

# Simultaneous Alignment and Structure Prediction of RNAs

Are Three Input Sequences Better than Two?\*

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## A Web Appendix: Supplementary Material

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**Table 1.** tRNA dataset.

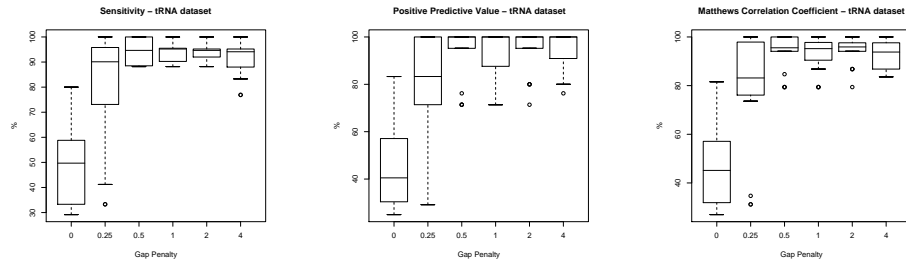
Id	Length	Description
RD0260	77	Asp Phage T5 (Virus)
RD0500	76	Asp <i>Haloferax volcanii</i> (Archae)
RD4800	71	Asp <i>Aedes albopictus</i> (Mitochondria, Animal)
RE2140	76	Glu <i>Synechocystis sp.</i> (Eubacteria)
RE6781	76	Glu <i>Hordeum vulgare</i> (Chloroplast)
RF6320	76	Phe <i>Schizosaccharomyces pombe</i> (Cytoplasm, Fungi)
RL0503	88	Leu <i>Haloferax volcanii</i> (Archae)
RL1141	89	Leu <i>Mycoplasma capricolum</i> (Eubacteria)
RS0380	88	Ser <i>Halobacterium cutirubrum</i> (Archae)
RS1141	92	Ser <i>Mycoplasma capricolum</i> (Eubacteria)

**Table 2.** 5S rRNA dataset.

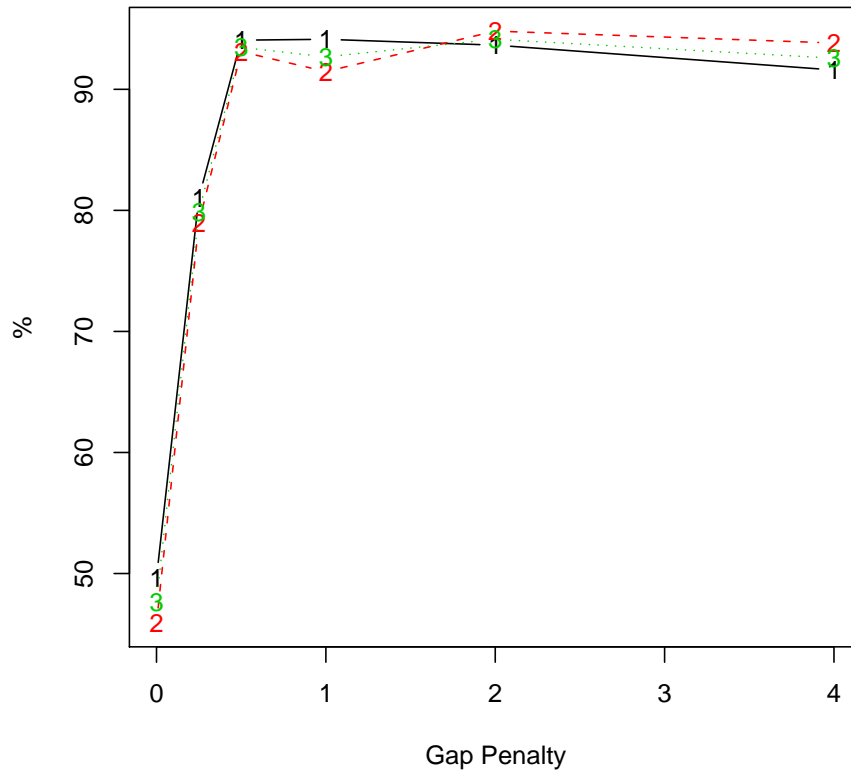
Id	Length	Description
AJ131594	117	<i>Delftia acidovorans</i>
AJ251080	117	<i>Geobacillus stearothermophilus</i>
K02682	120	<i>Micrococcus luteus</i>
M10816	119	<i>Geobacillus stearothermophilus</i>
M16532	121	<i>Thermus sp.</i>
M25591	117	<i>Geobacillus stearothermophilus</i>
V00336	120	<i>Escherichia coli</i>
X02024	119	<i>Sporosarcina pasteurii</i>
X02627	120	<i>Agrobacterium tumefaciens</i>
X04585	119	<i>Rhodobacter capsulatus</i>
X08000	122	<i>Arthrobacter oxydans</i>
X08002	122	<i>Arthrobacter globiformis</i>

**Table 3.** Sensitivity for the tRNA dataset.

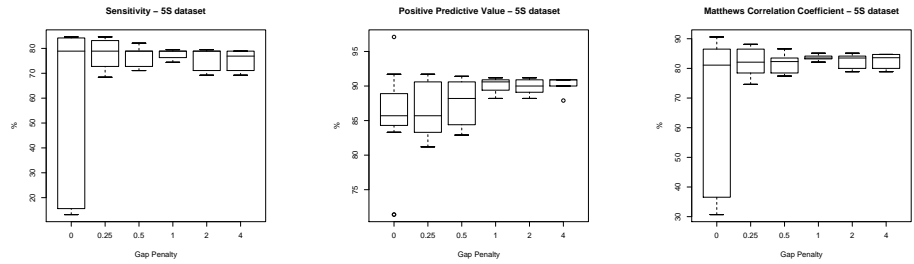
Id	$N_{xd}$	$N_d$	$\text{Min}_{xd}$	$\text{Min}_d$	$\text{Max}_{xd}$	$\text{Max}_d$	$\text{Ave}_{xd}$	$\text{Ave}_d$
RD0260	4	5	95	57	100	100	98.8	90.5
RD0500	4	5	76	47	95	95	81.0	80.0
RD4800	5	5	95	57	100	100	99.0	91.4
RE2140	2	4	100	95	100	100	100.0	98.8
RE6781	2	4	100	81	100	100	100.0	95.2
RF6320	4	5	95	47	100	100	96.4	89.5
RL0503	1	2	95	95	95	95	95.8	95.8
RL1141	2	3	92	68	92	92	92.0	84.0
RS0380	1	2	92	80	92	80	92.0	80.0
RS1141	2	3	88	65	88	92	88.5	82.1



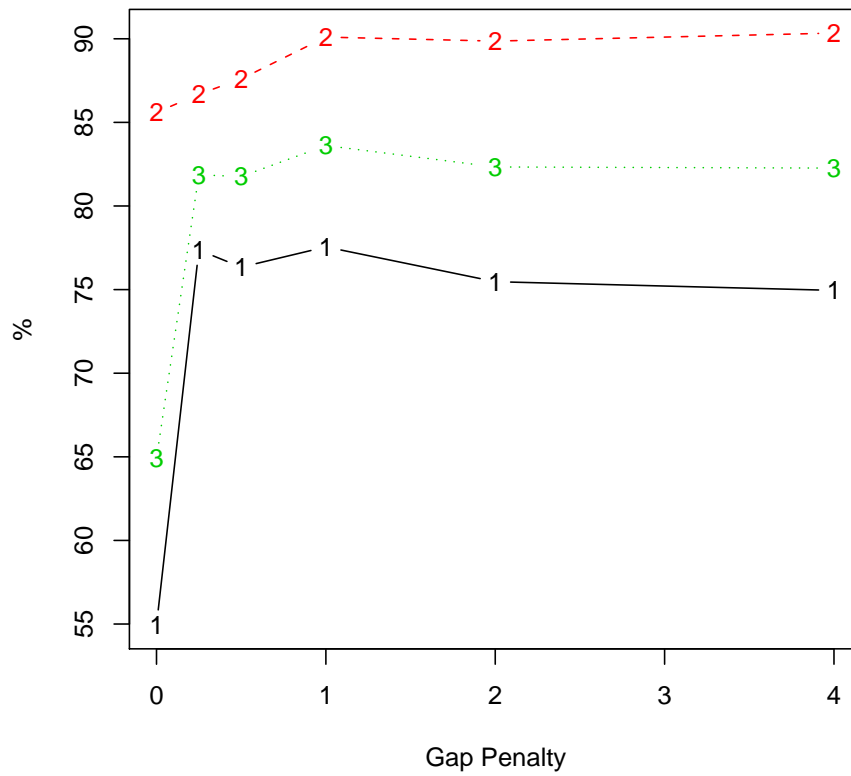
**tRNA dataset: 1 = Sensitivity, 2 = PPV, 3 = MCC**



**Fig. 1.** Effect of various gap penalty scores on PPV, sensitivity and MCC for the tRNA dataset.



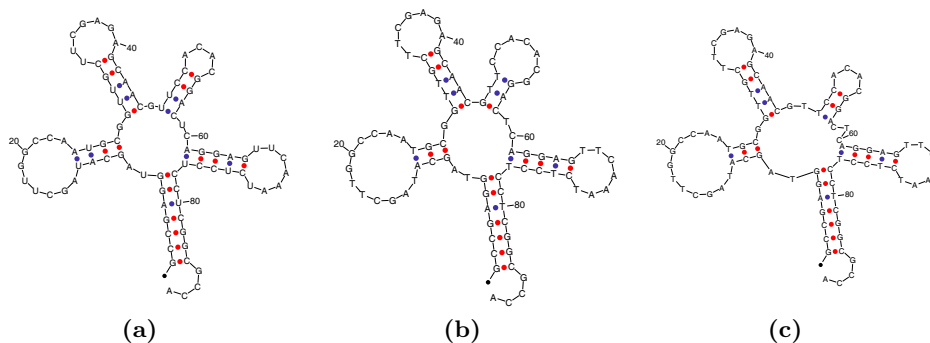
**5S dataset: 1 = Sensitivity, 2 = PPV, 3 = MCC**



**Fig. 2.** Effect of various gap penalty scores on MCC, PPV and Sensitivity for the 5S dataset.

**Table 4.** MCC for the tRNA dataset.

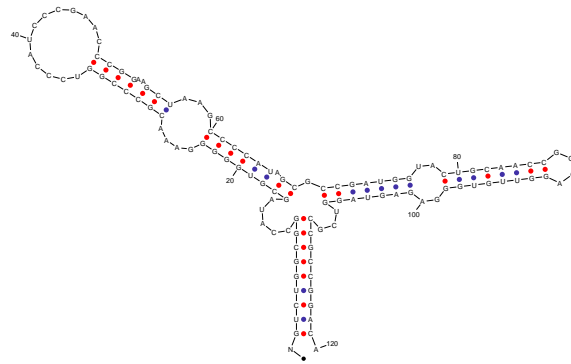
Id	$N_{xd}$	$N_d$	$Min_{xd}$	$Min_d$	$Max_{xd}$	$Max_d$	$Ave_{xd}$	$Ave_d$
RD0260	4	5	97	67	100	100	99.4	93.0
RD0500	4	5	76	46	97	97	81.6	80.4
RD4800	5	5	97	67	100	100	99.5	93.5
RE2140	2	4	100	97	100	100	100.0	99.4
RE6781	2	4	100	79	100	100	100.0	94.8
RF6320	4	5	95	46	100	100	96.4	89.3
RL0503	1	2	97	97	97	97	97.9	97.9
RL1141	2	3	95	69	95	95	95.9	87.1
RS0380	1	2	95	81	95	83	95.9	82.5
RS1141	2	3	94	68	94	96	94.1	86.1



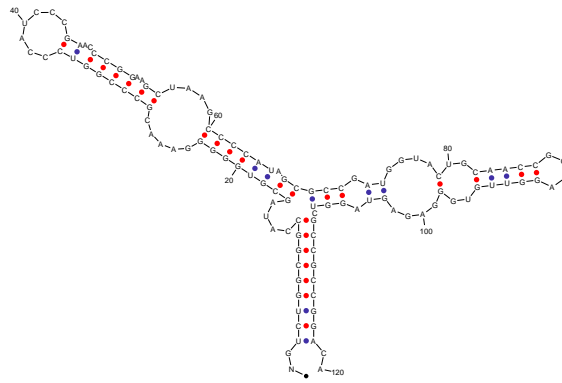
**Fig. 3.** Reference (a), Dynalign (b) and X-Dynalign (c) structures for the tRNA RS0380.

**Table 5.** Sensitivity for the 5S dataset.

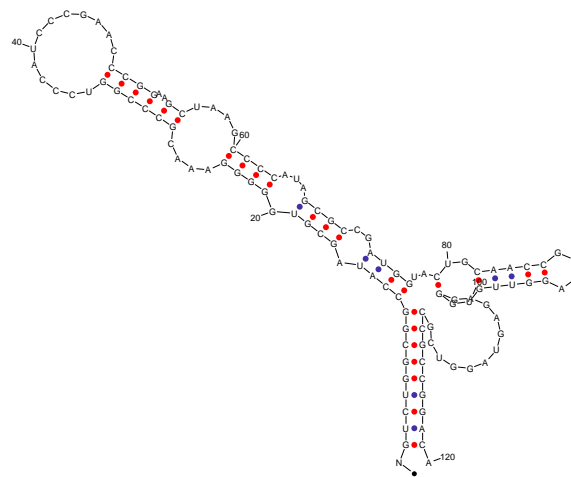
Id	$N_{xd}$	$N_d$	$Min_{xd}$	$Min_d$	$Max_{xd}$	$Max_d$	$Ave_{xd}$	$Ave_d$
AJ131594	2	3	86	86	86	89	86.8	87.7
AJ251080	6	5	76	76	78	84	77.2	79.4
D11460	6	5	73	63	76	81	74.6	71.1
K02682	8	9	53	79	84	89	76.3	84.3
M10816	3	4	76	76	78	84	77.2	80.9
M16532	1	2	82	71	82	76	82.1	74.3
M25591	6	5	76	76	78	84	76.7	79.4
V00336	3	4	62	57	82	90	75.8	78.8
X02024	9	6	76	73	78	84	77.2	76.8
X02627	1	2	84	87	84	89	84.6	88.5
X04585	2	3	63	63	84	81	73.7	74.6
X08000	5	5	74	74	74	79	74.4	77.5
X08002	5	5	74	74	74	79	74.4	77.5



(a)



(b)



(c)

**Fig. 4.** Reference (a), Dynalign (b) and X-Dynalign (c) secondary structures for the 5S rRNA K02682.

**Table 6.** MCC for the 5S dataset.

Id	$N_{xd}$	$N_d$	$\text{Min}_{xd}$	$\text{Min}_d$	$\text{Max}_{xd}$	$\text{Max}_d$	$\text{Ave}_{xd}$	$\text{Ave}_d$
AJ131594	2	3	93	89	93	93	93.2	91.0
AJ251080	6	5	83	79	84	85	83.5	82.1
D11460	6	5	80	64	81	85	80.8	75.1
K02682	8	9	58	85	92	93	82.4	88.1
M10816	3	4	83	80	84	86	83.7	84.3
M16532	1	2	87	74	87	81	87.9	78.0
M25591	6	5	81	79	83	85	83.0	82.1
V00336	3	4	68	61	90	94	83.5	84.8
X02024	9	6	83	79	84	86	83.4	81.1
X02627	1	2	92	90	92	93	92.0	92.2
X04585	2	3	67	65	89	87	78.4	78.5
X08000	5	5	82	82	82	83	82.1	83.2
X08002	5	5	82	82	82	83	82.1	83.2