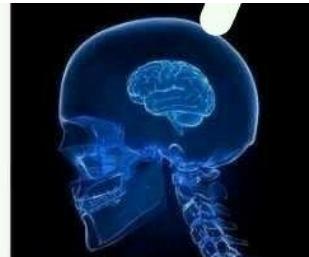


The 4 additional tasks

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1. Implement the constants as parameters



2. All-atom representation



3. KDE with R



4. Non-log formula



The 85 RNA atom types

```
{ "AC1'", "AC2", "AC2'", "AC3'", "AC4", "AC4'", "AC5",
"AC5'", "AC6", "AC8", "AN1", "AN3", "AN6", "AN7", "AN9",
"AO2'", "AO3'", "AO4'", "AO5'", "AOP1", "AOP2", "AP",
"CC1'", "CC2", "CC2'", "CC3'", "CC4", "CC4'", "CC5", "CC5'",
"CC6", "CN1", "CN3", "CN4", "CO2", "CO2'", "CO3'", "CO4'",
"CO5'", "COP1", "COP2", "CP", "GC1'", "GC2", "GC2'", "GC3'",
"GC4", "GC4'", "GC5", "GC5'", "GC6", "GC8", "GN1", "GN2",
"GN3", "GN7", "GN9", "GO2'", "GO3'", "GO4'", "GO5'", "GO6",
"GOP1", "GOP2", "GP", "UC1'", "UC2", "UC2'", "UC3'", "UC4",
"UC4'", "UC5", "UC5'", "UC6", "UN1", "UN3", "UO2", "UO2'",
"UO3'", "UO4", "UO4'", "UO5'", "UOP1", "UOP2", "UP"};
```

Non-log formula

Theoretical
structures

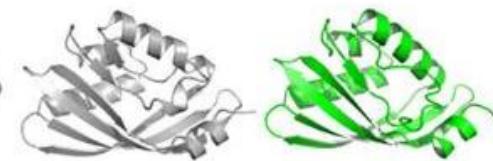


$$\bar{u}_{i,j}(r) = -kT \ln \left[\frac{f_{i,j}^{OBS}(r)}{f_{i,j}^{REF}(r)} \right]$$

Sippl's potentials



Incorrect



MODEL QUALITY ASSESSMENT

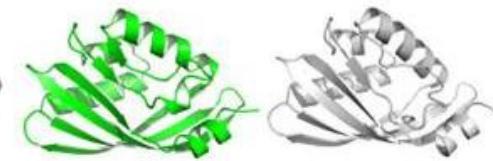


$$score = - \sum_{i,j} \frac{f_{i,j}^{OBS}(r) - f_{i,j}^{REF}(r)}{f_{i,j}^{REF}(r)}$$

Total information gain



Correct



Postic et al., 2020

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