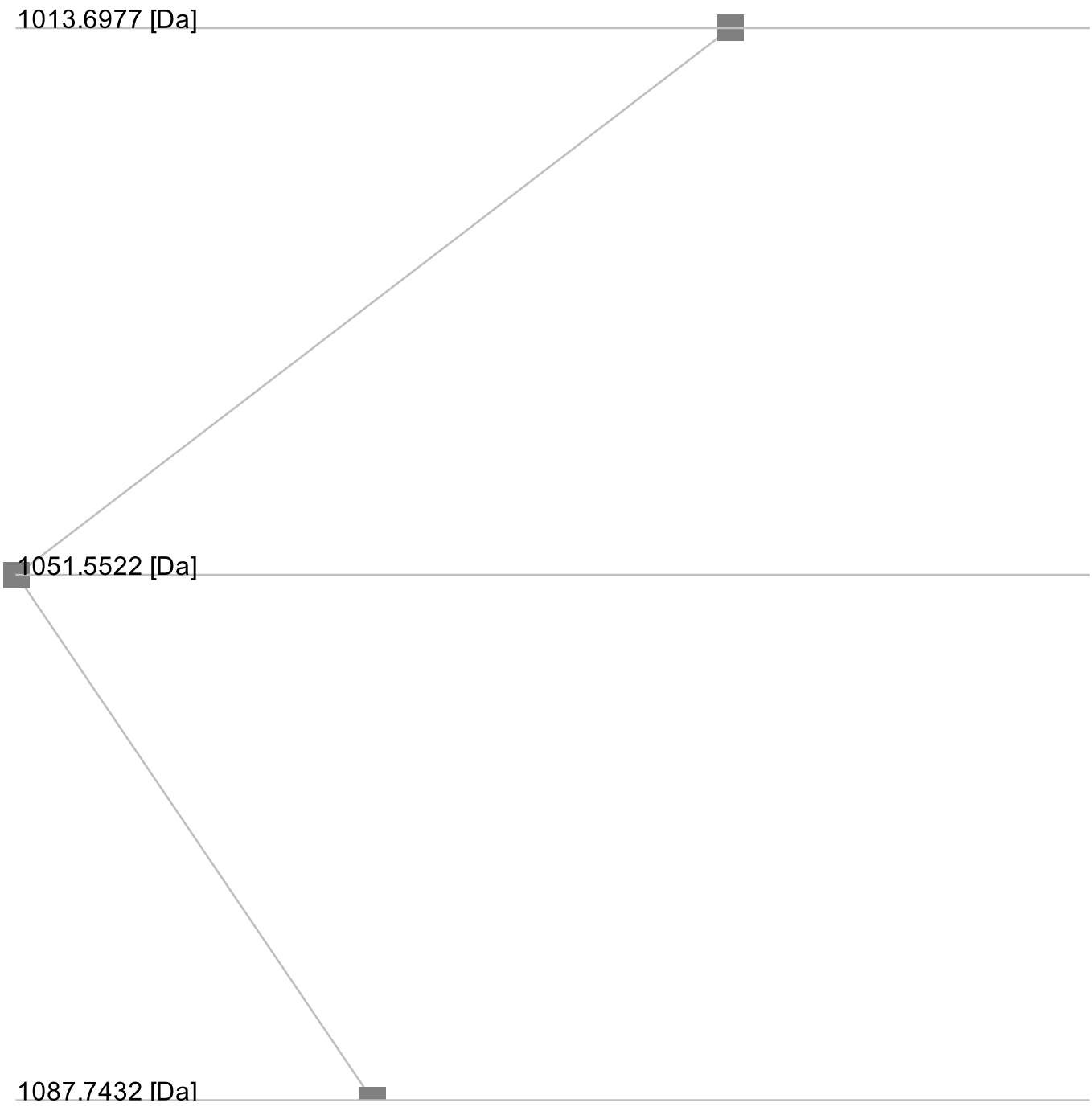
peptideNet ID : 26	
spectra in net : 4	pairs in net : 3
mass width of peptideNet : 18.0107 [Da]	
minimal mass : 1850.9507 [Da]	maximal mass : 1868.9615 [Da]



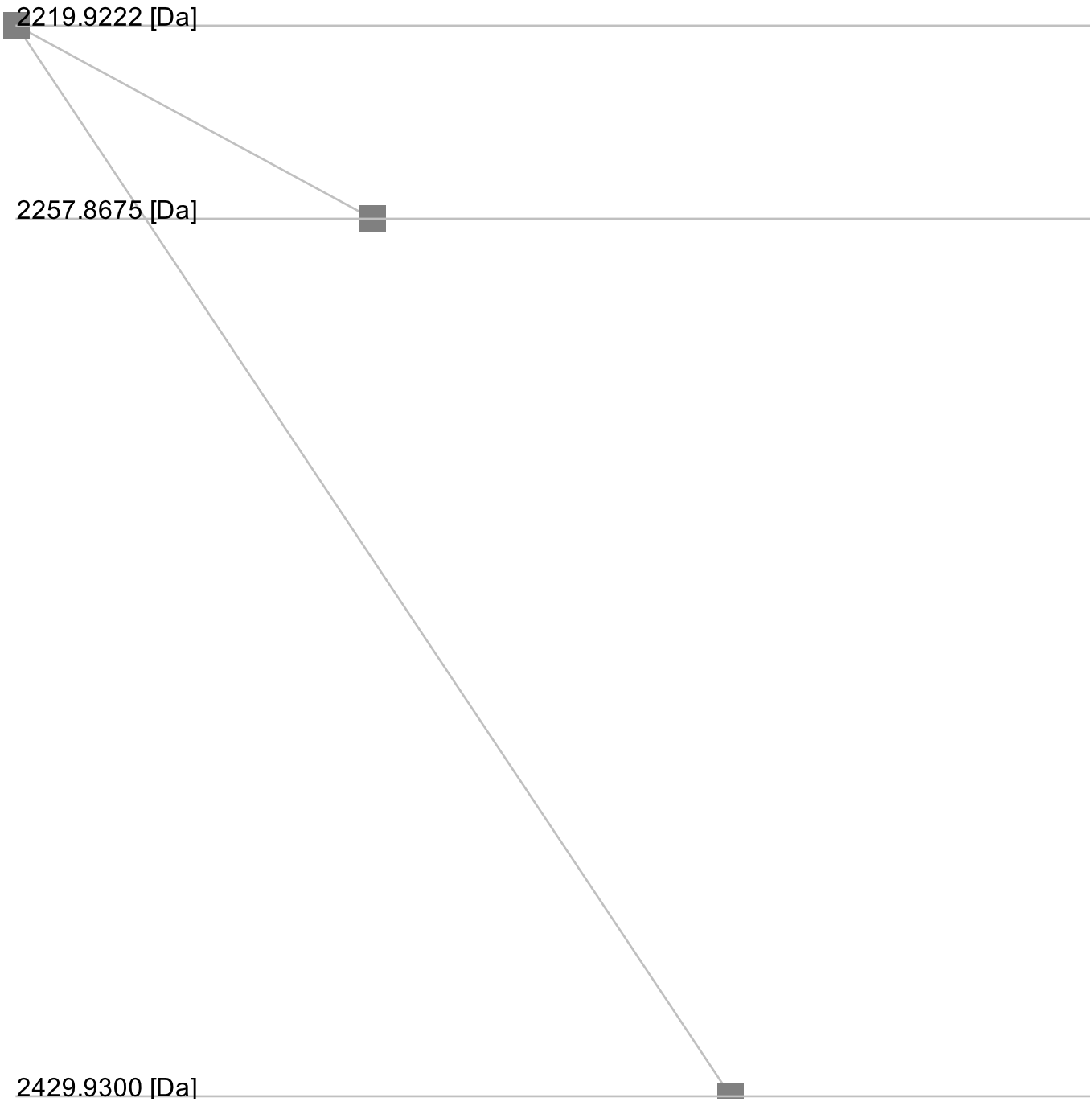
peptideNet ID : 5	
spectra in net : 3	pairs in net : 2
mass width of peptideNet : 83.0410 [Da]	
minimal mass : 2521.3555 [Da]	maximal mass : 2604.3965 [Da]



peptideNet ID : 10	
spectra in net : 3	pairs in net : 2
mass width of peptideNet : 74.0455 [Da]	
minimal mass : 1013.6977 [Da]	maximal mass : 1087.7432 [Da]



peptideNet ID : 25	
spectra in net : 3	pairs in net : 2
mass width of peptideNet : 210.0078 [Da]	
minimal mass : 2219.9222 [Da]	maximal mass : 2429.9300 [Da]



peptideNet ID : 22	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 323.2245 [Da]	
minimal mass : 1695.8620 [Da]	maximal mass : 2019.0865 [Da]

peptideNet ID : 3	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 74.0212 [Da]	
minimal mass : 759.2274 [Da]	maximal mass : 833.2485 [Da]

peptideNet ID : 9	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 83.0386 [Da]	
minimal mass : 2503.3457 [Da]	maximal mass : 2586.3843 [Da]

peptideNet ID : 2	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 31.0013 [Da]	
minimal mass : 1400.5871 [Da]	maximal mass : 1431.5884 [Da]

peptideNet ID : 11	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 58.1487 [Da]	
minimal mass : 836.4571 [Da]	maximal mass : 894.6058 [Da]

peptideNet ID : 13	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 18.0070 [Da]	
minimal mass : 3261.6031 [Da]	maximal mass : 3279.6101 [Da]

peptideNet ID : 1	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 15.9700 [Da]	
minimal mass : 2403.0621 [Da]	maximal mass : 2419.0320 [Da]

peptideNet ID : 15	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 34.9833 [Da]	
minimal mass : 1455.8376 [Da]	maximal mass : 1490.8208 [Da]

peptideNet ID : 7	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 15.0046 [Da]	
minimal mass : 2381.0806 [Da]	maximal mass : 2396.0852 [Da]

peptideNet ID : 20	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 43.0127 [Da]	
minimal mass : 2700.4090 [Da]	maximal mass : 2743.4217 [Da]

peptideNet ID : 21	
spectra in net : 2	pairs in net : 1
mass width of peptideNet : 30.0083 [Da]	
minimal mass : 969.6747 [Da]	maximal mass : 999.6830 [Da]