

## The NC Spectrum Graph – A “Real” Example

Define the “amino acid” alphabet  $\Sigma = \{a, b, c\}$  and the weight function  $w : \Sigma \rightarrow \mathbb{N}$  as  $w(a) = 40$ ,  $w(b) = 50$ ,  $w(c) = 70$ .

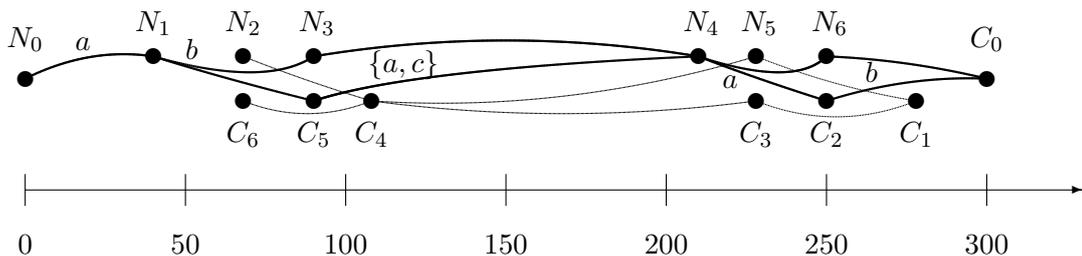
Let the parent mass be  $W = 318$  and assume the following ion masses to be measured: 41, 69, 91, 211, 229, 251.

Task: Reconstruct the original peptide sequence (if possible).

To construct the NC spectrum graph, define vertices  $N_0, N_1, \dots, N_6$  and  $C_0, C_1, \dots, C_6$  with the following coordinates:

index	$j$	0	1	2	3	4	5	6
mass	$w_j$	–	41	69	91	211	229	251
coord( $N$ -vertex)	$w_j - 1$	0	40	68	90	210	228	250
coord( $C$ -vertex)	$W - w_j + 1$	300	278	250	228	108	90	68

If one adds edges for amino acids whenever their coordinate difference equals an amino acid mass (or a combination of two), the graph looks as follows:



There are four possible paths from  $N_0$  to  $C_0$ , all of them corresponding to the sequence  $ab\{a, c\}ab$ :

1.  $N_0 - N_1 - N_3 - N_4 - N_6 - C_0$
2.  $N_0 - N_1 - C_5 - N_4 - N_6 - C_0$
3.  $N_0 - N_1 - N_3 - N_4 - C_2 - C_0$
4.  $N_0 - N_1 - C_5 - N_4 - C_2 - C_0$