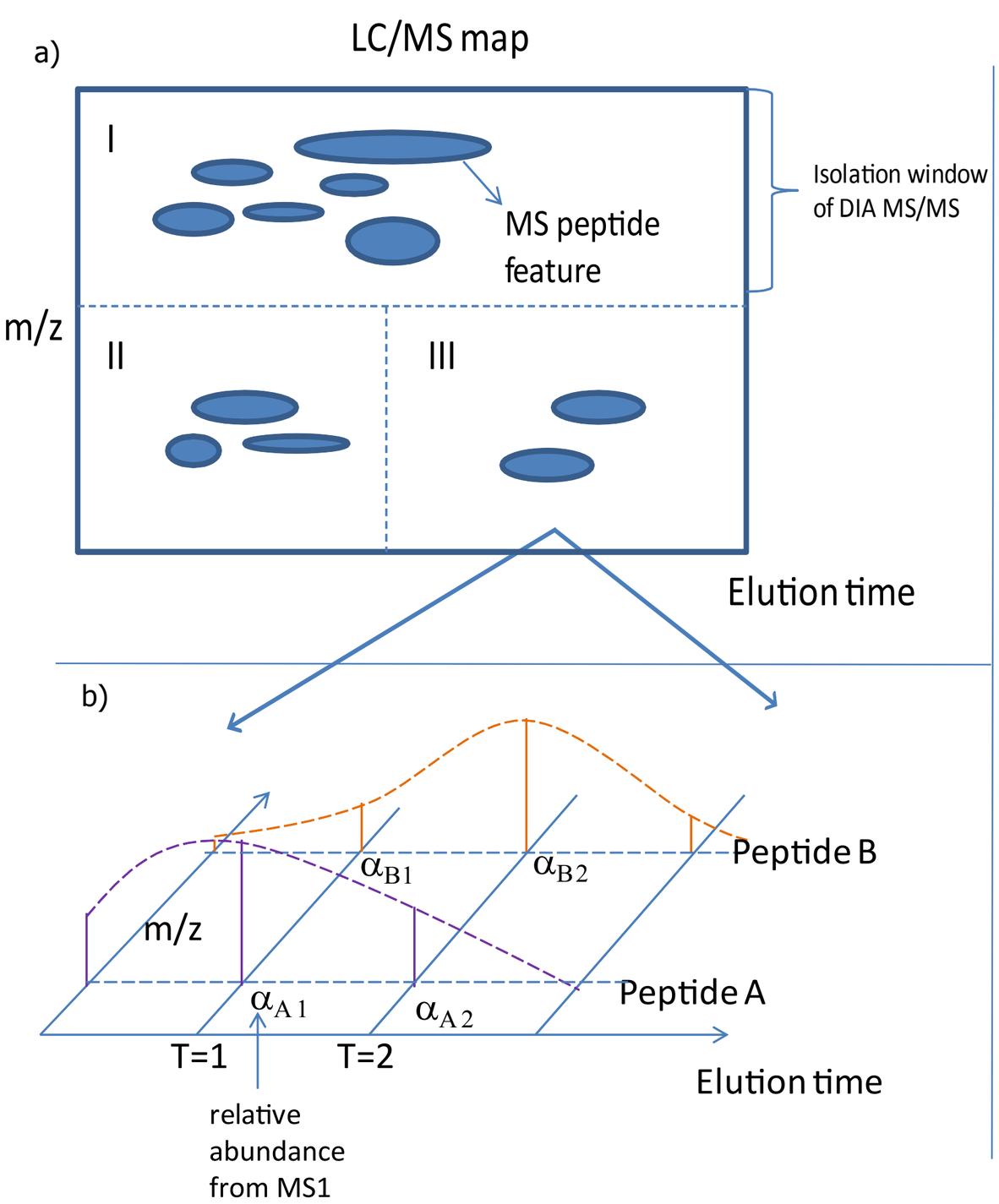

c)

Input:

MS/MS spectra at T=1: $M_1 = [m_{11} \ldots m_{1n}]$; T=2:$M_2=[m_{21} \ldots m_{2n}]$

Spectral-Library: {P,Q,R}; Mass(P)=Mass(R)=Mass(A); Mass(Q)=Mass(B)

α_{Ak} , α_{Bk} : measured MS1 abundances of peptides A,B at T=k

Consistency parameter c

Output:

α_{Pk}, α_{Qk}, α_{Rk} : estimated abundances of peptides P, Q, R in spectrum M_k

LP formulation:

Step 1: Define ε_i for each multiplexed spectrum M_i

$\varepsilon_1 = \sum (|m_{1i} - \alpha_{P1}p_i + \alpha_{Q1}q_i + \alpha_{R1}r_i|)$;

$\varepsilon_2 = \sum (|m_{2i} - \alpha_{P2}P_i + \alpha_{Q2}q_i + \alpha_{R1}r_i|)$

Step 2: Define δ_{Cij} for library candidate C and a pair of spectra M_i and M_j

$\delta_{P12} = |\alpha_{P1}/\alpha_{A1} - \alpha_{P2}/\alpha_{A2}|$;

$\delta_{Q12} = |\alpha_{Q1}/\alpha_{B1} - \alpha_{Q2}/\alpha_{B2}|$;

$\delta_{R12} = |\alpha_{R1}/\alpha_{A1} - \alpha_{R2}/\alpha_{A2}|$;

Final LP objective:

$\text{Min}((\varepsilon_1 + \varepsilon_2) + c(\delta_{P12} + \delta_{Q12} + \delta_{R12}))$