

Scheme 1. Comparison of algorithms among AF2, ESM2 and OpenFold.

	AlphaFold2	ESM2	OpenFold
Model Structure	b+c+d	a+e+f	b+c+d
Parameters	21 million	15 billion	93 million
Framework implementation	TensorFlow, Jax	PyTorch	PyTorch
Uses MSA	☑		☑
Uses Structure templates	☑		☑
Uses sequence	☑	☑	☑

- a. Sequence input.
- b. Three channel input.
- c. Transformer based prediction module.
- d. 3D structure equivalent module.
- e. Transformer based prediction model without using MSA.
- f. 3D equivalent structure module without using MSA.