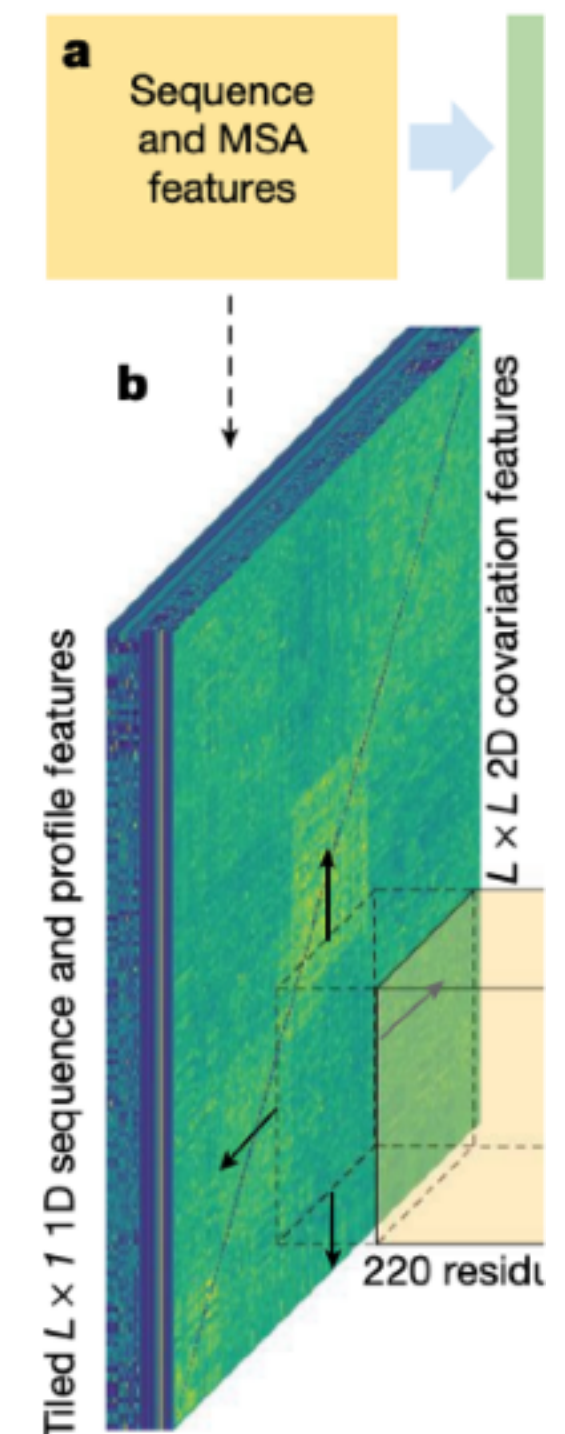
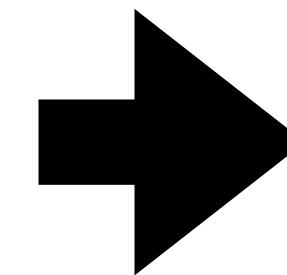


Feature engineering from AA sequence

- Using domain knowledge to create numeric representations of the protein sequence
- These representations contain information that may indicate inter-residue distances
- Eg. from known protein structures, how often does residue A come in contact with residue B

QTKCEKKKCV CENCERSTYL
SERKTMKFNERDSHVVC DKTC



Unsupervised learning of AA sequences

- Multiple sequence alignment [3] is an algorithm that uses many sample sequences of related proteins to infer residue contact
- Residue pairs that are consistent across sequences indicate that those residues may be in close contact (evolutionary covariation)
- Conversely, residues pairs that are uncorrelated are unlikely to be in contact

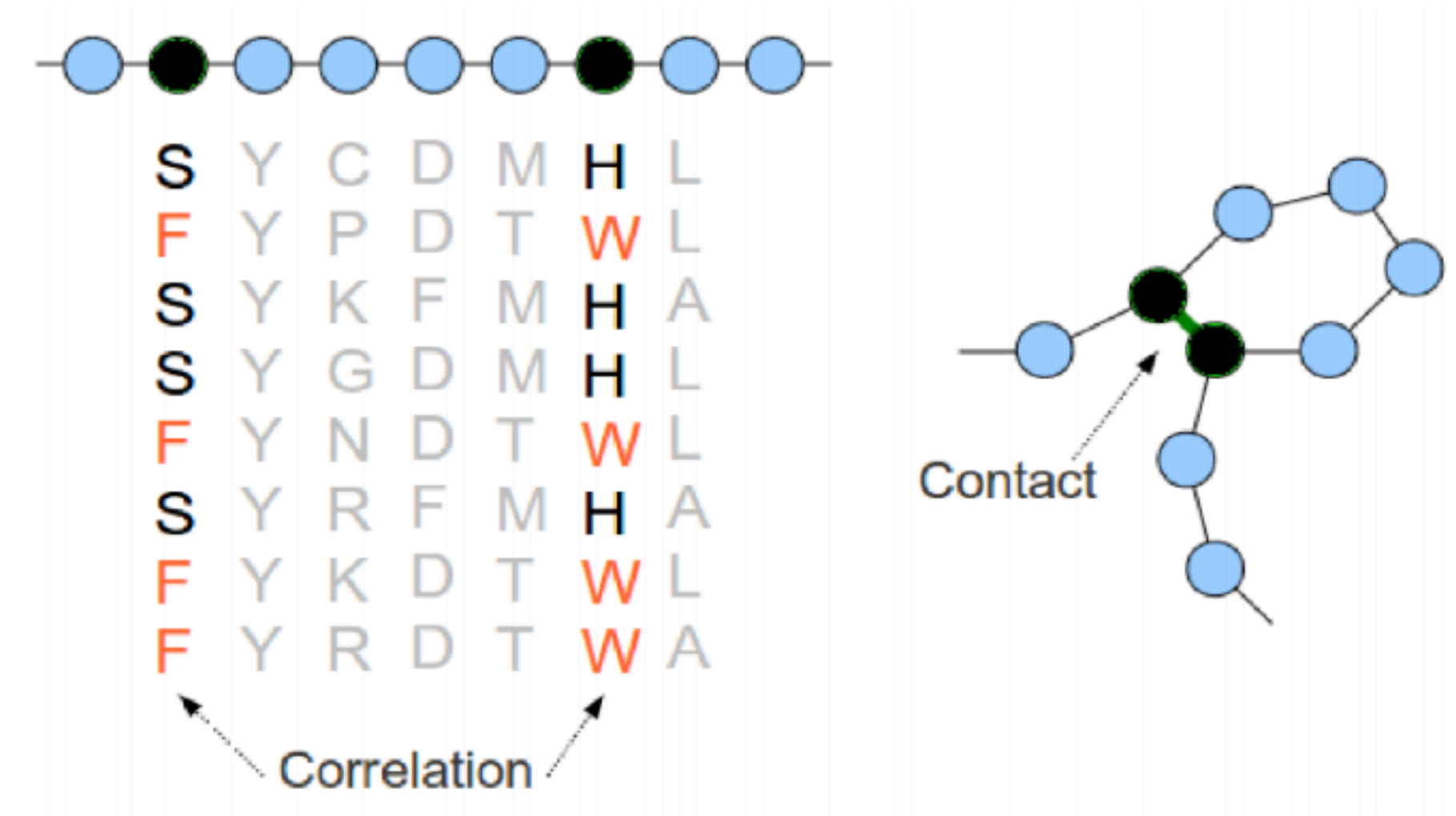


FIG. 1. (Color online) Left panel: small MSA with two positions of correlated amino-acid occupancy. Right panel: hypothetical corresponding spatial conformation, bringing the two correlated positions into direct contact.

[3] [Improved contact prediction in proteins: Using pseudolikelihoods to infer Potts models](#)