S1 Im3: Ten analyses with fragment ions of Im3

```
$ java -jar ProteinMassID.jar --benchmark

Please input the protein mass (Da):
9780

Please input the protein tolerance (Da):
10

Please enter the desired fragment ion tolerance for this benchmark:
1.5

Please enter fragment ion M/Z values, delimited by commas:
1813.8,2128.9,3881.3,4293.7,5158.0,6505.0,6619.9,6939.4,7645.1,7959.4,8022.7,8136.2,8583.3,8961.5

Please enter the desired input fasta file path:
C:\5008_RM7788.txt

Please enter the number of tables desired:
10

Please specify the desired benchmark oxidation state (o/r):
r

Beginning benchmark.
```

Table # 1 of randomly selected fragment ions (m/z A, B, C)

```
The randomly selected fragment ions were:
A: 1813.8
B: 8022.7
C: 8136.2
```

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,544,580	2,19,3	0	
E:	597,569,577	0,1,1	0	
N:	402,432,427	0,12,1	0	
D+E:	1148,1113,1154	3,34,7	0	
D+E+N:	1549,1543,1576	5,99,13	0	

Table # 2 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 4293.7
B: 8022.7
C: 8583.3

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	547,544,542	3,5,3	1	
E:	568,569,582	4,1,5	0	
N:	414,432,444	1,0,2	0	
D+E:	1113,1113,1124	13,9,10	1	
D+E+N:	1527,1543,1567	16,13,20	1	

Table # 3 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 3881.3
B: 6939.4
C: 8961.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	531,509,555	1,2,2	0	
E:	594,544,598	2,2,1	0	
N:	386,458,401	0,1,0	0	
D+E:	1124,1052,1153	8,10,7	1	
D+E+N:	1507,1510,1554	14,17,15	1	

Table # 4 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 1813.8
B: 2128.9
C: 6619.9

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,595,521	2,1,2	1	
E:	597,570,583	6,2,1	0	
N:	402,417,391	3,0,0	0	
D+E:	1148,1163,1104	12,7,5	1	
D+E+N:	1549,1580,1495	23,13,9	1	

Table # 5 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 1813.8
B: 3881.3
C: 5158.0

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,531,525	2,1,3	0	
E:	597,594,587	3,3,2	0	
N:	402,386,416	0,1,1	0	
D+E:	1148,1124,1112	11,7,10	1	
D+E+N:	1549,1507,1527	18,9,18	1	

Table # 6 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 1813.8
B: 6939.4
C: 7959.4

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,509,570	3,2,69	1	
E:	597,544,621	4,0,76	0	
N:	402,458,389	1,1,57	0	
D+E:	1148,1052,1190	7,6,146	1	
D+E+N:	1549,1510,1579	17,11,206	1	

Table # 7 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 4293.7
B: 5158.0
C: 8961.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	547,525,555	2,3,2	1	
E:	568,587,598	1,1,4	0	
N:	414,416,401	1,2,0	0	
D+E:	1113,1112,1153	7,7,7	1	

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D+E+N: 1527,1527,1554          11,16,12                    1
```

Table # 8 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 6619.9
B: 6939.4
C: 8136.2

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	521,509,580	1,1,1	0	
E:	583,544,577	1,2,2	0	
N:	391,458,427	2,1,0	0	
D+E:	1104,1052,1154	5,8,6	0	
D+E+N:	1495,1510,1576	10,20,11	0	

Table # 9 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 1813.8
B: 6939.4
C: 8961.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,509,555	3,2,3	1	
E:	597,544,598	4,2,1	0	
N:	402,458,401	1,1,2	0	
D+E:	1148,1052,1153	7,10,5	1	
D+E+N:	1549,1510,1554	17,17,11	1	

Table # 10 of randomly selected fragment ions (m/z A, B, C)

The randomly selected fragment ions were:
A: 1813.8
B: 6619.9
C: 8022.7

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,521,544	2,2,2	1	
E:	597,583,569	1,2,0	0	

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N:     402,391,432          0,0,0                   0
D+E:   1148,1104,1113       5,7,3                   1
D+E+N: 1549,1495,1543       9,8,5                   1


Benchmark complete.
```