

# Quality control metaproteomics

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```
##libraries
library(tidyverse)
library(here)

## input data
df_qc <- read.table(here::here("rawdata/summary.txt"),
                    header = TRUE,
                    sep="\t",
                    check.names = FALSE)

colnames(df_qc)
```

```
[1] "Raw file"
[2] "Experiment"
[3] "Fraction"
[4] "Enzyme"
[5] "Enzyme mode"
[6] "Enzyme first search"
[7] "Enzyme mode first search"
[8] "Use enzyme first search"
[9] "Variable modifications"
[10] "Fixed modifications"
[11] "Multi modifications"
[12] "Variable modifications first search"
[13] "Use variable modifications first search"
[14] "Requantify"
```

[15] "Multiplicity"  
[16] "Max. missed cleavages"  
[17] "Labels0"  
[18] "LC-MS run type"  
[19] "Time-dependent recalibration"  
[20] "MS"  
[21] "MS/MS"  
[22] "MS3"  
[23] "MS/MS Submitted"  
[24] "MS/MS Submitted (SIL)"  
[25] "MS/MS Submitted (ISO)"  
[26] "MS/MS Submitted (PEAK)"  
[27] "MS/MS Identified"  
[28] "MS/MS Identified (SIL)"  
[29] "MS/MS Identified (ISO)"  
[30] "MS/MS Identified (PEAK)"  
[31] "MS/MS Identified [%]"  
[32] "MS/MS Identified (SIL) [%]"  
[33] "MS/MS Identified (ISO) [%]"  
[34] "MS/MS Identified (PEAK) [%]"  
[35] "Peptide Sequences Identified"  
[36] "Peaks"  
[37] "Peaks Sequenced"  
[38] "Peaks Sequenced [%]"  
[39] "Peaks Repeatedly Sequenced"  
[40] "Peaks Repeatedly Sequenced [%]"  
[41] "Isotope Patterns"  
[42] "Isotope Patterns Sequenced"  
[43] "Isotope Patterns Sequenced (z>1)"  
[44] "Isotope Patterns Sequenced [%]"  
[45] "Isotope Patterns Sequenced (z>1) [%]"  
[46] "Isotope Patterns Repeatedly Sequenced"  
[47] "Isotope Patterns Repeatedly Sequenced [%]"  
[48] "Recalibrated"  
[49] "Av. Absolute Mass Deviation [ppm]"  
[50] "Mass Standard Deviation [ppm]"  
[51] "Av. Absolute Mass Deviation [mDa]"  
[52] "Mass Standard Deviation [mDa]"  
[53] "Label free norm param"

```

metadata <-read.table(here::here("rawdata/metadata_metapro.txt"),
                      header = TRUE,
                      sep="\t") %>%
  rename(sample=Probenname) %>%
  mutate(sample=str_replace_all(sample, "\\.", "_"))%>%
  separate(Abschnitt,
           into=c("region", "source",
                  sep=" "))
metadata

```

	sample	region	source
1	9_1	Stomach	Digesta <NA>
2	9_3	Stomach	Mucosa 1
3	9_4	Stomach	Mucosa 2
4	9_5	Stomach	Mucosa 3
5	9_6	Duodenum	Digesta <NA>
6	9_8	Duodenum	Mucosa <NA>
7	9_9	Jejunum	Digesta <NA>
8	9_11	Jejunum	Mucosa <NA>
9	9_12	Ileum	Digesta <NA>
10	9_14	Ileum	Mucosa <NA>
11	9_15	Colon	Digesta <NA>
12	9_17	Colon	Mucosa <NA>
13	9_18	Caecum	Digesta <NA>
14	9_2	Caecum	Mucosa <NA>
15	10_1	Stomach	Digesta <NA>
16	10_3	Stomach	Mucosa 1
17	10_4	Stomach	Mucosa 2
18	10_5	Stomach	Mucosa 3
19	10_6	Duodenum	Digesta <NA>
20	10_8	Duodenum	Mucosa <NA>
21	10_9	Jejunum	Digesta <NA>
22	10_11	Jejunum	Mucosa <NA>
23	10_12	Ileum	Digesta <NA>
24	10_14	Ileum	Mucosa <NA>
25	10_15	Colon	Digesta <NA>
26	10_17	Colon	Mucosa <NA>
27	10_18	Caecum	Digesta <NA>
28	10_2	Caecum	Mucosa <NA>
29	11_1	Stomach	Digesta <NA>
30	11_3	Stomach	Mucosa 1
31	11_4	Stomach	Mucosa 2

32	11_5	Stomach	Mucosa	3
33	11_6	Duodenum	Digesta	<NA>
34	11_8	Duodenum	Mucosa	<NA>
35	11_9	Jejunum	Digesta	<NA>
36	11_11	Jejunum	Mucosa	<NA>
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38	11_14	Ileum	Mucosa	<NA>
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40	11_17	Colon	Mucosa	<NA>
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42	11_2	Caecum	Mucosa	<NA>
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44	12_3	Stomach	Mucosa	1
45	12_4	Stomach	Mucosa	2
46	12_5	Stomach	Mucosa	3
47	12_6	Duodenum	Digesta	<NA>
48	12_8	Duodenum	Mucosa	<NA>
49	12_9	Jejunum	Digesta	<NA>
50	12_11	Jejunum	Mucosa	<NA>
51	12_12	Ileum	Digesta	<NA>
52	12_14	Ileum	Mucosa	<NA>
53	12_15	Colon	Digesta	<NA>
54	12_17	Colon	Mucosa	<NA>
55	12_18	Caecum	Digesta	<NA>
56	12_2	Caecum	Mucosa	<NA>
57	13_1	Stomach	Digesta	<NA>
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60	13_5	Stomach	Mucosa	3
61	13_6	Duodenum	Digesta	<NA>
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63	13_9	Jejunum	Digesta	<NA>
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74	14_5	Stomach	Mucosa	3

75	14_6	Duodenum	Digesta	<NA>
76	14_8	Duodenum	Mucosa	<NA>
77	14_9	Jejunum	Digesta	<NA>
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85	15_1	Stomach	Digesta	<NA>
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96	15_17	Colon	Mucosa	<NA>
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98	15_2	Caecum	Mucosa	<NA>
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103	16_6	Duodenum	Digesta	<NA>
104	16_8	Duodenum	Mucosa	<NA>
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116	17_5	Stomach	Mucosa	3
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118	17_8	Duodenum	Mucosa	<NA>
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143	19_4	Stomach	Mucosa	2
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152	19_17	Colon	Mucosa	<NA>
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157	20_4	Stomach	Mucosa	2
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171	21_4	Stomach	Mucosa	2
172	21_5	Stomach	Mucosa	3
173	21_6	Duodenum	Digesta	<NA>
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185	22_4	Stomach	Mucosa	2
186	22_5	Stomach	Mucosa	3
187	22_6	Duodenum	Digesta	<NA>
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193	22_15	Colon	Digesta	<NA>
194	22_17	Colon	Mucosa	<NA>
195	22_18	Caecum	Digesta	<NA>
196	22_2	Caecum	Mucosa	<NA>
197	22_21	Duodenum	Mucosa	<NA>
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199	23_3	Stomach	Mucosa	1
200	23_4	Stomach	Mucosa	2
201	23_5	Stomach	Mucosa	3
202	23_6	Duodenum	Digesta	<NA>
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204	23_9	Jejunum	Digesta	<NA>
205	23_11	Jejunum	Mucosa	<NA>
206	23_12	Ileum	Digesta	<NA>
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208	23_15	Colon	Digesta	<NA>
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210	23_18	Caecum	Digesta	<NA>
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213	24_3	Stomach	Mucosa	1
214	24_4	Stomach	Mucosa	2
215	24_5	Stomach	Mucosa	3
216	24_6	Duodenum	Digesta	<NA>
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225	24_2	Caecum	Mucosa	<NA>
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228	25_4	Stomach	Mucosa	2
229	25_5	Stomach	Mucosa	3
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234	25_12	Ileum	Digesta	<NA>
235	25_14	Ileum	Mucosa	<NA>
236	25_15	Colon	Digesta	<NA>
237	25_17	Colon	Mucosa	<NA>
238	25_18	Caecum	Digesta	<NA>
239	25_2	Caecum	Mucosa	<NA>
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241	26_3	Stomach	Mucosa	1
242	26_4	Stomach	Mucosa	2
243	26_5	Stomach	Mucosa	3
244	26_6	Duodenum	Digesta	<NA>
245	26_8	Duodenum	Mucosa	<NA>
246	26_9	Jejunum	Digesta	<NA>

247 26\_11 Jejunum Mucosa <NA>  
248 26\_12 Ileum Digesta <NA>  
249 26\_14 Ileum Mucosa <NA>  
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252 26\_18 Caecum Digesta <NA>  
253 26\_2 Caecum Mucosa <NA>  
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256 27\_4 Stomach Mucosa 2  
257 27\_5 Stomach Mucosa 3  
258 27\_6 Duodenum Digesta <NA>  
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269 28\_3 Stomach Mucosa 1  
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284 29\_4 Stomach Mucosa 2  
285 29\_5 Stomach Mucosa 3  
286 29\_6 Duodenum Digesta <NA>  
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289 29\_11 Jejunum Mucosa <NA>

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382	36_4	Stomach	Mucosa	2
383	36_5	Stomach	Mucosa	3
384	36_6	Duodenum	Digesta	<NA>
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386	36_9	Jejunum	Digesta	<NA>
387	36_11	Jejunum	Mucosa	<NA>
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410	38_4	Stomach	Mucosa	2
411	38_5	Stomach	Mucosa	3
412	38_6	Duodenum	Digesta	<NA>
413	38_8	Duodenum	Mucosa	<NA>
414	38_9	Jejunum	Digesta	<NA>
415	38_11	Jejunum	Mucosa	<NA>
416	38_12	Ileum	Digesta	<NA>
417	38_14	Ileum	Mucosa	<NA>
418	38_15	Colon	Digesta	<NA>

419 38\_17 Colon Mucosa <NA>  
420 38\_18 Caecum Digesta <NA>  
421 38\_2 Caecum Mucosa <NA>  
422 39\_1 Stomach Digesta <NA>  
423 39\_3 Stomach Mucosa 1  
424 39\_4 Stomach Mucosa 2  
425 39\_5 Stomach Mucosa 3  
426 39\_6 Duodenum Digesta <NA>  
427 39\_8 Duodenum Mucosa <NA>  
428 39\_9 Jejunum Digesta <NA>  
429 39\_11 Jejunum Mucosa <NA>  
430 39\_12 Ileum Digesta <NA>  
431 39\_14 Ileum Mucosa <NA>  
432 39\_15 Colon Digesta <NA>  
433 39\_17 Colon Mucosa <NA>  
434 39\_18 Caecum Digesta <NA>  
435 39\_2 Caecum Mucosa <NA>  
436 40\_1 Stomach Digesta <NA>  
437 40\_3 Stomach Mucosa 1  
438 40\_4 Stomach Mucosa 2  
439 40\_5 Stomach Mucosa 3  
440 40\_6 Duodenum Digesta <NA>  
441 40\_8 Duodenum Mucosa <NA>  
442 40\_9 Jejunum Digesta <NA>  
443 40\_11 Jejunum Mucosa <NA>  
444 40\_12 Ileum Digesta <NA>  
445 40\_14 Ileum Mucosa <NA>  
446 40\_15 Colon Digesta <NA>  
447 40\_17 Colon Mucosa <NA>  
448 40\_18 Caecum Digesta <NA>  
449 40\_2 Caecum Mucosa <NA>  
450 41\_1 Stomach Digesta <NA>  
451 41\_3 Stomach Mucosa 1  
452 41\_4 Stomach Mucosa 2  
453 41\_5 Stomach Mucosa 3  
454 41\_6 Duodenum Digesta <NA>  
455 41\_8 Duodenum Mucosa <NA>  
456 41\_9 Jejunum Digesta <NA>  
457 41\_11 Jejunum Mucosa <NA>  
458 41\_12 Ileum Digesta <NA>  
459 41\_14 Ileum Mucosa <NA>  
460 41\_15 Colon Digesta <NA>  
461 41\_17 Colon Mucosa <NA>

462	41_18	Caecum	Digesta	<NA>
463	41_2	Caecum	Mucosa	<NA>
464	42_1	Stomach	Digesta	<NA>
465	42_3	Stomach	Mucosa	1
466	42_4	Stomach	Mucosa	2
467	42_5	Stomach	Mucosa	3
468	42_6	Duodenum	Digesta	<NA>
469	42_8	Duodenum	Mucosa	<NA>
470	42_9	Jejunum	Digesta	<NA>
471	42_11	Jejunum	Mucosa	<NA>
472	42_12	Ileum	Digesta	<NA>
473	42_14	Ileum	Mucosa	<NA>
474	42_15	Colon	Digesta	<NA>
475	42_17	Colon	Mucosa	<NA>
476	42_18	Caecum	Digesta	<NA>
477	42_2	Caecum	Mucosa	<NA>
478	43_1	Stomach	Digesta	<NA>
479	43_3	Stomach	Mucosa	1
480	43_4	Stomach	Mucosa	2
481	43_5	Stomach	Mucosa	3
482	43_6	Duodenum	Digesta	<NA>
483	43_8	Duodenum	Mucosa	<NA>
484	43_9	Jejunum	Digesta	<NA>
485	43_11	Jejunum	Mucosa	<NA>
486	43_12	Ileum	Digesta	<NA>
487	43_14	Ileum	Mucosa	<NA>
488	43_15	Colon	Digesta	<NA>
489	43_17	Colon	Mucosa	<NA>
490	43_18	Caecum	Digesta	<NA>
491	43_2	Caecum	Mucosa	<NA>
492	44_1	Stomach	Digesta	<NA>
493	44_3	Stomach	Mucosa	1
494	44_4	Stomach	Mucosa	2
495	44_5	Stomach	Mucosa	3
496	44_6	Duodenum	Digesta	<NA>
497	44_8	Duodenum	Mucosa	<NA>
498	44_9	Jejunum	Digesta	<NA>
499	44_11	Jejunum	Mucosa	<NA>
500	44_12	Ileum	Digesta	<NA>
501	44_14	Ileum	Mucosa	<NA>
502	44_15	Colon	Digesta	<NA>
503	44_17	Colon	Mucosa	<NA>
504	44_18	Caecum	Digesta	<NA>

505	44_2	Caecum	Mucosa	<NA>
506	45_1	Stomach	Digesta	<NA>
507	45_3	Stomach	Mucosa	1
508	45_4	Stomach	Mucosa	2
509	45_5	Stomach	Mucosa	3
510	45_6	Duodenum	Digesta	<NA>
511	45_8	Duodenum	Mucosa	<NA>
512	45_9	Jejunum	Digesta	<NA>
513	45_11	Jejunum	Mucosa	<NA>
514	45_12	Ileum	Digesta	<NA>
515	45_14	Ileum	Mucosa	<NA>
516	45_15	Colon	Digesta	<NA>
517	45_17	Colon	Mucosa	<NA>
518	45_18	Caecum	Digesta	<NA>
519	45_2	Caecum	Mucosa	<NA>
520	46_1	Stomach	Digesta	<NA>
521	46_3	Stomach	Mucosa	1
522	46_4	Stomach	Mucosa	2
523	46_5	Stomach	Mucosa	3
524	46_6	Duodenum	Digesta	<NA>
525	46_8	Duodenum	Mucosa	<NA>
526	46_9	Jejunum	Digesta	<NA>
527	46_11	Jejunum	Mucosa	<NA>
528	46_12	Ileum	Digesta	<NA>
529	46_14	Ileum	Mucosa	<NA>
530	46_15	Colon	Digesta	<NA>
531	46_17	Colon	Mucosa	<NA>
532	46_18	Caecum	Digesta	<NA>
533	46_2	Caecum	Mucosa	<NA>
534	47_1	Stomach	Digesta	<NA>
535	47_3	Stomach	Mucosa	1
536	47_4	Stomach	Mucosa	2
537	47_5	Stomach	Mucosa	3
538	47_6	Duodenum	Digesta	<NA>
539	47_8	Duodenum	Mucosa	<NA>
540	47_9	Jejunum	Digesta	<NA>
541	47_11	Jejunum	Mucosa	<NA>
542	47_12	Ileum	Digesta	<NA>
543	47_14	Ileum	Mucosa	<NA>
544	47_15	Colon	Digesta	<NA>
545	47_17	Colon	Mucosa	<NA>
546	47_18	Caecum	Digesta	<NA>
547	47_2	Caecum	Mucosa	<NA>

548 48\_1 Stomach Digesta <NA>  
549 48\_3 Stomach Mucosa 1  
550 48\_4 Stomach Mucosa 2  
551 48\_5 Stomach Mucosa 3  
552 48\_6 Duodenum Digesta <NA>  
553 48\_8 Duodenum Mucosa <NA>  
554 48\_9 Jejunum Digesta <NA>  
555 48\_11 Jejunum Mucosa <NA>  
556 48\_12 Ileum Digesta <NA>  
557 48\_14 Ileum Mucosa <NA>  
558 48\_15 Colon Digesta <NA>  
559 48\_17 Colon Mucosa <NA>  
560 48\_18 Caecum Digesta <NA>  
561 48\_2 Caecum Mucosa <NA>  
562 49\_1 Stomach Digesta <NA>  
563 49\_3 Stomach Mucosa 1  
564 49\_4 Stomach Mucosa 2  
565 49\_5 Stomach Mucosa 3  
566 49\_6 Duodenum Digesta <NA>  
567 49\_8 Duodenum Mucosa <NA>  
568 49\_9 Jejunum Digesta <NA>  
569 49\_11 Jejunum Mucosa <NA>  
570 49\_12 Ileum Digesta <NA>  
571 49\_14 Ileum Mucosa <NA>  
572 49\_15 Colon Digesta <NA>  
573 49\_17 Colon Mucosa <NA>  
574 49\_18 Caecum Digesta <NA>  
575 49\_2 Caecum Mucosa <NA>  
576 50\_1 Stomach Digesta <NA>  
577 50\_3 Stomach Mucosa 1  
578 50\_4 Stomach Mucosa 2  
579 50\_5 Stomach Mucosa 3  
580 50\_6 Duodenum Digesta <NA>  
581 50\_8 Duodenum Mucosa <NA>  
582 50\_9 Jejunum Digesta <NA>  
583 50\_11 Jejunum Mucosa <NA>  
584 50\_12 Ileum Digesta <NA>  
585 50\_14 Ileum Mucosa <NA>  
586 50\_15 Colon Digesta <NA>  
587 50\_17 Colon Mucosa <NA>  
588 50\_18 Caecum Digesta <NA>  
589 50\_2 Caecum Mucosa <NA>  
590 51\_1 Stomach Digesta <NA>

591	51_3	Stomach	Mucosa	1
592	51_4	Stomach	Mucosa	2
593	51_5	Stomach	Mucosa	3
594	51_6	Duodenum	Digesta	<NA>
595	51_8	Duodenum	Mucosa	<NA>
596	51_9	Jejunum	Digesta	<NA>
597	51_11	Jejunum	Mucosa	<NA>
598	51_12	Ileum	Digesta	<NA>
599	51_14	Ileum	Mucosa	<NA>
600	51_15	Colon	Digesta	<NA>
601	51_17	Colon	Mucosa	<NA>
602	51_18	Caecum	Digesta	<NA>
603	51_2	Caecum	Mucosa	<NA>
604	52_1	Stomach	Digesta	<NA>
605	52_3	Stomach	Mucosa	1
606	52_4	Stomach	Mucosa	2
607	52_5	Stomach	Mucosa	3
608	52_6	Duodenum	Digesta	<NA>
609	52_8	Duodenum	Mucosa	<NA>
610	52_9	Jejunum	Digesta	<NA>
611	52_11	Jejunum	Mucosa	<NA>
612	52_12	Ileum	Digesta	<NA>
613	52_14	Ileum	Mucosa	<NA>
614	52_15	Colon	Digesta	<NA>
615	52_17	Colon	Mucosa	<NA>
616	52_18	Caecum	Digesta	<NA>
617	52_2	Caecum	Mucosa	<NA>
618	53_1	Stomach	Digesta	<NA>
619	53_3	Stomach	Mucosa	1
620	53_4	Stomach	Mucosa	2
621	53_5	Stomach	Mucosa	3
622	53_6	Duodenum	Digesta	<NA>
623	53_8	Duodenum	Mucosa	<NA>
624	53_9	Jejunum	Digesta	<NA>
625	53_11	Jejunum	Mucosa	<NA>
626	53_12	Ileum	Digesta	<NA>
627	53_14	Ileum	Mucosa	<NA>
628	53_15	Colon	Digesta	<NA>
629	53_17	Colon	Mucosa	<NA>
630	53_18	Caecum	Digesta	<NA>
631	53_2	Caecum	Mucosa	<NA>
632	54_1	Stomach	Digesta	<NA>
633	54_3	Stomach	Mucosa	1

634	54_4	Stomach	Mucosa	2
635	54_5	Stomach	Mucosa	3
636	54_6	Duodenum	Digesta	<NA>
637	54_8	Duodenum	Mucosa	<NA>
638	54_9	Jejunum	Digesta	<NA>
639	54_11	Jejunum	Mucosa	<NA>
640	54_12	Ileum	Digesta	<NA>
641	54_14	Ileum	Mucosa	<NA>
642	54_15	Colon	Digesta	<NA>
643	54_17	Colon	Mucosa	<NA>
644	54_18	Caecum	Digesta	<NA>
645	54_2	Caecum	Mucosa	<NA>
646	55_1	Stomach	Digesta	<NA>
647	55_3	Stomach	Mucosa	1
648	55_4	Stomach	Mucosa	2
649	55_5	Stomach	Mucosa	3
650	55_6	Duodenum	Digesta	<NA>
651	55_8	Duodenum	Mucosa	<NA>
652	55_9	Jejunum	Digesta	<NA>
653	55_11	Jejunum	Mucosa	<NA>
654	55_12	Ileum	Digesta	<NA>
655	55_14	Ileum	Mucosa	<NA>
656	55_15	Colon	Digesta	<NA>
657	55_17	Colon	Mucosa	<NA>
658	55_18	Caecum	Digesta	<NA>
659	55_2	Caecum	Mucosa	<NA>
660	56_1	Stomach	Digesta	<NA>
661	56_3	Stomach	Mucosa	1
662	56_4	Stomach	Mucosa	2
663	56_5	Stomach	Mucosa	3
664	56_6	Duodenum	Digesta	<NA>
665	56_8	Duodenum	Mucosa	<NA>
666	56_9	Jejunum	Digesta	<NA>
667	56_11	Jejunum	Mucosa	<NA>
668	56_12	Ileum	Digesta	<NA>
669	56_14	Ileum	Mucosa	<NA>
670	56_15	Colon	Digesta	<NA>
671	56_17	Colon	Mucosa	<NA>
672	56_18	Caecum	Digesta	<NA>
673	56_2	Caecum	Mucosa	<NA>