

Quantitative Stable Isotope Probing

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Supplemental Information

This file contains the code used in QIIME to analyze the sequencing data, including all steps used in that analysis. This file also contains a table (Table S1), which summarizes results from the bioinformatics statistics.

QIIME Code and Analysis Steps

Sequence preparation

Paired end reads were stitched as described in supplementary methods. These files were edited to contain valid post-split-libraries sequence identifiers (a QIIME requirement).

Get valid post-split-libraries sequence identifiers:

```
In [1]: from bipy.parse.fasta import MinimalFastaParser
```

```
In [2]: infp = "RAV241_246_tgen_newStitched.fa"
```

```
In [3]: ofp = infp + '.fna'
```

```
23
24 In [4]: of = open(ofp, 'w')
25
26 In [5]: for seq_id, seq in MinimalFastaParser(open(infp)):
27     ....:     seq_id = seq_id.split(':')[0]
28     ....:     of.write('>%s\n%s\n' % (seq_id, seq))
29     ....:
30
31 In [6]: of.close()
32
33 In [9]: infps = ["RAV247_252_tgen_newStitched.fa",
34 "RAV253_257_tgen_newStitched.fa"]
35
36 In [10]: for infp in infps:
37     ....:     ofp = infp + '.fna'
38     ....:     of = open(ofp, 'w')
39     ....:     for seq_id, seq in MinimalFastaParser(open(infp)):
40     ....:         seq_id = seq_id.split(':')[0]
41     ....:         of.write('>%s\n%s\n' % (seq_id, seq))
42     ....:     of.close()
43     ....:
44
45 # Sanity check
46 In [13]: !count_seqs.py -i "RAV*"
```

47

48 1053070 : RAV253_257_tgen_newStitched.fa (Sequence lengths
49 (mean +/- std): 415.9885 +/- 12.3755)

50 1053070 : RAV253_257_tgen_newStitched.fa.fna (Sequence lengths
51 (mean +/- std): 415.9885 +/- 12.3755)

52

53 3125131 : RAV247_252_tgen_newStitched.fa (Sequence lengths
54 (mean +/- std): 413.0582 +/- 17.0290)

55 3125131 : RAV247_252_tgen_newStitched.fa.fna (Sequence lengths
56 (mean +/- std): 413.0582 +/- 17.0290)

57

58 5200677 : RAV241_246_tgen_newStitched.fa (Sequence lengths
59 (mean +/- std): 412.6679 +/- 15.8659)

60 5200677 : RAV241_246_tgen_newStitched.fa.fna (Sequence lengths
61 (mean +/- std): 412.6679 +/- 15.8659)

62

63 Iterative [open-reference OTU picking](#)

64 echo "pick_open_reference_otus.py -i
65 /home/caporaso/analysis/2014.02.17-
66 hungate/Tgen_Stitch/RAV241_246_tgen_newStitched.fa.fna,/home/cap
67 oraso/analysis/2014.02.17-
68 hungate/Tgen_Stitch/RAV247_252_tgen_newStitched.fa.fna,/home/cap
69 oraso/analysis/2014.02.17-

```
70 hungate/Tgen_Stitch/RAV253_257_tgen_newStitched.fa.fna -r
71 /data/gg_13_8_otus/rep_set/97_otus.fasta -o
72 /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/ucrssi/ -p
73 /home/caporaso/analysis/uc_fast_params.txt -a05" | qsub -keo -N
74 hungate-otus
```

75

```
76 echo "pick_open_reference_otus.py -i
77 /home/caporaso/analysis/2014.02.17-
78 hungate/Tgen_Stitch/RAV241_246_tgen_newStitched.fa.fna,/home/cap
79 oraso/analysis/2014.02.17-
80 hungate/Tgen_Stitch/RAV247_252_tgen_newStitched.fa.fna,/home/cap
81 oraso/analysis/2014.02.17-
```

```
82 hungate/Tgen_Stitch/RAV253_257_tgen_newStitched.fa.fna -r
83 /data/gg_13_8_otus/rep_set/97_otus.fasta -o
84 /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/ucrssi/ -p
85 /home/caporaso/analysis/uc_fast_params.txt -a05 -f" | qsub -keo
86 -N hungate-otus
```

87

88 **Diversity analyses**

```
89 echo "core_diversity_analyses.py -i
90 /home/caporaso/analysis/2014.02.17-
91 hungate/Tgen_Stitch/ucrssi/otu_table_mc2_w_tax_no_pynast_failures
92 .biom -o /home/caporaso/analysis/2014.02.17-
```

```
93  hungate/Tgen_Stitch/ucrсс/cd_4049/ -e 4049 -m
94  /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/hungate-
95  dob-map.tsv -t /home/caporaso/analysis/2014.02.17-
96  hungate/Tgen_Stitch/ucrсс/rep_set.tre -a0 5 -c sample-
97  num,fraction-num,week-num,control-or-priming,combo-trt-
98  code,isotope-trt" | qsub -keo -N cd4049
99  # killed the above bc the sample-num boxplots were taking way
100 too long (~30 hours and weighted unifrac still wasn't done) - we
101 can add sample-num,fraction-num back later if we need to.
102
103 echo "core_diversity_analyses.py -i
104 /home/caporaso/analysis/2014.02.17-
105 hungate/Tgen_Stitch/ucrсс/otu_table_mc2_w_tax_no_pynast_failures
106 .biom -o /home/caporaso/analysis/2014.02.17-
107 hungate/Tgen_Stitch/ucrсс/cd_4049/ -e 4049 -m
108 /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/hungate-
109 dob-map.tsv -t /home/caporaso/analysis/2014.02.17-
110 hungate/Tgen_Stitch/ucrсс/rep_set.tre -a0 5 -c week-num,control-
111 or-priming --recover_from_failure" | qsub -keo -N cd4049
112
113 # re-run with isotope-trt,combo-trt-code added as categories
114 echo "core_diversity_analyses.py -i
115 /home/caporaso/analysis/2014.02.17-
116 hungate/Tgen_Stitch/ucrсс/otu_table_mc2_w_tax_no_pynast_failures
```

```
117 .biom -o /home/caporaso/analysis/2014.02.17-
118 hungate/Tgen_Stitch/ucrсс/cd_4049/ -e 4049 -m
119 /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/hungate-
120 dob-map.tsv -t /home/caporaso/analysis/2014.02.17-
121 hungate/Tgen_Stitch/ucrсс/rep_set.tre -a0 5 -c isotope-
122 trt,combo-trt-code --recover_from_failure" | qsub -keo -N cd4049
123
124 # re-run with comb-week-control added as a category
125 echo "core_diversity_analyses.py -i
126 /home/caporaso/analysis/2014.02.17-
127 hungate/Tgen_Stitch/ucrсс/otu_table_mc2_w_tax_no_pynast_failures
128 .biom -o /home/caporaso/analysis/2014.02.17-
129 hungate/Tgen_Stitch/ucrсс/cd_4049/ -e 4049 -m
130 /home/caporaso/analysis/2014.02.17-hungate/Tgen_Stitch/hungate-
131 dob-map.tsv -t /home/caporaso/analysis/2014.02.17-
132 hungate/Tgen_Stitch/ucrсс/rep_set.tre -a0 5 -c week-num,control-
133 or-priming,comb-week-control,isotope-trt,combo-trt-code --
134 recover_from_failure" | qsub -keo -N cd4049
135
136 # run locally to generate rarefaction plots with continuous
137 coloring
138 ## NEED TO RE-RUN FOR LAST ITERATION OF CORE DIV!
139 cd cd_4049/arare_max4049/
140 mv alpha_rarefaction_plots/ alpha_rarefaction_plots_discrete
```

```
141 make_prefs_file.py -m ../hungate-dob-map.tsv -o prefs.txt
142 make_rarefaction_plots.py -i alpha_div_collated/ -m ../hungate-
143 dob-map.tsv -o alpha_rarefaction_plots/ -p prefs.txt
144
145 Comparison of uclust consensus taxonomic assignment with RDP taxonomic
146 assignment
147 parallel_assign_taxonomy_rdp.py -i
148 /home/caporaso/analysis/2014.02.17-
149 hungate/Tgen_Stitch/ucrss/rep_set.fna -o
150 /home/caporaso/analysis/2014.02.17-
151 hungate/Tgen_Stitch/ucrss/rdp_assigned_taxonomy/ -c 0.50 -O 25
152
153 biom add-metadata -i /home/caporaso/analysis/2014.02.17-
154 hungate/Tgen_Stitch/ucrss//otu_table_mc2.biom --observation-
155 metadata-fp /home/caporaso/analysis/2014.02.17-
156 hungate/Tgen_Stitch/ucrss/rdp_assigned_taxonomy/rep_set_tax_assi
157 gnments.txt -o /home/caporaso/analysis/2014.02.17-
158 hungate/Tgen_Stitch/ucrss//otu_table_mc2_w_rdptax.biom --sc-
159 separated taxonomy --observation-header OTUID,taxonomy
160
161 filter_otus_from_otu_table.py -i
162 /home/caporaso/analysis/2014.02.17-
163 hungate/Tgen_Stitch/ucrss//otu_table_mc2_w_rdptax.biom -o
```

```
164 /home/caporaso/analysis/2014.02.17-
165 hungate/Tgen_Stitch/ucrssl/otu_table_mc2_w_rdptax_no_pynast_fail
166 ures.biom -e /home/caporaso/analysis/2014.02.17-
167 hungate/Tgen_Stitch/ucrssl/pynast_aligned_seqs/rep_set_failures.f
168 asta
169
170 biom summarize-table -i /home/caporaso/analysis/2014.02.17-
171 hungate/Tgen_Stitch/ucrssl/otu_table_mc2_w_rdptax_no_pynast_fail
172 ures.biom -o /home/caporaso/analysis/2014.02.17-
173 hungate/Tgen_Stitch/ucrssl/otu_table_mc2_w_rdptax_no_pynast_fail
174 ures.txt
175
176 summarize_taxa_through_plots.py -i
177 /home/caporaso/analysis/2014.02.17-
178 hungate/Tgen_Stitch/ucrssl/otu_table_mc2_w_rdptax_no_pynast_failu
179 res.biom -o /home/caporaso/analysis/2014.02.17-
180 hungate/Tgen_Stitch/ucrssl/rdp_taxa_plots/
181
182 compare_taxa_summaries.py -i /home/caporaso/analysis/2014.02.17-
183 hungate/Tgen_Stitch/ucrssl/rdp_taxa_plots/otu_table_mc2_w_rdptax_
184 no_pynast_failures_L2.txt,/home/caporaso/analysis/2014.02.17-
185 hungate/Tgen_Stitch/ucrssl/cd_4049/taxa_plots/table_mc4049_sorted
186 _L2.txt -o rdp_v_uclust_tax_L2 -m paired
```



```
187 compare_taxa_summaries.py -i /home/caporaso/analysis/2014.02.17-
188 hungate/Tgen_Stitch/ucrss/rdp_taxa_plots/otu_table_mc2_w_rdptax_
189 no_pynast_failures_L3.txt,/home/caporaso/analysis/2014.02.17-
190 hungate/Tgen_Stitch/ucrss/cd_4049/taxa_plots/table_mc4049_sorted
191 _L3.txt -o rdp_v_uclust_tax_L3 -m paired
192 compare_taxa_summaries.py -i /home/caporaso/analysis/2014.02.17-
193 hungate/Tgen_Stitch/ucrss/rdp_taxa_plots/otu_table_mc2_w_rdptax_
194 no_pynast_failures_L4.txt,/home/caporaso/analysis/2014.02.17-
195 hungate/Tgen_Stitch/ucrss/cd_4049/taxa_plots/table_mc4049_sorted
196 _L4.txt -o rdp_v_uclust_tax_L4 -m paired
197 compare_taxa_summaries.py -i /home/caporaso/analysis/2014.02.17-
198 hungate/Tgen_Stitch/ucrss/rdp_taxa_plots/otu_table_mc2_w_rdptax_
199 no_pynast_failures_L5.txt,/home/caporaso/analysis/2014.02.17-
200 hungate/Tgen_Stitch/ucrss/cd_4049/taxa_plots/table_mc4049_sorted
201 _L5.txt -o rdp_v_uclust_tax_L5 -m paired
202 compare_taxa_summaries.py -i /home/caporaso/analysis/2014.02.17-
203 hungate/Tgen_Stitch/ucrss/rdp_taxa_plots/otu_table_mc2_w_rdptax_
204 no_pynast_failures_L6.txt,/home/caporaso/analysis/2014.02.17-
205 hungate/Tgen_Stitch/ucrss/cd_4049/taxa_plots/table_mc4049_sorted
206 _L6.txt -o rdp_v_uclust_tax_L6 -m pair
```

Table S1. Statistical analysis of QIIME output, showing confidence levels in taxonomic assignments.

Taxonomic level	Pearson r	95% Confidence Interval (lower bound)	95% Confidence Interval (upper bound)	Nonparametric p-value
Phylum	0.9996	0.9996	0.9996	< 0.001
Class	0.9993	0.9992	0.9993	< 0.001
Order	0.9990	0.9990	0.9990	< 0.001
Family	0.9822	0.9821	0.9824	< 0.001
Genus	0.9616	0.9613	0.9618	< 0.001

Table S2. qPCR analysis of the 16S gene for each density fraction

#SampleID	Tube	glucose	water	density-g- p-mL	16S-qPCR- copynum- p-uL
1.2	1	none	nat abun	1.69581	195379.5
1.21	1	none	nat abun	1.69249	282486.0
1.22	1	none	nat abun	1.69139	310844.9
1.23	1	none	nat abun	1.69139	250752.9
1.24	1	none	nat abun	1.68586	208810.1
1.25	1	none	nat abun	1.68586	143032.8
1.26	1	none	nat abun	1.68255	70350.8
1.27	1	none	nat abun	1.68034	25598.2
1.28	1	none	nat abun	1.67703	16908.1
1.29	1	none	nat abun	1.67703	10827.1
1.3	1	none	nat abun	1.67482	6074.6
2.12	2	none	nat abun	1.71437	702.0
2.13	2	none	nat abun	1.71003	5511.1
2.14	2	none	nat abun	1.70895	5792.9
2.15	2	none	nat abun	1.70569	19987.9
2.16	2	none	nat abun	1.70243	102398.0
2.17	2	none	nat abun	1.69917	255659.7
2.18	2	none	nat abun	1.69483	182935.5
2.19	2	none	nat abun	1.69049	176871.6
2.2	2	none	nat abun	1.68397	102896.8
3.09	3	none	nat abun	1.72026	1130.2
3.11	3	none	nat abun	1.71262	1394.5
3.12	3	none	nat abun	1.70934	2519.9
3.13	3	none	nat abun	1.70715	6733.9
3.16	3	none	nat abun	1.69514	129206.6
3.17	3	none	nat abun	1.69186	199474.9
3.18	3	none	nat abun	1.68858	262653.9
3.19	3	none	nat abun	1.69077	117614.2
3.2	3	none	nat abun	1.68422	85964.5
3.21	3	none	nat abun	1.68312	35034.3
3.22	3	none	nat abun	1.67875	11926.9
3.23	3	none	nat abun	1.67875	6396.0
4.09	4	none	97% 18O	1.73826	290.3
4.11	4	none	97% 18O	1.73392	1023.7
4.12	4	none	97% 18O	1.73283	1218.4
4.13	4	none	97% 18O	1.72849	887.2
4.17	4	none	97% 18O	1.71872	8307.4
4.18	4	none	97% 18O	1.71329	13351.7

4.19	4	none	97% 180	1.71329	25963.7
4.2	4	none	97% 180	1.71329	57820.1
4.21	4	none	97% 180	1.70786	28942.1
4.22	4	none	97% 180	1.70243	64547.1
4.23	4	none	97% 180	1.70026	140311.0
4.24	4	none	97% 180	1.69809	80501.2
4.25	4	none	97% 180	1.69374	107908.5
4.26	4	none	97% 180	1.68940	65896.6
5.09	5	none	97% 180	1.71707	19109.6
5.1	5	none	97% 180	1.71271	29223.8
5.11	5	none	97% 180	1.71052	66513.6
5.12	5	none	97% 180	1.71052	33385.8
5.13	5	none	97% 180	1.70398	103146.4
5.15	5	none	97% 180	1.69852	298566.4
5.16	5	none	97% 180	1.69415	387737.3
5.17	5	none	97% 180	1.69197	142507.7
5.18	5	none	97% 180	1.68651	127473.3
5.19	5	none	97% 180	1.68324	35066.6
5.2	5	none	97% 180	1.68215	243.1
5.22	5	none	97% 180	1.67778	11177.9
5.23	5	none	97% 180	1.67669	5510.4
5.24	5	none	97% 180	1.67342	3741.1
6.08	6	none	97% 180	1.72013	6266.3
6.09	6	none	97% 180	1.71683	7994.9
6.1	6	none	97% 180	1.71244	13189.6
6.11	6	none	97% 180	1.70804	25158.1
6.12	6	none	97% 180	1.70475	40810.3
6.13	6	none	97% 180	1.70475	54854.2
6.14	6	none	97% 180	1.69706	68266.3
6.15	6	none	97% 180	1.69376	72412.2
6.16	6	none	97% 180	1.69157	106788.2
6.17	6	none	97% 180	1.68827	146010.1
6.18	6	none	97% 180	1.68388	140868.6
6.19	6	none	97% 180	1.67949	79977.4
6.2	6	none	97% 180	1.67839	42703.1
6.21	6	none	97% 180	1.67399	26187.2
6.22	6	none	97% 180	1.66850	13974.0
7.09	7	nat abund	nat abund	1.72342	1190.0
7.1	7	nat abund	nat abund	1.71793	782.5
7.11	7	nat abund	nat abund	1.71463	1902.5
7.12	7	nat abund	nat abund	1.71134	1983.5
7.13	7	nat abund	nat abund	1.70695	4275.2
7.14	7	nat abund	nat abund	1.70695	8413.3

7.16	7	nat abun	nat abun	1.69596	59229.8
7.17	7	nat abun	nat abun	1.69267	148575.9
7.18	7	nat abun	nat abun	1.68827	297527.8
7.19	7	nat abun	nat abun	1.68498	268087.0
7.2	7	nat abun	nat abun	1.68168	208338.7
7.21	7	nat abun	nat abun	1.67839	12.7
7.22	7	nat abun	nat abun	1.67290	65751.2
8.11	8	nat abun	nat abun	1.71263	158.8
8.14	8	nat abun	nat abun	1.70173	40839.2
8.15	8	nat abun	nat abun	1.69737	99724.5
8.16	8	nat abun	nat abun	1.69737	255649.3
8.17	8	nat abun	nat abun	1.69192	438744.1
8.18	8	nat abun	nat abun	1.68865	208369.4
8.19	8	nat abun	nat abun	1.68539	180135.9
8.2	8	nat abun	nat abun	1.68430	92049.3
8.21	8	nat abun	nat abun	1.68103	55443.6
8.23	8	nat abun	nat abun	1.67776	7937.9
8.24	8	nat abun	nat abun	1.67885	2304.6
9.12	9	nat abun	nat abun	1.71825	1053.6
9.14	9	nat abun	nat abun	1.71500	2202.3
9.15	9	nat abun	nat abun	1.71175	2934.1
9.16	9	nat abun	nat abun	1.70849	10164.9
9.18	9	nat abun	nat abun	1.70199	71409.6
9.19	9	nat abun	nat abun	1.69765	158480.9
9.2	9	nat abun	nat abun	1.69440	206591.6
9.21	9	nat abun	nat abun	1.69006	231657.2
9.22	9	nat abun	nat abun	1.68247	107583.0
10.1	10	nat abun	97% 18O	1.71934	8574.1
10.11	10	nat abun	97% 18O	1.71717	32940.5
10.12	10	nat abun	97% 18O	1.71283	8644.2
10.13	10	nat abun	97% 18O	1.71175	48513.4
10.14	10	nat abun	97% 18O	1.70741	66720.1
10.15	10	nat abun	97% 18O	1.70524	78419.9
10.16	10	nat abun	97% 18O	1.70091	181429.5
10.17	10	nat abun	97% 18O	1.69765	236561.7
10.18	10	nat abun	97% 18O	1.69440	116247.8
10.19	10	nat abun	97% 18O	1.69115	110746.8
10.2	10	nat abun	97% 18O	1.68898	30122.2
10.21	10	nat abun	97% 18O	1.68681	57095.4
10.22	10	nat abun	97% 18O	1.68356	24712.8
11.12	11	nat abun	97% 18O	1.70834	122343.3
11.13	11	nat abun	97% 18O	1.71052	372085.0
11.14	11	nat abun	97% 18O	1.71162	113722.0

11.15	11	nat abun	97% 18O	1.69961	250492.1
11.16	11	nat abun	97% 18O	1.70070	322448.0
11.17	11	nat abun	97% 18O	1.69634	233383.9
11.18	11	nat abun	97% 18O	1.69197	208305.1
11.19	11	nat abun	97% 18O	1.68870	139133.9
11.2	11	nat abun	97% 18O	1.68761	66842.3
11.21	11	nat abun	97% 18O	1.68979	50910.1
11.22	11	nat abun	97% 18O	1.68542	15927.7
11.23	11	nat abun	97% 18O	1.67887	25189.2
12.1	12	nat abun	97% 18O	1.72344	4379.1
12.11	12	nat abun	97% 18O	1.72015	8095.0
12.12	12	nat abun	97% 18O	1.71796	18464.9
12.13	12	nat abun	97% 18O	1.71467	36486.5
12.14	12	nat abun	97% 18O	1.71028	59608.8
12.15	12	nat abun	97% 18O	1.70590	84484.4
12.16	12	nat abun	97% 18O	1.70590	120118.3
12.17	12	nat abun	97% 18O	1.70261	118149.3
12.18	12	nat abun	97% 18O	1.69712	118360.1
12.19	12	nat abun	97% 18O	1.69603	158605.8
12.2	12	nat abun	97% 18O	1.68835	141594.1
12.21	12	nat abun	97% 18O	1.68616	40408.2
12.22	12	nat abun	97% 18O	1.67958	43900.3
13.1	13	99% 13C	nat abun	1.72706	7834.4
13.11	13	99% 13C	nat abun	1.72377	11034.9
13.12	13	99% 13C	nat abun	1.72268	9234.6
13.14	13	99% 13C	nat abun	1.71282	15236.5
13.15	13	99% 13C	nat abun	1.71063	33436.6
13.16	13	99% 13C	nat abun	1.70735	23708.5
13.17	13	99% 13C	nat abun	1.70516	89965.6
13.18	13	99% 13C	nat abun	1.70078	64620.8
13.19	13	99% 13C	nat abun	1.69640	116417.8
13.2	13	99% 13C	nat abun	1.69640	216161.8
13.21	13	99% 13C	nat abun	1.69202	188690.3
13.22	13	99% 13C	nat abun	1.68326	98145.5
13.23	13	99% 13C	nat abun	1.67997	43639.0
14.1	14	99% 13C	nat abun	1.72978	3879.6
14.11	14	99% 13C	nat abun	1.72647	6395.8
14.15	14	99% 13C	nat abun	1.71323	11466.4
14.16	14	99% 13C	nat abun	1.70771	16896.9
14.17	14	99% 13C	nat abun	1.70661	17100.7
14.18	14	99% 13C	nat abun	1.70109	54519.2
14.19	14	99% 13C	nat abun	1.69889	68095.2
14.2	14	99% 13C	nat abun	1.69447	82815.7

14.21	14	99% 13C	nat abund	1.69447	533396.7
14.22	14	99% 13C	nat abund	1.69006	781146.9
14.23	14	99% 13C	nat abund	1.68454	330091.1
14.24	14	99% 13C	nat abund	1.68344	175264.4
14.25	14	99% 13C	nat abund	1.68013	197046.9
14.26	14	99% 13C	nat abund	1.67903	140984.1
15.08	15	99% 13C	nat abund	1.72909	28284.9
15.09	15	99% 13C	nat abund	1.72476	29998.7
15.11	15	99% 13C	nat abund	1.71934	25057.6
15.13	15	99% 13C	nat abund	1.71392	60574.8
15.14	15	99% 13C	nat abund	1.71175	151498.5
15.15	15	99% 13C	nat abund	1.70849	138528.8
15.16	15	99% 13C	nat abund	1.70633	220243.4
15.17	15	99% 13C	nat abund	1.70307	324151.5
15.18	15	99% 13C	nat abund	1.69982	715222.5
15.19	15	99% 13C	nat abund	1.69657	146343.4
15.2	15	99% 13C	nat abund	1.69332	821646.7
15.21	15	99% 13C	nat abund	1.69223	652432.3
15.24	15	99% 13C	nat abund	1.68356	268143.0