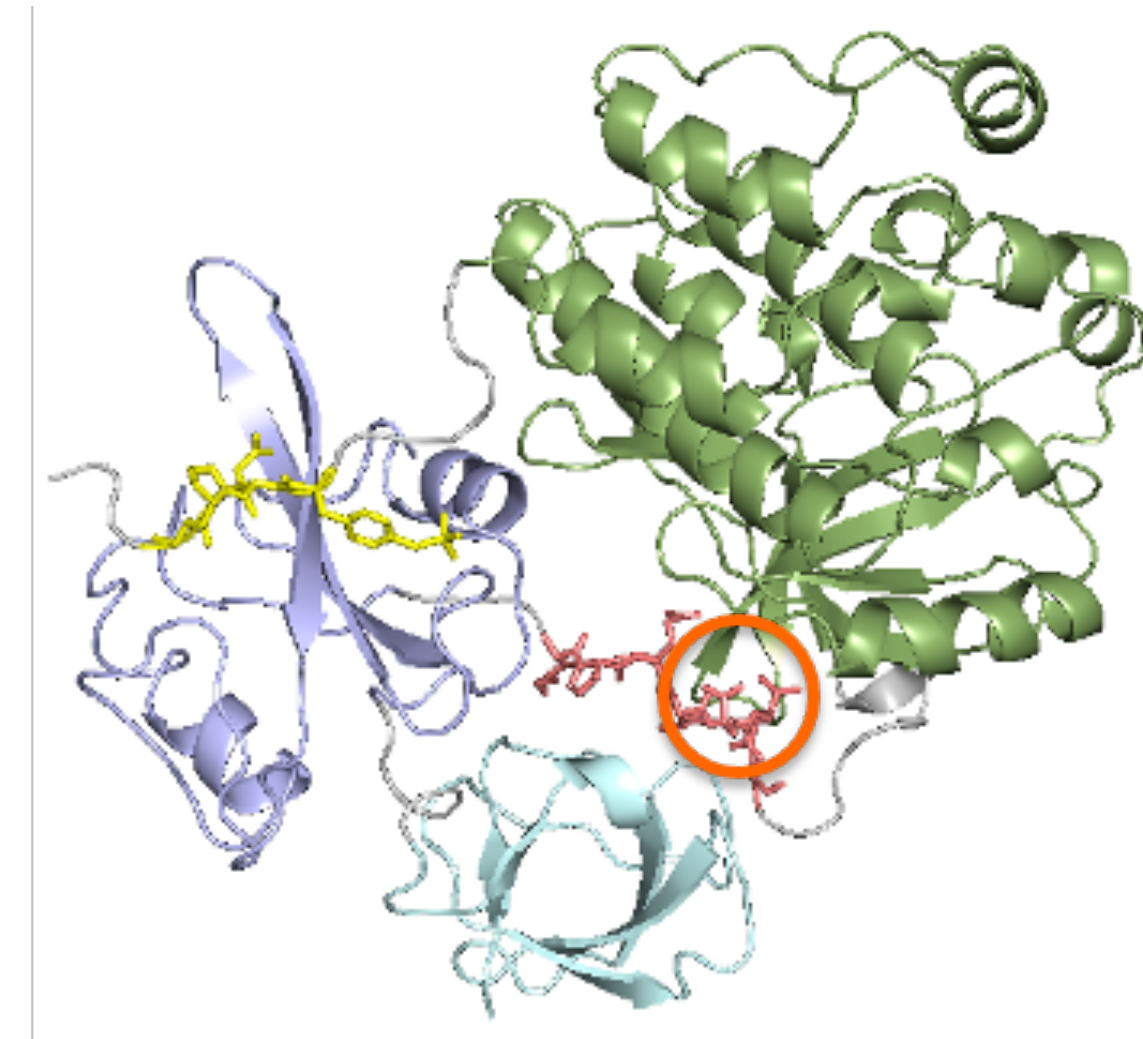
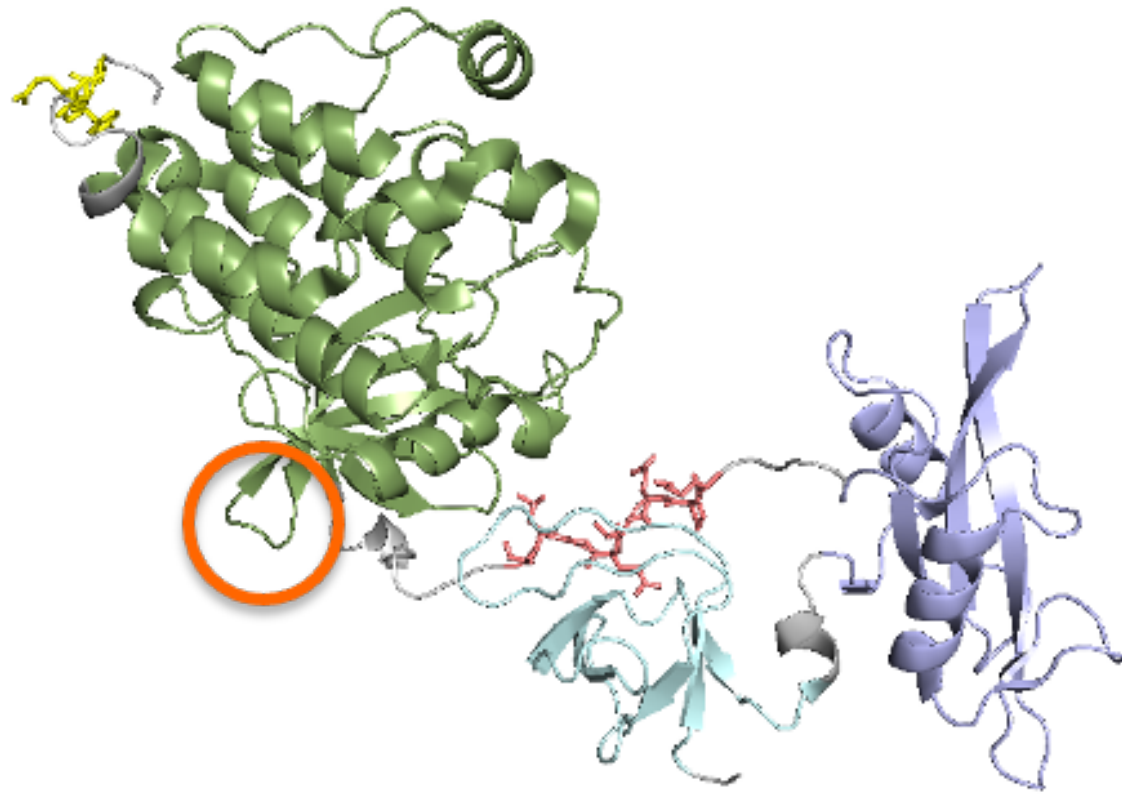
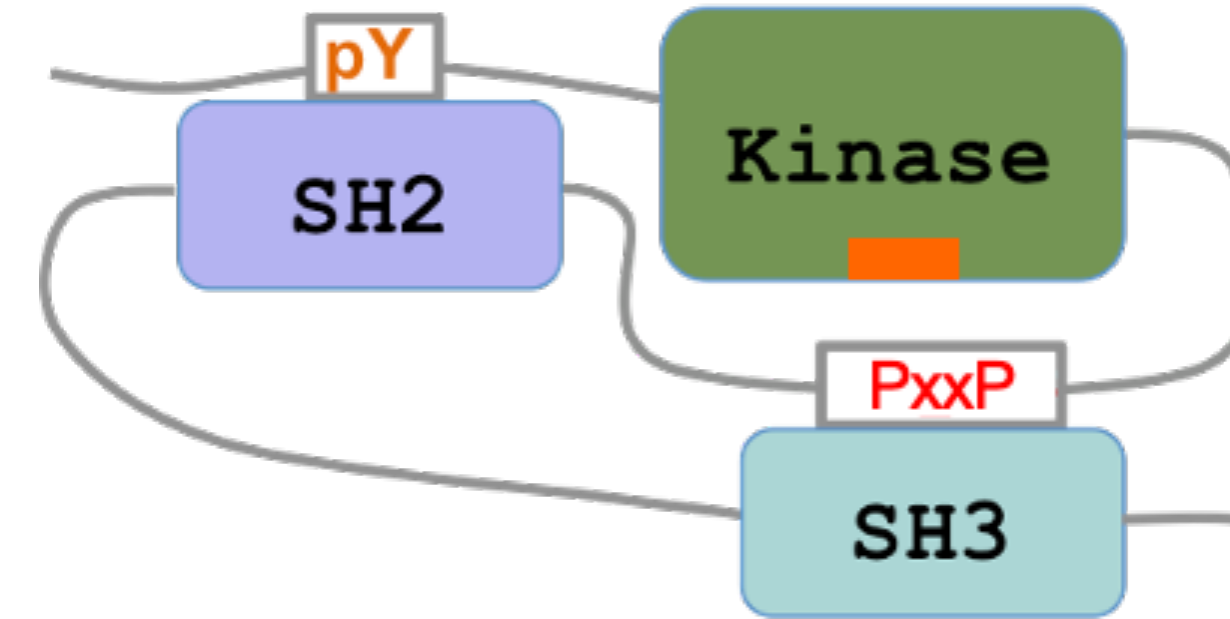
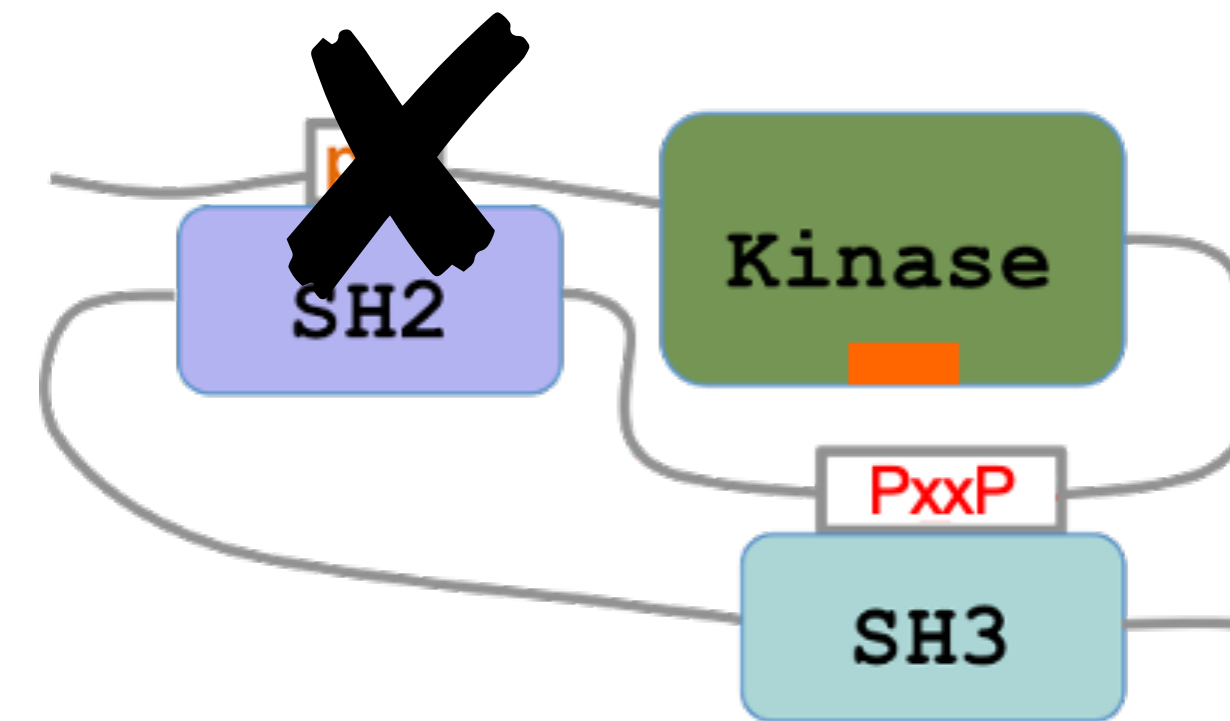
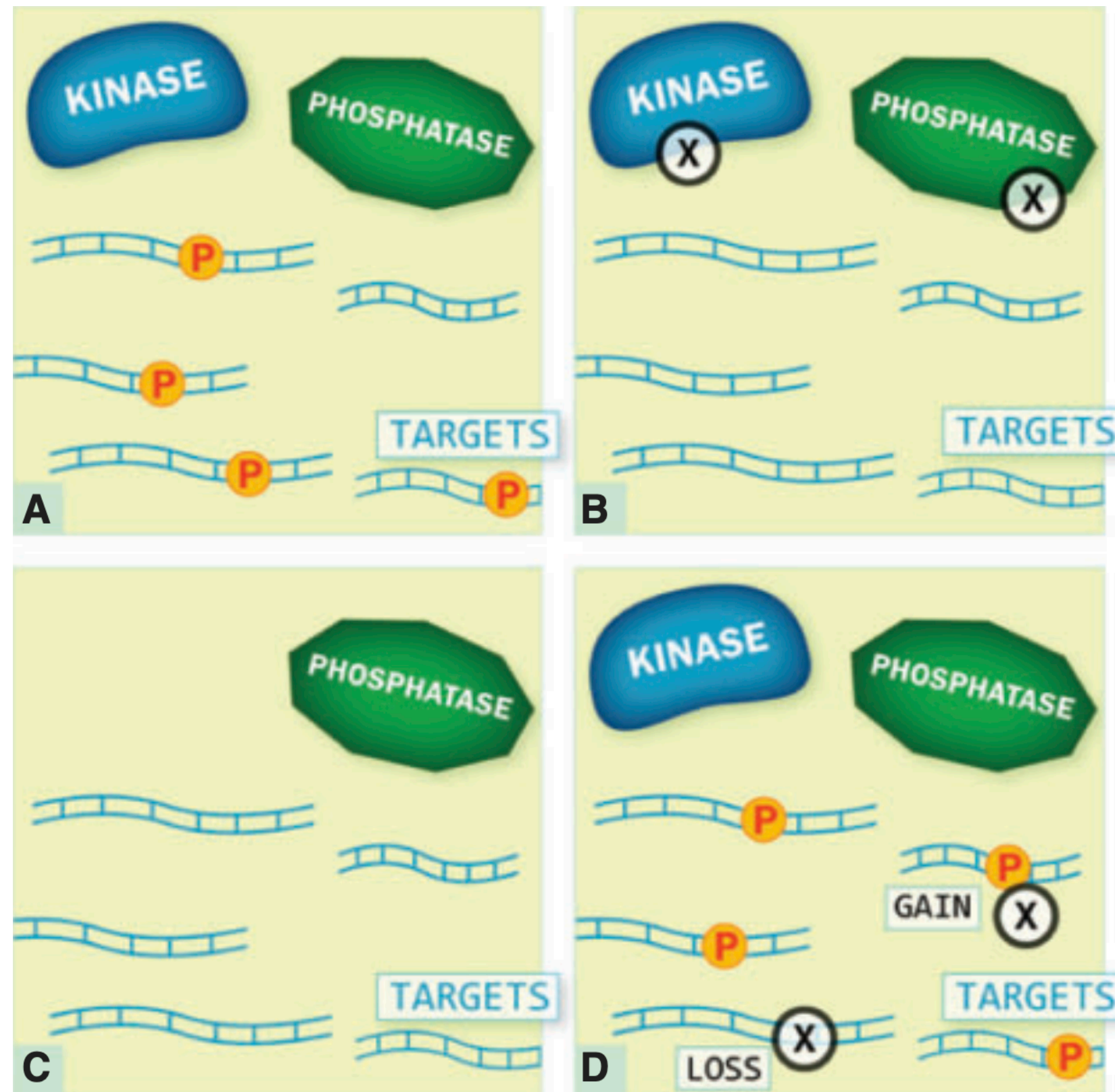


# Modularity in Proteins: c-Src





# Modeling Phosphorylated Peptides to Protein Domains

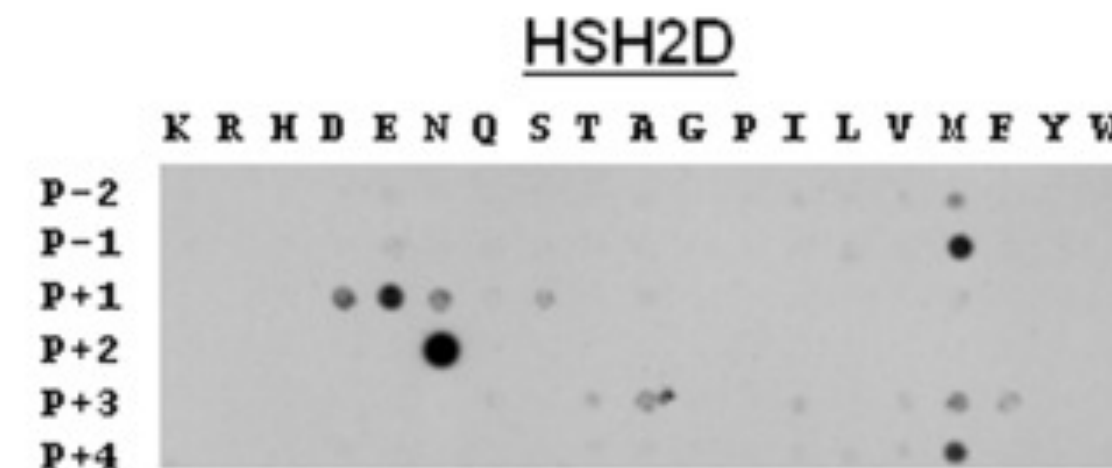
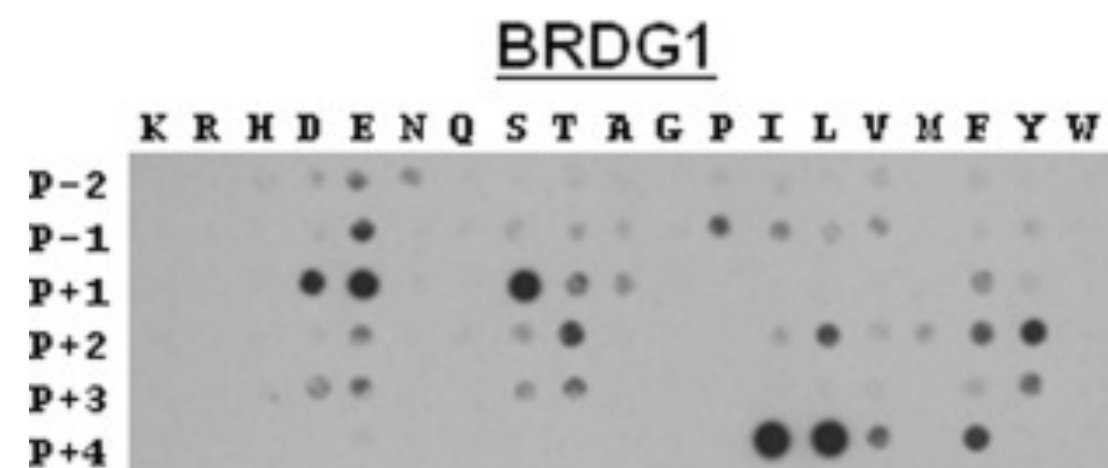
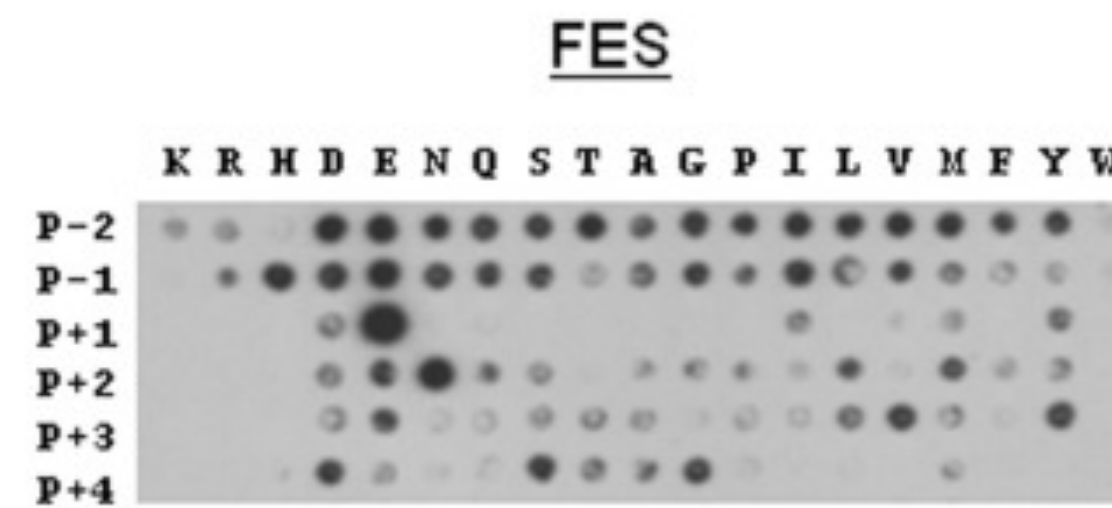
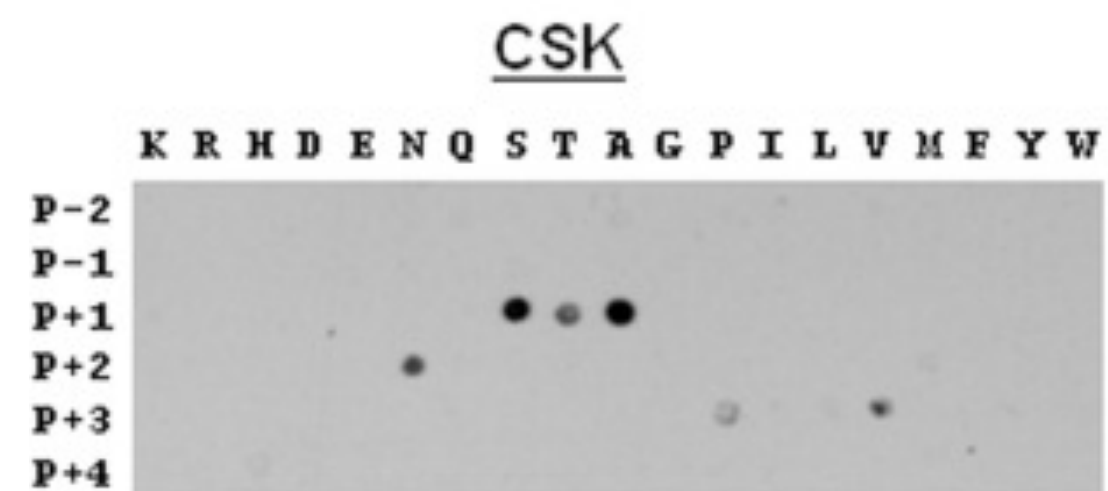
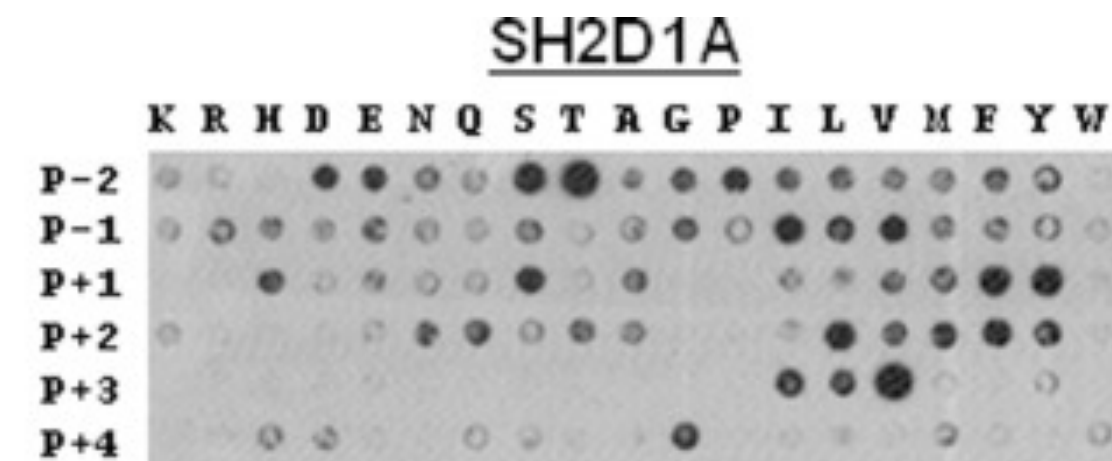
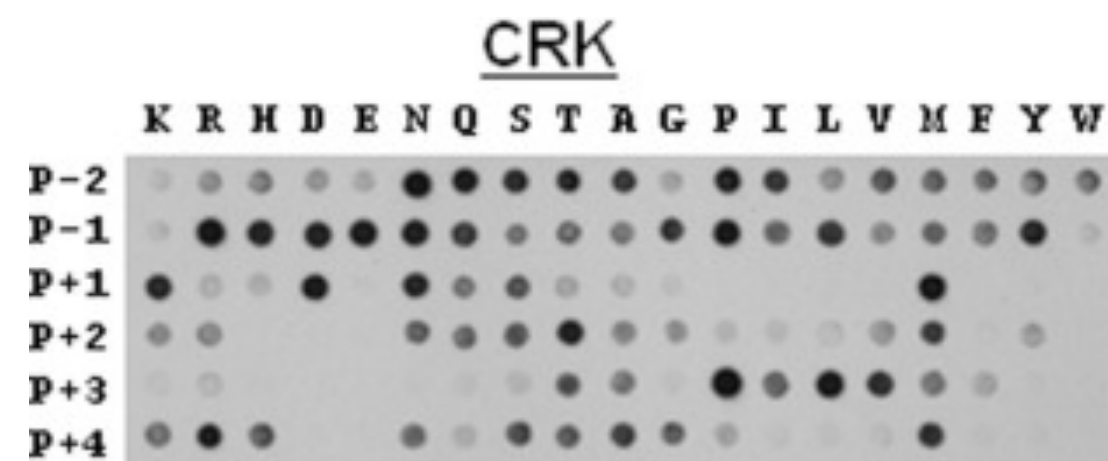


**A**

				LIR autophagy										TSTF $\chi$ ----- $\chi\phi\chi\phi$									
				PTB/apoPTB										NP $\chi$ Y									
$\beta_1$	P05556	752-798	K L L M I I H D R R E F A K F E K E K M N A K W D T G E N P I Y K S A V T T V V - - - - -											N P K Y E G K - - - - -									
$\beta_2$	P05107	724-769	K A L I H L S D L R E Y R R F E K E K L K S Q W N N - D N P L F K S A T T T V M - - - - -											N P K F A E S - - - - -									
$\beta_3$	P05106	742-788	K L L I T I H D R K E F A K F E E R A R A K W D T A N N P L Y K E A T S T F T - - - - -											N I T Y R G T - - - - -									
$\beta_5$	P18084	743-799	K L L V T I H D R R E F A K F Q S E R S R A R Y E M A S N P L Y R K P I S T H T V D F T F N K F - - - - -											N K S Y N G T V D - - - - -									
$\beta_6$	P18564	731-788	K L L V S F H D R K E V A K F E A E R S K A K W Q T G T N P L Y R G S T S T F K - - - - -											N V T Y K H R E K Q K V D L S T D C - - - - -									
$\beta_7$	P26010	747-798	R L S V E I Y D R R E Y S R F E K E Q Q L N W K Q D S N P L Y K S A I T T T I - - - - -											N P R F Q E A D S P T L - - - - -									

Cytosolic C terminus

# Modeling Phosphorylated Peptides to Protein Domains



- From Spot Array we know different phosphopeptides have different affinities for their target domain
- This experiments give only relative affinities
- Time consuming, expensive



# Modeling Phosphorylated Peptides to Protein Domains

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- AlphaFold does not model amino acid modification
- AlphaFold is not appropriate to study single mutations in the global structure
- Molecular Dynamics (GROMACS) can model phosphorylation sites
  - CHARMM-GUI is necessary to create the topology files