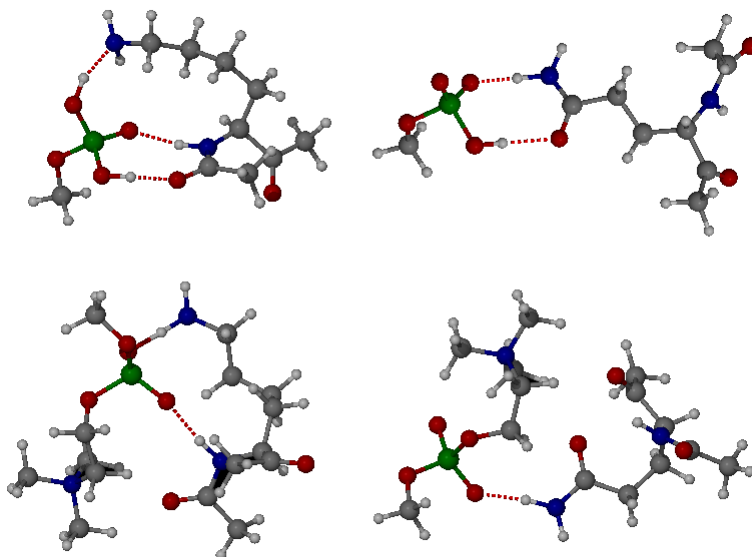


## **Anion Transport Properties of Amine and Amide-Sidechained Peptides is Affected by Phospholipid Composition**

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### Computational studies.



*Figure 1S* Calculation results for four model complexes: phosphate-lysine (upper left), phosphocholine-lysine (lower left), phosphate-glutamine (upper right) and phosphocholine-glutamine (lower right).

The key features of the computational models are summarized below. The caveats concerning both the gas phase and the choice of models must be borne in mind. The model phosphate-lysine complex (upper left panel) is dominated by an H-bonded salt bridge that is formed between ammonium and phosphate. The bridged hydrogen is calculated to be closer to the phosphate oxygen (H-O, 1.02 Å) than to the ammonium nitrogen (H-N, 1.71 Å, other two N-H, 1.02 Å). This could reflect the difference in electronegativity between O and N or could suggest proton transfer. A hydrogen-bonded double bridge exists between phosphate and *N*-terminus acetamide (O-H, 1.85 and 1.65 Å respectively) but this is an artifact of the acetylated model.

The model phosphocholine-lysine complex (lower left panel) shows a bridge between phosphate oxygen and ammonium nitrogen. The bridged hydrogen is 1.41 Å from oxygen (O-H, 1.41 Å) and 1.14 Å from nitrogen (N-H, 1.14 Å). The other two N-H bonds are 1.02 Å. This indicates that the interaction between phosphate and ammonium is much stronger in this case than in the model phosphocholine-ammonium complex. The computational model is therefore consistent with the experimental results recorded in the previous section.

The stabilizing force in the model phosphate-glutamine complex (upper right panel) is a doubly bridged hydrogen bond (O-H, 1.57 and 1.93 Å respectively). The model phosphocholine-glutamine complex shows only one hydrogen bond (O-H, 1.76 Å). The calculations show that the interaction between phosphate and the glutamine sidechain amide is more favorable than the corresponding phosphocholine interaction. This is also in accord with the experimental results.