

## S2 ImBac: Ten analyses with fragment ions of ImBac

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

```
Please input the protein mass (Da):
```

```
9650
```

```
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:
```

```
2675.4,2904.5,3076.2,3853.5,5657.5,5772.8
```

```
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: 2675.4

B: 3076.2

C: 5657.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,505,574	0,1,5	0	
E:	569,619,607	3,2,2	0	
N:	455,389,454	0,2,0	0	
D+E:	1119,1124,1178	6,8,10	1	
D+E+N:	1573,1511,1630	10,14,20	1	

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

The randomly selected fragment ions were:

A: 2904.5  
B: 3076.2  
C: 5657.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	533,505,574	4,1,0	0	
E:	626,619,607	1,2,2	0	
N:	416,389,454	1,2,0	0	
D+E:	1159,1124,1178	8,8,4	0	
D+E+N:	1574,1511,1630	23,14,9	1	

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

The randomly selected fragment ions were:

A: 3076.2  
B: 5657.5  
C: 5772.8

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	505,574,515	1,28,2	0	
E:	619,607,621	2,1,2	0	
N:	389,454,418	2,17,1	1	
D+E:	1124,1178,1135	8,61,8	1	
D+E+N:	1511,1630,1552	14,134,10	2	

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

The randomly selected fragment ions were:

A: 2675.4  
B: 2904.5  
C: 3853.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,533,564	9,0,3	0	
E:	569,626,609	2,5,2	0	
N:	455,416,400	2,1,0	0	
D+E:	1119,1159,1173	22,11,7	0	
D+E+N:	1573,1574,1572	43,16,12	1	

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

The randomly selected fragment ions were:

A: 2675.4

B: 5657.5

C: 5772.8

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,574,515	5,28,3	2	
E:	569,607,621	2,1,0	0	
N:	455,454,418	0,17,3	0	
D+E:	1119,1178,1135	10,61,7	2	
D+E+N:	1573,1630,1552	20,134,15	3	

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

The randomly selected fragment ions were:

A: 2904.5

B: 3076.2

C: 5772.8

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	533,505,515	4,2,1	0	
E:	626,619,621	1,2,2	0	
N:	416,389,418	1,1,0	0	
D+E:	1159,1124,1135	8,8,7	0	
D+E+N:	1574,1511,1552	23,10,14	1	

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

The randomly selected fragment ions were:

A: 2675.4

B: 2904.5

C: 3853.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,533,564	9,0,3	0	
E:	569,626,609	2,5,2	0	
N:	455,416,400	2,1,0	0	
D+E:	1119,1159,1173	22,11,7	0	
D+E+N:	1573,1574,1572	43,16,12	1	

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

The randomly selected fragment ions were:

A: 3076.2

B: 5657.5

C: 5772.8

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	505,574,515	1,28,2	0	
E:	619,607,621	2,1,2	0	
N:	389,454,418	2,17,1	1	
D+E:	1124,1178,1135	8,61,8	1	
D+E+N:	1511,1630,1552	14,134,10	2	

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

The randomly selected fragment ions were:

A: 2675.4

B: 2904.5

C: 5772.8

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,533,515	9,1,3	0	
E:	569,626,621	2,2,0	0	
N:	455,416,418	2,0,3	0	
D+E:	1119,1159,1135	22,7,7	0	
D+E+N:	1573,1574,1552	43,14,15	2	

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

The randomly selected fragment ions were:

A: 2675.4

B: 2904.5

C: 5657.5

	1_A,B,C	2_AB,BC,AC	3_ABC	(#of fragment ions)
D:	551,533,574	9,0,5	0	
E:	569,626,607	2,2,2	0	
N:	455,416,454	2,0,0	0	
D+E:	1119,1159,1178	22,4,10	0	
D+E+N:	1573,1574,1630	43,9,20	1	

Benchmark complete.