

# Analysis Parameters and Results

Used databases (path from local filesystem):

D:\\tRNAs\_small\_sample.txt

20 structures can be considered for the analysis;

0 structures must be ignored (these are prohibited in the used SCFG model).

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**Probabilities of Production Rules**

Considered production rule	Relative frequency	Floating point approximation
1. $S \rightarrow TAC$	1	1.000000000
2. $T \rightarrow TAC$	0	0
3. $T \rightarrow C$	1	1.000000000
4. $C \rightarrow C \mid$	$\frac{13}{33}$	0.3939393939
5. $C \rightarrow \text{epsilon}$	$\frac{20}{33}$	0.6060606061
6. $A \rightarrow (L)$	1	1.000000000
7. $L \rightarrow (L)$	$\frac{341}{421}$	0.8099762470
8. $L \rightarrow M$	$\frac{20}{421}$	0.04750593824
9. $L \rightarrow P$	0	0
10. $L \rightarrow Q$	0	0
11. $L \rightarrow R$	0	0
12. $L \rightarrow F$	$\frac{60}{421}$	0.1425178147
13. $L \rightarrow G$	0	0
14. $G \rightarrow (L) \mid$	0	0
15. $G \rightarrow (L) B \mid \mid$	0	0
16. $G \rightarrow \mid (L)$	0	0
17. $G \rightarrow \mid \mid B (L)$	0	0
18. $B \rightarrow B \mid$	0	0
19. $B \rightarrow \text{epsilon}$	0	0
20. $F \rightarrow \mid \mid \mid$	0	0
21. $F \rightarrow \mid \mid \mid \mid$	0	0
22. $F \rightarrow \mid \mid \mid \mid H$	1	1.000000000
23. $H \rightarrow H \mid$	$\frac{9}{13}$	0.6923076923
24. $H \rightarrow \text{epsilon}$	$\frac{4}{13}$	0.3076923077
25. $P \rightarrow \mid (L) \mid$	0	0
26. $P \rightarrow \mid (L) \mid \mid$	0	0
27. $P \rightarrow \mid \mid (L) \mid$	0	0
28. $P \rightarrow \mid \mid (L) \mid \mid$	0	0

29. $Q \rightarrow \mid \mid (L) K \mid \mid \mid$	0	0
30. $Q \rightarrow \mid \mid \mid J (L) K \mid \mid$	0	0
31. $R \rightarrow \mid (L) K \mid \mid \mid$	0	0
32. $R \rightarrow \mid \mid \mid J (L) \mid$	0	0
33. $J \rightarrow J \mid$	0	0
34. $J \rightarrow \text{epsilon}$	0	0
35. $K \rightarrow K \mid$	0	0
36. $K \rightarrow \text{epsilon}$	0	0
37. $M \rightarrow U (L) U (L) N$	1	1.000000000
38. $N \rightarrow U (L) N$	$\frac{1}{2}$	0.500000000
39. $N \rightarrow U$	$\frac{1}{2}$	0.500000000
40. $U \rightarrow U \mid$	$\frac{157}{237}$	0.6624472574
41. $U \rightarrow \text{epsilon}$	$\frac{80}{237}$	0.3375527426

Remark: Probabilities are equal to zero in cases where no structure of the input made use of the corresponding rule.

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**Averaged Free Energy Contributions**

Considered Parameter	Floating point value	Rational approximation
ldeh	5.91667	$\frac{71}{12}$
ldehPerNuc	0.819974	$\frac{6199}{7560}$
tmseh	-1.37833	$-\frac{827}{600}$
GGGLoopBonus	0	0
cHairpinOf3	Indeterminate	Indeterminate
cHairpin	0	0
cHairpinPerNuc	0	0
termAUpenHL	Indeterminate	Indeterminate
tetra	Indeterminate	Indeterminate
se	-2.67742	$-\frac{83}{31}$
seBulge	Indeterminate	Indeterminate
ldeb	Indeterminate	Indeterminate
ldebPerNuc	Indeterminate	Indeterminate
termAUpenBL	Indeterminate	Indeterminate
ile1x1	Indeterminate	Indeterminate
ile2x2	Indeterminate	Indeterminate
ile1x2	Indeterminate	Indeterminate
ldei	Indeterminate	Indeterminate
ldeiPerNuc	Indeterminate	Indeterminate
asym	Indeterminate	Indeterminate
tmsei	Indeterminate	Indeterminate
tbplxNil	Indeterminate	Indeterminate
MBLinitiation	5.	5
MBLOffset	3.4	$\frac{17}{5}$
MBLFreeBasePenalty	0	0
MBLHelixPenalty	0.4	$\frac{2}{5}$
stackingMulti	-0.865	$-\frac{173}{200}$
termAUpenML	0.125	$\frac{1}{8}$
stackingExterior	-1.7	$-\frac{17}{10}$
termAUpenEL	0	0

Remark: Parameters are indeterminate in cases where no structure of the input showed the appropriate motif. However, in such a case the probabilities of the corresponding rules of our stochastic grammar are equal to zero such that the missing parameter value is of no importance.

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## Asymptotical Free Energy Results

### ▪ Expected Values

Static Model:

$$-0.4284343499 n - 3.238831948 + O\left[\frac{1}{n}\right]^1$$

Dynamic Model:

$$-0.4256571092 n - 3.466478768 + O\left[\frac{1}{n}\right]^1$$

### ▪ Variances

Static Model:

$$4.29598885 n + O\left[\frac{1}{n}\right]^0$$

Dynamic Model:

$$4.72662620 n + O\left[\frac{1}{n}\right]^0$$