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A homology model for 16S rRNA tertiary structure of *Frankia*

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Abstract

Tertiary structure determination of biomolecule is important for knowing their function. Although different experimental prediction methods are present computational approach has an important role. *Frankia sp.*, is a nitrogen fixing bacterium promoting soil fertility.16S ribosomal nucleic acid molecule is not only important as a molecular signature for classification and identification of organisms but has a great impact on protein synthesis. Here we have developed 3D structure of 16S rRNA of three different strains of *Frankia* viz. *Frankia* sp. strain HFPCcl3, *Frankia alni* strain ACN14a and *Frankia* sp. strain EAN1pec through knowledge based coarsed to atomic approach. The occurrence of tertiary structural motifs like C-loop, E-loop, GNRA tetraloop, hook-turn, sarcin-ricin motif, K-turn, reverse K-turn were examined. The presence of such sort of motif stabilizes the complexed RNA structures through their Watson-Crick, Non-Watson Crick, tandem sheared stacking packages. Among them E-loop, K-turn, sarcin-ricin motif have significant functional importance for transporting the biomolecules, RNA-protein interaction, RNA-RNA interaction/RNA-drug interaction accordingly.

Keywords: Homology modeling, *Frankia*, 16S rRNA, GNRA, NMR,

The 16S rRNA acts as a novel model for not only taxonomic differentiation but also for understanding the clinical microbiology and infectious diseases and also for identifying the non-cultured bacteria (Clarridge III 2004). 16S rRNA genes can also be assigned as 16S rDNA genes. Both are in interchangeable form. It is most stable among all genetic material during evolution (Goudarzi *et al.* 2006) and thus is used for not only comparing among all bacterial world but also with the 16S rRNA genes of archeobacteria as well as 18S rRNA genes of eukaryotes (Clarridge III 2004). It also has functional association with protein synthesis and may directly or indirectly involve in the translational machineries to regulate the mRNA translation into proteins. But their function in protein synthesis is still unclear to us (Saraiya *et al.* 2009). There are limited numbers of tertiary structural information available in structural database relative to primary structure available in the sequence database. Since tertiary structure carry much more conserved structural-functional relationship in comparison to primary structure so there has a need to develop a 3D structure based analysis to explore its new look. Generally like protein the primary structure of RNA folds into its much more compact form and thus introduce the ribosomal subunit for interacting remotely. The building blocks of RNA structure are RNA-motifs. According to the Leontis *et al.* (2003) RNA motifs are the directed and the ordered arrays of non-WC base pairs forming distinctive folding of the phosphodiester backbones of the interacting RNA strands. The specific motif comprised with similar tertiary conformation with its similar sort of tertiary interaction i.e. they are much more conserved part of a structure. Here our main objective is to design 3D structure of 16S rRNA of three different *Frankia* strains from its 1D information. The three different *Frankia* strains are *Frankia alni* ACN14a, *Frankia sp.* Ccl3 and *Frankia sp.* EAN1pec. *Frankia sp.* are facultative symbiont of actinorhizal plants. By late 19's century scientists have discovered that it has a capability to fix environmental nitrogen into the root nodules of non-leguminous plants (Benson and Silvester 1993). Thus it may arise its importance in ecological as well as in agricultural field in future. It can be used as a reducer of soil-droughts. Nitrogen fixative genes share a common evolutionary history with 16S rRNA. So the development of tertiary structure is much more prevalent over its primary one. Homology model of 16S rRNA structure was generated through *In-silico* approach. There are a number of solved 16S rRNA structure of different bacteria existed in structural database. But they were predicted through crystallography or NMR method. Both are time consuming and expensive one to use where as computational approach not only reduces the cost but also a faster one in this new emerging field.

Materials and Methods

The 16S rRNA gene sequences in FASTA format for the following organisms were taken from IMG database (http://img.jgi.doe.gov/). They are *Frankia alni* ACN14a, *Frankia sp.* Ccl3 and *Frankia sp.* EAN1pec.

The secondary structures of all 16S rRNA were predicted through MFold web server of Mr. Zuker Version 2.3(http://mfold.rna.albany.edu//?q=mfold/RNA

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Table 1: Number of loop, helix and single strand segment

Strain	Loop	Helix	SSS*
ACN14a	23	58	111
Ccl3	18	51	100
EAN1pec	20	54	102

*SSS=single strand segment

-Folding-Form2.3). The folding temperature was changed into 30°C and other default parameters were used. The coarsed-grained structures of each all were generated by NAST (Nucleic Acid Simulation Tool). The full atomic structure of the above said generated coarse-grained structure were further evolved through the coarse to atomic package of NAST. Finally full 3D structure of 16S rRNA of the above three strains were obtained and here I have used 2QAL (PDB ID) as reference 16S rRNA model for structure prediction through homology modeling concept. 2QAL contains the 16S rRNA of *E. coli*. Energy Minimization of the generated 3D structure was performed with Gromacs package where it was modified with Amber Force Field 99 which is a nucleic acid supported force field. We have used the Gromacs 4.0.7 and fftw of 3.3.2 version in Ubuntu Linux Platform. The above three structures were energy minimized in Vacuum to get a much more stabilized and accepted form. The structures were then further validated through RCSB validation server (http://deposit.pdb.org/validate/). The structures were then annotated by RNAview software package which reveals their intra-atomic configuration in detail. Again the inbuilt tertiary structural features were studied from the generated 3D structures through RNAMotifScan to get into the structural-functional relationship.

Results and Discussion

We restricted our study to three different strains of *Frankia sp.* to understand their structural inbuilt of 16S rRNA for their functional importance at 3D level relative to 1D. According to the analysis of primary structure so far studied, it is revealed that among the *Frankia alni* ACN14a, *Frankia sp.* Ccl3 and *Frankia sp.* EAN1pec the 16S rRNA primary structure is 97.8-98.9% conserved signifies their evolutionary sequence level conservation irrespective to the other factors (Mastronunzio *et al.* 2008) The generated 2D structure have their Gibb's free energy of -668.48kcal/mol, -662.44kcal/mol and -661.24kcal/mol for 16S rRNA of *Frankia alni* ACN14a, *Frankia sp.* Ccl3 and *Frankia sp.* EAN1pec respectively at 30 °C. The negative Gibb's free energy of the generated secondary structures reveal about their stable conformation. The stable 2D conformation selection for tertiary structure prediction is much more important as it incorporate the primary building blocks like helix, loop.

These secondary structures were further used to develop the tertiary one. We have developed 3D structure of 16S rRNA of three different strains of *Frankia sp.* through knowledge based coarsed to atomic approach by NAST and c2a package (Jonikas *et al.* 2009). The energy minimized homology model have their potential energy of 1.505e+05 kJ/mol, 3.09e+05kJ/mol and 1.69e+kJ/mol for 16S rRNA of *Frankia alni* ACN14a, *Frankia sp.* Ccl3 and *Frankia sp.* EAN1pec respectively. The validated report shows that the structures have 10-15% of outliers need to refine them in future as it is out of scope of present platform available so far. The annotated analysis of these partially stabilized structure shows their brief details of intra-atomic configuration which are given in a Table 1a,1b and 1c .

We analyzed the building blocks of RNA architecture i.e. the 3D motifs in these experimentally derived 16S rRNA tertiary structure. The result demonstrate that each of the three generated model consists of C-loop, E-loop, GNRA, K-turn, reverse K-turn, sarcin-ricin, hook-turn like most conserved 3D building blocks which are shown by Table 2. The presence of number of C-loops in all three structures show that the bases in the longer strand form non-WC base pairs with the bases in the shorter strand. There are also unpaired bases present as extruded. They have their unique functional importance in living creatures. Structural stability and conservation depends on the presence of structural motifs like C-loop, E-loop, GNRA, K-turn, reverse K-turn, hook-turn.

C-loop motif is an internal loop which is asymmetrical in nature. The presence of C-loop in the stem-loop structure reveals its importance in the tertiary interaction between the two hairpins. It also helps to twist the helical stem between two WC base pairs (Lescoute *et al.* 2005). Here the presence of WC base-pair acts as helix twister. The complex form of its tertiary nature stabilizes the 3D structure of the whole molecule. C-loop in 16S rRNA has affinity to interact with protein and it also acts as a complex in between the threonine synthetase and the synthetase itself. Thus it performs certain sort of cell regulation (Leontis and Westhof 2003).

GNRA is tetraloop in nature. In GNRA N stands for any nucleic acid and R stands for purine bases. It has a functional importance for tetraloop-tetraloop receptor interactions. It is thermodynamically stable in nature relative to the other tetraloops. There are high percentage of GNRA exists in RNA molecules e.g. 70% of tetraloop belongs to GNRA/ UNCG family in ribosomal RNA (Hendrix *et al.* 2005).

K-turns or kinks are recurrent internal loops which produce pointed kinks or twist in the helical region in

Table 2 Overview of base pair types

Strain	Base pair types												
	WW		HH		SS		WH		WS		HS		standard
	cis	trans	cis	trans	cis	trans	cis	trans	cis	trans	cis	trans	
ACN14a	108	6	1	1	1	0	5	27	8	3	5	13	95
Ccl3	94	10	0	0	1	1	3	30	8	5	3	26	76
EAN1pec	90	6	0	0	2	3	2	30	5	5	8	27	83

Table 3 Glycosyl-conformation (syn base-position) in 16SrRNA of *Frankia*

Strain	Syn base-position
ACN14a	77, 93, 101, 114, 146, 147, 156, 169, 192, 207, 221, 248, 250, 254, 264, 276, 300, 301, 315, 331, 347, 366, 380, 381, 383, 388, 405, 407, 423, 446, 447, 489, 490, 503, 515, 516, 526, 554, 596, 597, 608, 610, 623, 628, 640, 642, 658, 667, 680, 707, 715, 734, 780, 819, 820, 822, 829, 834, 839, 882, 891, 929, 997, 1000, 1032, 1038, 1099, 1100, 1138, 1168, 1209, 1210, 1234, 1261, 1262, 1264, 1291, 1293, 1301, 1334, 1336, 1343, 1346, 1392, 1397, 1400, 1410, 1420, 1471, 1487, 1489
Ccl3	20, 28, 29, 31, 38, 47, 62, 64, 112, 114, 122, 126, 127, 137, 141, 209, 218, 229, 247, 254, 286, 307, 308, 311, 323, 324, 325, 367, 378, 418, 425, 427, 507, 552, 562, 584, 586, 612, 630, 642, 689, 713, 714, 729, 733, 751, 753, 766, 767, 790, 794, 822, 823, 824, 825, 833, 850, 851, 852, 853, 857, 866, 870, 916, 931, 934, 945, 946, 971, 973, 1049, 1074, 1098, 1133, 1154, 1161, 1164, 1178, 1185, 1186, 1197, 1198, 1203, 1215, 1221, 1231, 1232, 1235, 1246, 1249, 1265, 1266, 1282, 1294, 1295, 1312, 1321, 1334, 1341, 1344, 1345, 1362, 1364, 1403, 1407, 1429, 1454, 1463
EAN1pec	16, 17, 26, 27, 59, 82, 100, 101104, 114, 116, 129, 145, 168, 171, 184, 185, 187, 191, 208, 211, 213, 223, 226, 253, 272, 304, 305, 314, 374, 414, 415, 419, 423, 477, 483, 488, 515, 539, 559, 596, 596, 596, 598, 653, 656, 658, 724, 773, 783, 850, 859, 866, 867, 894, 895, 897, 927, 950, 995, 1003, 1014, 1029, 1055, 1062, 1065, 1079, 1088, 1103, 1104, 119, 1124, 1127, 1146, 1156, 1158, 1186, 1213, 1215, 1221, 1222, 1225, 1290, 1297, 1324, 1340, 1344, 1347, 1363, 1374, 1375, 1388, 1393, 1411, 1436, 1440, 1442, 1446, 1463, 1464, 1465, 1466, 1479, 1481

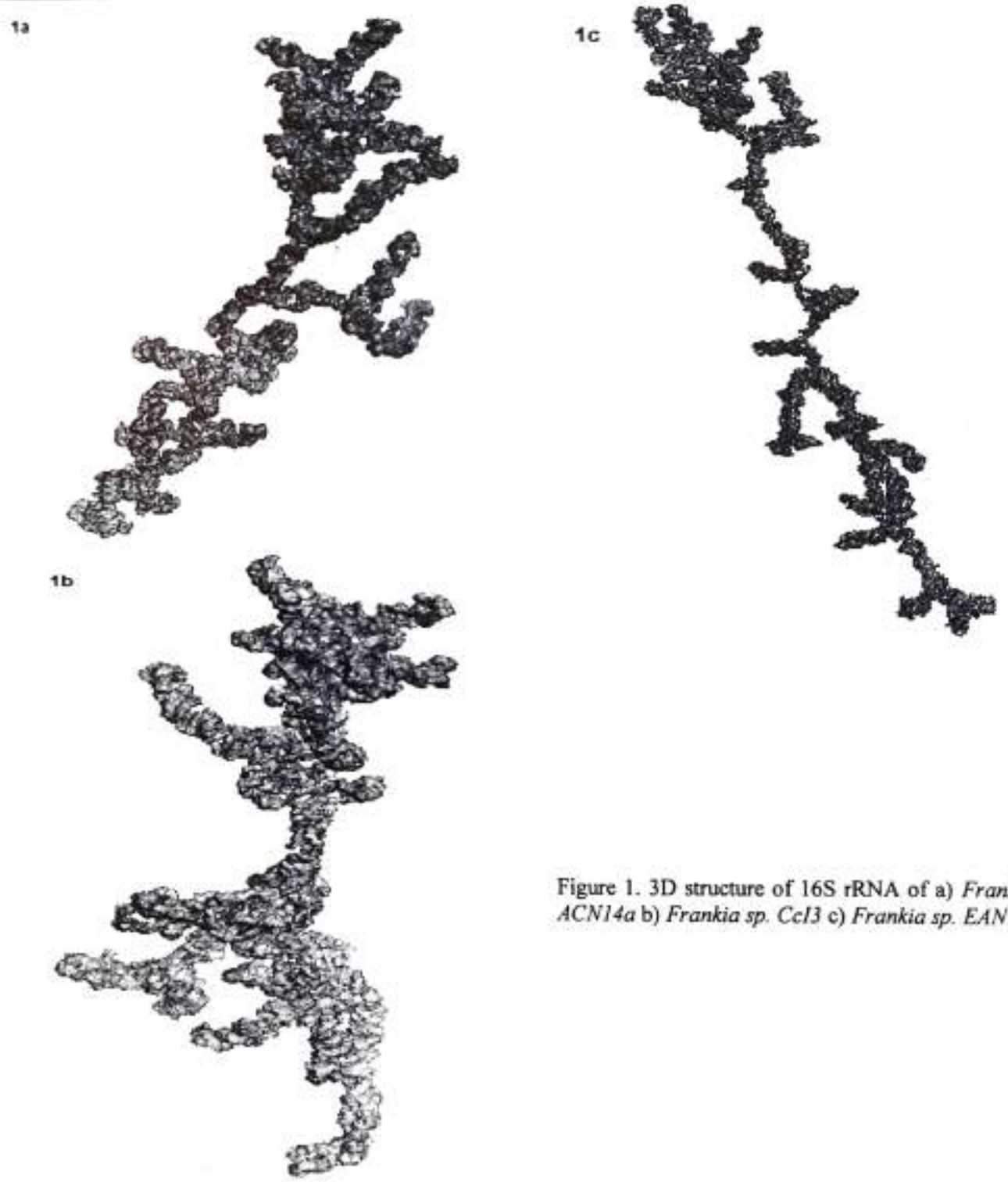

Figure 1. 3D structure of 16S rRNA of a) *Frankia alni ACN14a* b) *Frankia sp. Ccl3* c) *Frankia sp. EAN1pec*

Table 4 Structural motifs for 16srRNA of *Frankia*

Tertiary Motif	ACN14a	CcI3	EAN1pec
C-Loop	X409-X423/X392-X405	Y639-Y646/Y676-Y686	Z554-Z572/Z582-Z598
	X1164-X1174/X1149-X1158	Y1163-Y1177/Y1145-Y1160	Z243-Z253/Z225-Z238
	X128-X143/X149-X168	Y1062-Y1067/Y1038-Y1054	Z944-Z948/Z1173-Z1177
	X1090-X1095/X34-X41	Y775-Y790/Y899-Y911	Z480-Z497/Z468-Z479
	X1448-X1456/X1394-X1403	Y1303-Y1321/Y1334-Y1350	Z160-Z168/Z175-Z183
	X661-X677/X645-X657	Y552-Y558/Y609-Y616	Z546-Z552/Z257-Z263
	X1476-X1482/X1489-X1495	Y105-Y121/Y93-Y115	Z361-Z364/Z353-Z356
	X785-X796/X762-X773	Y410-Y421/Y394-Y405	Z502-Z514/Z522-Z538
	X3-X7/X1370-X1374	Y699-Y710/Y625-Y635	Z694-Z705/Z613-Z624
	X183-X191/X170-X178	Y1256-Y1262/Y1207-Y1213	Z802-Z812/Z790-Z795
	X302-X306/X319-X323	Y1430-Y1447/Y1388-Y1405	Z634-Z649/Z652-Z670
	X589-X607/X563-X582	Y518-Y530/Y156-Y166	Z988-Z1001/Z952-Z970
	X225-X231/X214-X219	Y639-Y646/Y676-Y686	Z1277-Z1293/Z1258-Z1274
	X1278-X1290/X1307-X1325	Y1163-Y1177/Y1145-Y1160	Z554-Z572/Z582-Z598
	X884-X898/X844-X850	Y1062-Y1067/Y1038-Y1054	Z243-Z253/Z225-Z238
	X1108-X1118/X1125-X1139	Y775-Y790/Y899-Y911	Z944-Z948/Z1173-Z1177
	X409-X423/X392-X405	Y1303-Y1321/Y1334-Y1350	Z480-Z497/Z468-Z479
	X1164-X1174/X1149-X1158	Y552-Y558/Y609-Y616	Z160-Z168/Z175-Z183
	X128-X143/X149-X168	Y105-Y121/Y93-Y115	Z546-Z552/Z257-Z263
	X1090-X1095/X34-X41	Y410-Y421/Y394-Y405	Z361-Z364/Z353-Z356
	X1448-X1456/X1394-X1403	Y699-Y710/Y625-Y635	Z502-Z514/Z522-Z538
	X661-X677/X645-X657	Y1256-Y1262/Y1207-Y1213	Z694-Z705/Z613-Z624
	X1476-X1482/X1489-X1495	Y1430-Y1447/Y1388-Y1405	Z802-Z812/Z790-Z795
	X785-X796/X762-X773	Y518-Y530/Y156-Y166	Z634-Z649/Z652-Z670
	X3-X7/X1370-X1374		Z988-Z1001/Z952-Z970
	X183-X191/X170-X178		Z1277-Z1293/Z1258-Z1274
	X302-X306/X319-X323		
	X589-X607/X563-X582		
	X225-X231/X214-X219		
	X1278-X1290/X1307-X1325		
	X884-X898/X844-X850		
	X1108-X1118/X1125-X1139		
	X409-X423/X392-X405		
	X1164-X1174/X1149-X1158		
	X128-X143/X149-X168		
E-Loop	X251-X255/X241-X247	Y474-Y502/Y170-Y195	Z225-Z238/Z243-Z253
	X563-X571/X599-X607	Y495-Y502/Y170-Y175	Z1075-Z1080/Z1106-Z1111
	X1370-X1374/X3-X7	Y411-Y419/Y396-Y404	Z833-Z836/Z779-Z782
	X1476-X1481/X1490-X1495	Y236-Y243/Y255-Y257	Z1478-Z1487/Z1465-Z1473
	X225-X231/X214-X219	Y23-Y31/Y1181-Y1188	Z546-Z551/Z258-Z263
	X413-X422/X393-X402	Y302-Y308/Y317-Y323	Z808-Z811/Z791-Z795
	X302-X306/X319-X323	Y518-Y524/Y160-Y166	Z228-Z234/Z246-Z251
	X645-X651/X671-X677	Y552-Y557/Y610-Y616	Z694-Z704/Z615-Z624
	X56-X62/X962-X967	Y845-Y847/Y894-Y896	Z510-Z514/Z522-Z526
	X333-X335/X326-X328	Y676-Y686/Y640-Y646	Z1173-Z1177/Z944-Z948
	X183-X191/X170-X178	Y699-Y706/Y630-Y635	Z749-Z751/Z744-Z746
	X844-X848/X895-X898	Y590-Y593/Y579-Y582	Z468-Z476/Z486-Z497
	X409-X414/X401-X405	Y41-Y43/Y1092-Y1094	Z1277-Z1284/Z1266-Z1274
	X280-X283/X286-X289	Y111-Y115/Y117-Y121	Z160-Z167/Z176-Z183
	X589-X591/X580-X582	Y775-Y779/Y907-Y911	Z906-Z909/Z1188-Z1191
	X251-X255/X241-X247	Y186-Y193/Y478-Y484	Z353-Z356/Z361-Z364
	X563-X571/X599-X607	Y1317-Y1321/Y1334-Y1338	Z1052-Z1054/Z1043-Z1045
	X1370-X1374/X3-X7	Y1274-Y1283/Y1286-Y1295	Z1106-Z1111/Z1075-Z1080
	X1476-X1481/X1490-X1495	Y105-Y109/Y93-Y97	Z243-Z249/Z231-Z238
	X225-X231/X214-X219	Y1049-Y1054/Y1062-Y1066	Z510-Z514/Z522-Z526
	X413-X422/X393-X402	Y1388-Y1390/Y1445-Y1447	Z1188-Z1191/Z906-Z909
	X302-X306/X319-X323	Y643-Y646/Y676-Y679	Z1173-Z1177/Z944-Z948
	X645-X651/X671-X677	Y1334-Y1338/Y1317-Y1321	Z257-Z262/Z547-Z552

Continued to next page

Table 4 *continued*

	X56-X62/X962-X967	Y590-Y593/Y579-Y582	Z808-Z811/Z791-Z795
	X333-X335/X326-X328	Y170-Y175/Y495-Y502	Z694-Z704/Z615-Z624
	X183-X191/X170-X178	Y474-Y483/Y187-Y195	Z361-Z364/Z353-Z356
	X844-X848/X895-X898	Y552-Y557/Y610-Y616	Z468-Z476/Z486-Z497
	X409-X414/X401-X405	Y845-Y847/Y894-Y896	Z1277-Z1284/Z1266-Z1274
	X280-X283/X286-X289	Y117-Y121/Y111-Y115	Z160-Z167/Z176-Z183
	X589-X591/X580-X582	Y699-Y706/Y630-Y635	Z1052-Z1054/Z1043-Z1045
	X251-X255/X241-X247	Y775-Y779/Y907-Y911	Z589-Z598/Z554-Z561
	X563-X571/X599-X607	Y396-Y404/Y411-Y419	Z582-Z586/Z568-Z572
	X1370-X1374/X3-X7	Y22-Y25/Y1186-Y1189	Z634-Z640/Z664-Z670
	X1476-X1481/X1490-X1495	Y41-Y43/Y1092-Y1094	Z1075-Z1080/Z1106-Z1111
	X225-X231/X214-X219	Y254-Y257/Y235-Y243	Z944-Z948/Z1173-Z1177
	X413-X422/X393-X402	Y1445-Y1447/Y1388-Y1390	Z228-Z234/Z246-Z251
	X333-X335/X326-X328	Y1049-Y1054/Y1062-Y1066	Z522-Z526/Z510-Z514
	X1476-X1481/X1490-X1495	Y317-Y323/Y302-Y308	Z906-Z909/Z1188-Z1191
	X214-X219/X225-X231	Y93-Y97/Y105-Y109	Z257-Z262/Z547-Z552
	X302-X306/X319-X323	Y1286-Y1295/Y1274-Y1283	Z619-Z624/Z694-Z700
	X580-X582/X589-X591	Y522-Y530/Y156-Y162	Z792-Z795/Z802-Z810
	X393-X402/X413-X422	Y1163-Y1169/Y1154-Y1160	Z486-Z497/Z468-Z476
	X895-X898/X844-X848	Y676-Y686/Y640-Y646	Z1043-Z1045/Z1052-Z1054
	X599-X607/X563-X571	Y495-Y502/Y170-Y175	Z1266-Z1274/Z1277-Z1284
	X3-X7/X1370-X1374	Y236-Y243/Y255-Y257	Z175-Z182/Z161-Z168
	X645-X651/X671-X677	Y579-Y582/Y590-Y593	Z353-Z356/Z361-Z364
	X130-X138/X154-X162	Y1317-Y1321/Y1334-Y1338	Z554-Z561/Z589-Z598
	X170-X178/X183-X191	Y894-Y896/Y845-Y847	Z569-Z574/Z580-Z585
	X280-X283/X286-X289	Y609-Y616/Y552-Y558	Z664-Z670/Z634-Z640
	X454-X459/X425-X431	Y111-Y115/Y117-Y121	
	X34-X41/X1090-X1095	Y907-Y911/Y775-Y779	
	X69-X75/X943-X950	Y411-Y419/Y396-Y404	
	X1285-X1290/X1307-X1314	Y1092-Y1094/Y41-Y43	
		Y22-Y25/Y1186-Y1189	
		Y1274-Y1283/Y1286-Y1295	
		Y105-Y109/Y93-Y97	
		Y1049-Y1054/Y1062-Y1066	
		Y302-Y308/Y317-Y323	
		Y1388-Y1390/Y1445-Y1447	
		Y478-Y484/Y186-Y193	
		Y699-Y706/Y630-Y635	
GNRA	X281-X283/X286-X288	Y1157-Y1160/Y1163-Y1164	Z1272-Z1274/Z1277-Z1279
			Z744-Z746/Z749-Z751
K-turn	X409-X423/X392-X405	Y410-Y421/Y394-Y405	Z580-Z598/Z554-Z574
	X1489-X1495/X1476-X1482	Y631-Y645/Y677-Y704	Z522-Z538/Z502-Z514
	X225-X231/X214-X219		Z243-Z253/Z225-Z238
	X664-X689/X636-X655		Z1075-Z1080/Z1106-Z1111
			Z175-Z183/Z160-Z168
Hook-turn	X425-X431/X454-X459	Y474-Y483/Y187-Y195	Z1106-Z1111/Z1075-Z1080
	X943-X950/X69-X75	Y1317-Y1321/Y1334-Y1338	Z1181-Z1191/Z906-Z915
	X563-X571/X599-X607	Y105-Y109/Y93-Y97	Z547-Z552/Z257-Z262
	X214-X219/X225-X231	Y1445-Y1447/Y1388-Y1390	Z589-Z598/Z554-Z561
	X302-X306/X319-X323	Y552-Y558/Y609-Y616	Z230-Z235/Z245-Z251
	X409-X414/X400-X405	Y590-Y593/Y579-Y582	Z1435-Z1445/Z1388-Z1397
	X21-X31/X1178-X1189	Y1049-Y1054/Y1062-Y1066	Z944-Z948/Z1173-Z1177
	X789-X796/X762-X769	Y899-Y909/Y777-Y790	Z582-Z586/Z568-Z572
	X1476-X1481/X1490-X1495	Y317-Y323/Y302-Y308	Z522-Z526/Z510-Z514
	X183-X191/X170-X178	Y1286-Y1295/Y1274-Y1283	Z1277-Z1284/Z1266-Z1274
	X326-X328/X333-X335	Y640-Y646/Y676-Y686	Z1258-Z1268/Z1282-Z1293
	X130-X141/X150-X162	Y1163-Y1169/Y1154-Y1160	Z1043-Z1045/Z1052-Z1054
	X3-X7/X1370-X1374	Y894-Y896/Y845-Y847	Z791-Z795/Z802-Z811
	X671-X677/X645-X651	Y699-Y710/Y625-Y635	Z353-Z356/Z361-Z364
	X1307-X1320/X1282-X1290	Y394-Y402/Y413-Y421	Z614-Z624/Z694-Z705
	X1164-X1174/X1150-X1158	Y170-Y175/Y495-Y502	Z664-Z670/Z634-Z640
	X286-X289/X280-X283	Y1178-Y1188/Y23-Y31	Z277-Z280/Z271-Z274
	X580-X582/X589-X591	Y518-Y524/Y160-Y166	Z468-Z476/Z486-Z497
	X844-X848/X895-X898	Y1109-Y1112/Y1133-Y1135	Z160-Z167/Z176-Z183
		Y1430-Y1435/Y1398-Y1405	Z1029-Z1032/Z1037-Z1040
		Y117-Y121/Y111-Y115	Z833-Z836/Z779-Z782
		Y1256-Y1262/Y1207-Y1213	
		Y41-Y43/Y1092-Y1094	

the RNA structure. K-turn is generally helix-loop-helix element which also revealed in our designed structure. It presents in the minor groove side of 16S rRNA and thus helps to fold the RNA structure in more complexed form. The number of listed K-turns comprised with two stems of which one bears connonical base-pairs and the other with non-cannonical base-pair. It helps to come closer two minor groove. It has functional importance to produce local as well as long range tertiary interaction to stabilize the complexed RNA structure (Leontis and Westhof 2003) and may participate in protein-RNA interaction (Szep *et al.* 2003).

Reverse kink-turn produce bend at the major groove of complexed structure. Thus it recalled as independent RNA-motifs (Leontis and Westhof 2003).

Sarcin-ricin motif is generally prevalent in 23S rRNA but in some 16S rRNA also include such kind of motif for its functional importance. 16S rRNA of *Frankia* CCI3 *and* EAN1pec. has very low percentage of existence of this motif where as *Frankia* ACN14a haven't for a single one. It is also reported that *Frankia* sp. is antibiotic resistance [] but the molecular basis of the symbiosis is largely unknown because genetic manipulation of *Frankia* has not been possible. But why *Frankia* ACN14a haven't such sort of structural motif is still unclear to us. They have the major functional significance for RNA-RNA, RNA-protein, RNA-drug interactions (Leontis *et al.* 2002). Thus it has a major target for pharmaceutical field.

E-loop is generally important for its transport activity. It has co-relation with transporters mainly ABC-transporters (Okuda *et al.* 2010). Thus the high percentage of existence of such kind of motif reveals that it may involve in signal peptide transport in some way or may involve for its symbiotic association through transportation machineries.

Hook-turn presents at the end of helix having hook like conformation i.e. it bears a sharp turn like a hook mainly at the end of WC- basepair of helix which ends with G on short strand-site or else A on large-strand side (Szep *et al.* 2003). They stabilize the structures through RNA-tertiary interactions but not used as cap for helical segments.

Conclusion

The tertiary structure prediction reveals that atomic constitution of 16S rRNA is too large to handle in a single platform relative to present RNA webservices. There is need to develop a service for such sort of large molecules to achieve a much more stabilized structure through *In-silico* approach. A short survey of tertiary structural motif shows that the sarcin-ricin motif, K-motif, E-loop should be examined in more detail in future. Our main objective for future case studies are exploring functional importance in much more detailed fashion. Here we give some pictorial representation of 16s rRNA of *Frankia sp.* with a structural-functional association.

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