International Conference on Recent Trends in Data Science and its Applications
DOI: rp-9788770040723.069

An Analysis in the Identification of Secondary RNA Structure Using Energy Algorithm

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Abstract—RNA particles have several varieties of important activities within animals' bodies, involving genetic control, processing, and nutrient production. Because various foldable configurations of molecular RNA are so important for biological functioning, a considerable lot more work has gone into creating precise algorithms that predict RNA supplementary organization using overall basis sequences. The lowest complimentary resource forecasts predicated upon closest neighbour physicochemical characteristics were commonly employed. Techniques that use partitioning functional computations to discover overall organization having maximal anticipated correctness but rather simulated anticipated precision approaches have already been suggested. Considering databases containing established target architectures, advancements throughout predictions algorithms were often appraised employing sensitivities, positively predicting values, especially associated harmonized maximum, specifically F-measure. Because comparable evaluations track development towards increasing environmental quality for computationally forecasting techniques, this seems application have this essential to understanding exactly performance measurements change with changing references collections but also only when enhancements throughout techniques specific environmental characteristics result throughout scientifically meaningful increases. Without regard to this same most recent database but also energetic characteristics, this study extends fundamental knowledge regarding MFE and MEA-based approaches.

Keywords—Secondary RNA sequences; Potential energies; Performance Measures; MFE and MEA approaches

I. INTRODUCTION

RNA proteins were required for a variety of important tasks within every species' body. Certain compounds, such particular, play an important role during genetic translations so well both acting either catalysis but honesty and integrity moderators on genes activation [1]. Considering molecules architecture determines functionality, much has a considerable lot of money is invested in computer approaches that anticipate RNA intermediate architecture, which may then be used to estimate the fundamental framework [2]. The objective was to use theoretically sound methods to evaluate the overall advantages of certain contemporary advancements throughout intermediate structural predictions.

Considering basic foundation sequences, researchers concentrate upon thermochemical inspired techniques towards forecasting pseudoknot complimentary subsequent architectures [3]. This minimal free energy (MFE) organization having regard for the closest neighbouring heat transfer models is found using another commonly employed approach. Both improved maximum expected accuracy (MEA-based) and also greatest pseudo-anticipated reliability were two significant breakthroughs throughout intermediate architecture predictions. Those techniques provide greater averaged correctness over conventional MFE algorithms upon fundamental energies components but also improve (pseudo) anticipated basis pairing correctness being any proportion variable bases pairing possibilities determined utilizing another partitioning functional methodology.

II. RELATED WORKS

Several probability simulations describing architectures are used to anticipate RNA intermediate organization. However, because these statistical techniques were essentially based upon actual macroeconomic framework, designers will not incorporate them throughout any subsequent assessments [4]. Further advancement was that estimate for additional energetic characteristics employing government calculation algorithms from relational isothermal but also architectural information [5]. Inferring parametric settings using energy acquired utilizing optically melted studies is much atomic architectural information. These 2 collections of temperature characteristics were referred to known as BL but also CG, respectively, following this Boltzmann possibility but also constrained generating procedures that were employed to derive these. When compared to conventional Original specifications, those variable groupings resulted in considerable advances in overall MFE methodology predictions efficiency, having both BL characteristics marginally superior to those overall CG variables [6].Here and throughout, the accuracy of a prediction refers to its Measure, which is the harmonic mean of sensitivity and positive predictive value. This research

DOI: rp-9788770040723.069

evaluates algorithmic effectiveness upon individual categories identify RNAs, including genomic regions and transferring RNAs, also much its general median performance across RNAs across various categories. MFE approaches without regard of various variants of original variables, by much as relatively latest BL but also CG specifications using information spanning single RNA classifications on much as huge databases which contain numerous RNA categories to address important concerns [7-8].

Several major conclusions are presented. Firstly, designers demonstrate whether F-measure precision across experimental big databases was expected likely constitute trustworthy estimations of overall demographic precision, particularly this same notion because slightly elevated intervals breadth in F-measure computed employing this same bootstrapping maximum approach were around relatively limited, 2% spread. Over fewer courses, averaged reliability was lower dependable [9]. Given another population comprising 89 Category I introns having recently been employed throughout benchmarks methods, confident estimates with overall MEA but also MFE comprise approximately 8 % variance. Secondly, throughout perspective in total forecasting efficiency, they were an obvious "champion," notably this same pseudo-MEA-based technique [10-11]. This same corresponding exactness of this same MFE but rather Types single sample self-frameworks, moreover, becomes dependent on this same underpinning power generation specifications: that used a factorization experiment, designers encounter that this same correctness of MFE-based estimation on everything with us other humongous databases becomes preferable on 2 of this same 4 electricity input variables which humans regard, at a numerically considerable standard [12]. While MEA-based prediction is better than MFE-based prediction on a third parameter set. Ultimately, while employing this same fourth variable, this same BL* radiation variables, combined Types of self but also MFE approaches obtain overall best reliability. The authors developed Rsample, an algorithm for predicting various RNA structures from experimental data for sequences that populate several forms at equilibrium. They've shown that they can simulate RNA sequences using SHAPE mapping data with high accuracy [13-14].

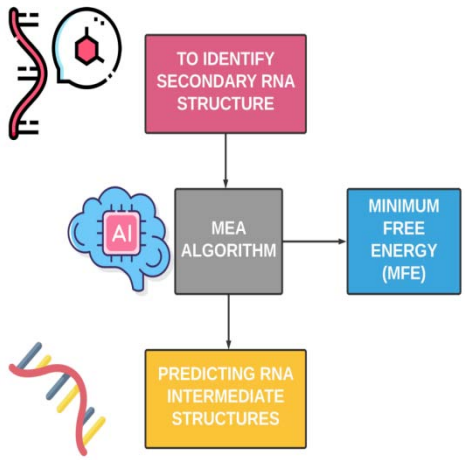

Fig.1. Proposed architecture of RNA secondary prediction using ML

III. Proposed Methods

S-Full includes another collection comprising 3,245 RNA strands with associated supplementary properties culled through several varieties of different credible repositories. Segments within the above but also comparable databases have a maximum limited value of 700 characters; although in certain circumstances, bigger sequencing, including instance 16S Ribosomal RNA segments, be partitioned to achieve compliance. Throughout S-Full, this same overall frequency for every nucleotide was 270nt. 16S Ribosomal RNA, 23S Ribosomal RNA, 5S Ribosomal RNA, Group I organelle, Group II transposon, Ribonuclease P RNA, Signals Identification RNA, but instead Transfers RNA are some of the several types of nucleotide RNA. • MA represents another subgroup for this same S-Full collection, comprising only individual S-Full sequences found within specific RNA categories covered by MT. This MA collection was created such that researchers could investigate different methods around these same categories despite employing that many RNAs representing various categories were feasible. These conclusions were based upon this limited version from this MT collection wherein particular sequencing characters appear written in smaller cases, suggesting indicates its basis was stranded within the original comparison framework. Researchers made projections based upon such fundamental knowledge. Designers, on the other hand, have simply used such knowledge, consequently, overall consistency metrics using actual MT collection remain differently.

This thermodynamics modelling comprises made up of characteristics, which are tiny compositional themes like stacking pairings, and constant temperature transition variables, which are assigned to each characteristic. This same Taylor 99, this same final version humans employ, was the greatest extensively represented energies models in RNA intermediate structural predictions. This framework comprises about 7600 characteristics predicated upon Anderson's closest neighbours constraints, which were to represent this same premise because this durability for any foundation pairing and the circle is determined by their sequencing and structural sequencing surrounding nearby repeats with unattached nucleotides. Another of these architectural patterns, concentric layering, was created using basic characteristics from another later edition of these same Taylor models, Turner2004. This Turner99 designer's characteristics are being used throughout this majority of all these same architectural motifs. Because the majority half these characteristics were Turner99 characteristics because this same concentric layering pattern was never featured within every alternative model humans investigate, humans additionally designate this characteristic collection utilized under this same Turner99. Characteristics that help determine the architecture of RNA. However, researchers need cannot include these characteristics throughout the current study even before they were irrelevant to the overall computation of any partitioning functional however and also, as a result, to the overall probabilities determination needed by using MEA technique.

They look at several different techniques for predicting RNA intermediate structures. This former forecasts

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supplementary formations containing this same minimum free energy (MFE) with a certain thermodynamics framework. The following methodology was another maximum expected accuracy (MEA), which improves predicted basis pairing correctness by any proportion on basis pairing probability computed utilizing termed partitioning functional technique. Regarding usage utilizing these MultiRNAFoldmodelling, researchers built using MEA algorithms. For such consequence, scientists experimented simply exclusively using either safe and EMEA techniques, however additionally produced this same UBC MFA MFE program but instead, another unique version for MEA termed UBC MBA. Whenever this same g component of this same rsMEA was adjusted to 1, this delivers the overall highest forecasting performance. As this result, designers adjusted g equal 1 within UBC MBA as well. This extended median estimation technique was this next technique will look examine. One such approach was comparable with previous MEA methodology, however instead infers architectural configuration using base-pairing possibilities using another slightly alternative objectives functional, notably using brightness estimation.

Overall structurally predicting efficiency is determined using 3 initiatives: sensitivities positively predicting values but rather PPV, but also F-measure, whose integrates sensitivities but also PPV together any singular metric. That percentage between accurately forecast basis pairings over this same overall bases pairings within overall standard architecture was the response. This percentage accurately expected bases pairings irrespective of overall forecasted bases pairings were known simply as PPV. This same harmonized average between this sensitivity and PPV termed measures F-measure. Whenever sensitivities and PPV were both identical, one such number equals the overall numerical median. Whenever 1 among these integers approaches 0, meanwhile, these same F-measure increases lower under overall numerical means. Humans chose to use F-measure over traditional Pearson correlations coefficients primarily because makes was easier can compare their conclusions against theirs.

$$\text{Sensitivity} = \frac{No.of\ Correctly\ \ predicted\ \ base\ pairs}{No.of\ \ base\ \ pairs\ \ in\ reference\ \ \ structure} \quad (1)$$

$$\text{PPV} = \frac{No.of\ Correctly\ \ predicted\ \ base\ pairs}{No.of\ \ predicted\ \ \ base\ pairs} \quad (2)$$

$$\text{F-score} = \frac{2*Sensitivity\ *PPV}{Sensitivity\ *PPV} \quad (3)$$

Table 1 shows estimated averaged normalizing commonalities, which typically lie amongst 0 but also person, with an overall value approaching something indicating meaning individual segments within this collection were comparable. Whenever si seems to be 0 across every RNA category, the overall weighted average matches this same balanced averages, whereas whenever it reaches across every course, this matches this same overall ordinary approximate. Considering those other circumstances, this same S-weighted average's frequency might be somewhere around either approximate but also balanced averaged.

TABLE 1. RNA INFORMATION SOURCES

RNA class	No. in MT	Mean ± std of length	Average similarity	No. in MA	Mean ± std of length	Average similarity
16S Ribosomal RNA	87	367.97±157.13	0.61	671	486.34±112.01	0.60
23S Ribosomal RNA	25	459.6±149.54	0.52	162	443.47±118.88	0.55
5S Ribosomal RNA	312	128.5±2.70	0.87	130	110.98±2.98	0.87
Group 1 intron	13	351.84±65.20	0.60	87	358.98±113.01	0.60
Group 2 intron	2	657.9±71.65	0.72	2	571±46.05	0.71
Ribonuclease P RNA	7	374.30±40.54	0.75	398	331.79±53.50	0.71
Signal Recognition RNA	88	262.87±60.35	0.73	354	225.02±110.55	0.62
Transfer RNA	481	75.84±3.9	0.98	479	76.15±5.60	0.97
Total	1112			2207		

IV. RESULTS AND DISCUSSION

This is critical to understanding comprehend because these metrics differ based upon actual comparable information employed. We'll look to examine whether correctness measurements differ based on the energy modelling employed subsequently throughout the following chapter. This background information from Table 2 reveals even between furthermore MA and MT datasets overall must be potentially large disparities regarding algorithmic performance across Nucleotide classifications. By illustrating, while implementing default BL* configuration one DNA polymerase P RNA, UBC MBA obtains an F-measure of 0.471 on the MT collection against 0.643 with matching MA database, total differential equal nearly 17%.

TABLE 2. PERFORMANCE MEASURES

RNA class	Class size	Mean ± std of length	ubcMEA	ubcMFE	gC-gI	gC pMFmeas	RsMEA	rsMFE
16S Ribosomal RNA	87	367.97±157.13	0.686	0.631	0.648	0.649	0.579	0.579
23S Ribosomal RNA	25	459.6±149.54	0.701	0.684	0.691	0.745	0.674	0.647
5S Ribosomal RNA	312	128.5±2.70	0.741	0.746	0.757	0.764	0.614	0.614
Group 1 intron	13	351.84±65.20	0.701	0.645	0.784	0.709	0.647	0.579
Group 2 intron	2	657.9±71.65	0.720	0.761	0.798	0.764	0.756	0.731
Ribonuclease P RNA	7	374.30±40.54	0.541	0.484	0.468	0.487	0.547	0.547
Signal Recognition RNA	88	262.87±60.35	0.647	0.648	0.617	0.679	0.518	0.567
Transfer RNA	481	75.84±3.9	0.719	0.776	0.781	0.794	0.794	0.726
Unweighted Avg			0.659	0.667	0.648	0.698	0.647	0.674
Weighted Avg			0.725	0.735	0.712	0.746	0.669	0.664
S-Weighted Avg			0.679	0.647	0.647	0.687	0.603	0.598

Table.1 shows this same differentiation throughout accuracies on its MT instead of MA data points on relational this same DNA polymerase P RNA but rather this same Group 1 ubcMEA, UBC MFA, but rather GC-pm means software, which uses this same BL* specifications, but rather towards this same rsMEA but a rather safe machine learning, has used its Turner99 specifications, for this same ubcMEA, UBC MFA, but rather higher the discrepancy in Fig.2, the farther those spots were towards those highlighted diagonally lines. Every one among these 10 information samples shows an overall discrepancy equal to less than 3.2

DOI: rp-9788770040723.069

%. Those findings show why someone could indeed derive significant inferences concerning this same typical accuracy for identifying a given methodology upon the whole demographic within a specific RNA category depending hardly alone on this same general correctness for presently accessible information absent additional quantitative research.

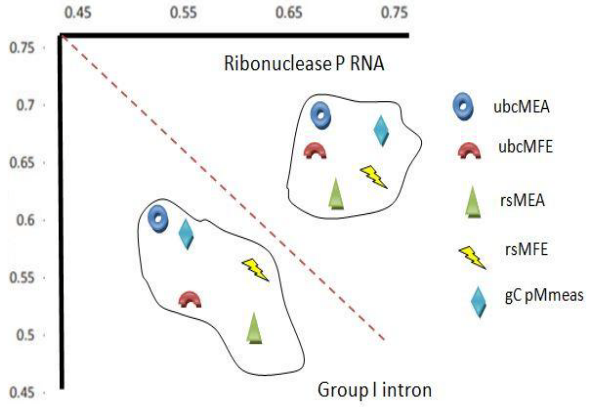

Fig.2. Comparative analysis

TABLE 3. PERFORMANCE ANALYSIS OF PROPOSED WITH EXISTING METHODS

RNA class	Class size	Mean ± std of length	ubcMEA	ubcMFE	gC-gI	gC pMFmeas	RsMEA	rsMFE
16S Ribosomal RNA	671	486.34±112.01	0.657	0.620	0.634	0.651	0.547	0.517
23S Ribosomal RNA	162	443.47±118.88	0.701	0.681	0.698	0.721	0.615	0.647
5S Ribosomal RNA	130	110.98±2.98	0.742	0.741	0.720	0.764	0.615	0.624
Group 1 intron	87	358.98±113.01	0.701	0.641	0.647	0.709	0.678	0.594
Group 2 intron	2	571±46.05	0.715	0.734	0.684	0.714	0.765	0.706
Ribonuclease P RNA	398	331.79±53.50	0.451	0.454	0.505	0.449	0.507	0.518
Signal Recognition RNA	354	225.02±110.55	0.678	0.619	0.614	0.679	0.579	0.517
Transfer RNA	479	76.15±5.60	0.721	0.768	0.734	0.798	0.701	0.714
Unweighted Avg			0.66	0.654	0.657	0.684	0.671	0.621
Weighted Avg			0.701	0.754	0.726	0.734	0.614	0.687
S-Weighted Avg			0.660	0.674	0.648	0.648	0.624	0.583

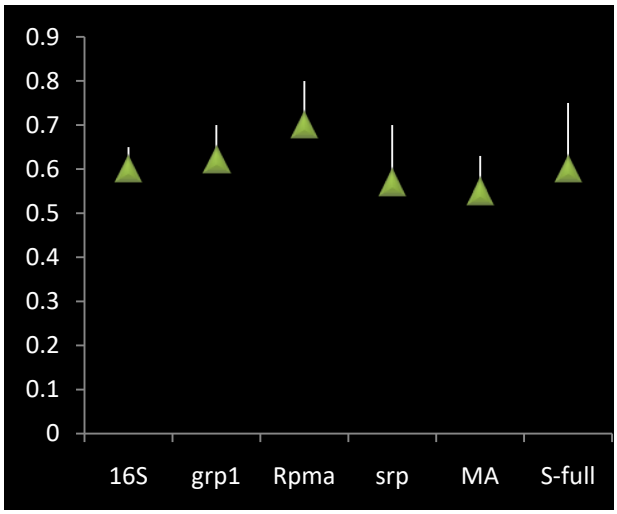

Fig.3. Bootstrap performance over proposed method

Fig.3 displays an estimated 95 % probability of bootstrapping maximum credibility ranges for applying UBC MBA but also UBC MFA methods upon specific RNA subclasses including overall MA but also S-Full databases utilizing this same BL* sensitivity combination. Table 3 shows that BL* characteristic collection's 90 % probability bootstrapping maximum credibility ranges both generating UBC MFA but phase which means flow cytometry procedures. Firstly, both MA and S-Full settings' test statistics possess a maximum mean diameter of around 0.018, demonstrating, therefore, their median reliability assessed using those collections was expected would constitute a very reasonable approximation - around 1% - for overall precision for any community containing Biomolecules reflected under those pairs. Particular classification intermediate thicknesses sometimes are substantially wider, for example, 0.075 using UBC MBA upon any Groups I transposon category, implying, therefore, averaged correctness was a hardly very credible estimate on any product's ultimate efficiency across certain categories. A 0.02 differential overall correctness was deemed substantial within certain relevant studies requiring using application of more sophisticated quantitative approaches. Secondly, overall breadth within RNA subclass probability intervals may always absolutely decline while the overall population in that category grows. Even though its Transporter RNA classification includes around 1.2 twice more numerous RNAs than its Endonuclease P RNA category, this same DNA polymerase P RNA category has maximum probability intervals thickness approximately 0.01 smaller than this same Transport RNA category using this same UBC MBA methodology. Probability intervals thicknesses need thereby be accounted covered by parameters relevant to all individual subclasses additional beyond course number. UbcMEA but instead UBC MFA procedures have 95 percentage bootstrapping probability ranges.

Each hypothesis indicates that categories having more structural similarities maintain lower confident windows because this same probability region approaches 0 breadth towards extreme limiting whenever every sequencing within a given category becomes comparable. Fixtures 1 information, by this same other hand, showed never show exhibit strong link amongst averaged standardized resemblance but also credibility intervals breadth, particularly among categories that were neither very dissimilar overall magnitude. Within this Massachusetts collection, by illustration, individuals Utilizing available 0.001 but also Transporter Deoxyribonucleic acid (DNA classifications possess comparable dimensions, even though identical DNA processor P RNA subcategory has had far lower adjusted weight. Furthermore, the overall breadth of estimated credibility intervals using this same UBC MFA method is generally similar to those from that whole UBC MBA but also GC-pm means algorithms for every particular information, although unless actual intervals locations might seem somewhat dissimilar. Under their DNA polymerase Pg Ribosome category, for illustration, median averaged F-measures from UBC MBA and UBC MFA differed by approximately 0.04, although their credibility intervals thicknesses remain similar. That instance, amongst these three methods, overall least but also maximum confident intervals thicknesses that its 16S Ribosomal RNA classification were 0.026 and 0.030, accordingly, indicating significant differential equal lower about 0.01 % spacing breadth under a particular classification.

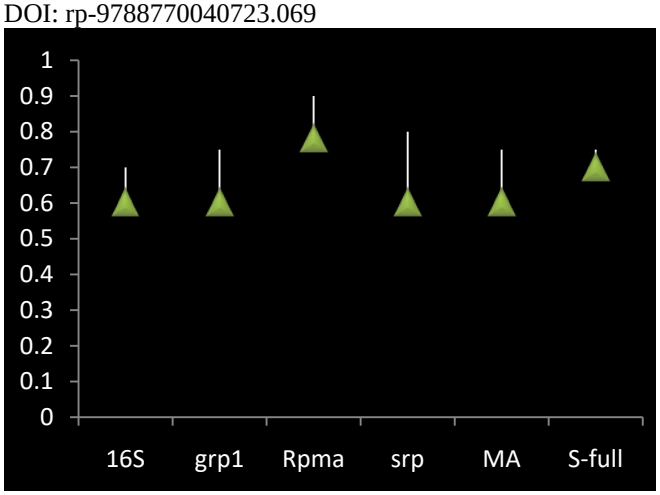

Fig.4. Bootstrapping maximum uncertainty ranges

Using experimental ubcMEA, UBC MFA, and GC-PMFmeas techniques, Fig.4 displays the estimated breadth of the credibility regions vs overall sizes among distinct RNA subclasses. This could be seen, practically the majority set observed locations from those 3 techniques were similar equal height within their respective dimensions, showing either ubcMEA, UBC MFA, but also GC-PMFmeas possess the same breadth. Another key takeaway from this graph was generally, while 1 might anticipate, overall breadth is median probability intervals shrink when total amount individual RNAs having every particular class throughout this same precedent collection is larger, although were noticeable outliers following such a tendency, especially groups smaller than 500.

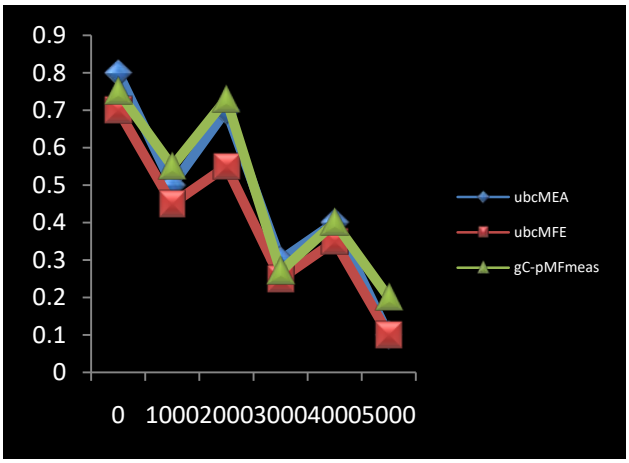

Fig.5. Comparison analysis of performance measures

Furthermore, they see found, dependent upon our power models, MFE occasionally outperforms MEA across any certain category with RNAs but also conversely (shown Start Fig.5). In that instance, MFE beats MEA by about 0.02 while applying standard BL* variable collection with their collection of endonuclease RNAs, but MEA improves Interventions made besides 0.04 because once employing its Complete Newton 98 variables. Furthermore, they find to show this same comparative effectiveness using MEA vs MFE is dependent upon particular physicochemical variable collection employed, particularly, therefore, ubcMBA but instead, UBC MFA using this same BL* information group is much more accurate than rsMEA utilizing standard Turner99 information setting.

V. Conclusions

Scientific advancements using computerized techniques, especially heat transfer computations, have helped intermediary superstructure predictions make substantial advances. Throughout this paper, researchers demonstrate whether GC-pm means without this same BL* variable setting beats most previous MFE and previously unapproached they looked quite considerably. Nevertheless, dependent upon the particular thermodynamics input variable employed, overall comparative effectiveness between Stereotypes with MFE approaches varies. Under this same Turner99 simulation, for instance, Previously un techniques greatly outperform the lowest freed energetic approaches, although this same converse holds applicable for many simulations, while overall differential throughout effectiveness among Stereotype versus MFE approaches using their strongest thermostatic framework, BL*, seems minimal. These observations show suggesting having a varied array of computational approaches would continue will have been useful while thermodynamics simulations advance. Designers additionally demonstrated potential relevance for evaluating overall correctness using certain strategies but abrading thermodynamics simulations utilizing huge information. Humans demonstrated that this same ordinary highest consistency template per cent range test statistics on with us 2 greatest information - frames, MA but rather S-Full, possess constricted dimensions, implying that this same ordinary precision assessed on such pairs possess become probable to be great projections of this same error margins of this same community of RNA particles consumers reflect. Distance lengths remained substantially greater across numerous among those individual RNA subclasses evaluated throughout the research article, without little evident association among probability distance length but also category number but rather a median normalization resemblance.

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