

poster

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Mass Spectrometry Analysis of Toxin

This poster examines a data set which was created by a Mass Spectrometry(MS) analysis of a sample. The MS data has been processed by PEAKS DeNovo Assembly to determine the peptides which are likely contained in the sample. By matching these peptides against a database, it should be possible to determine the contents of the sample and find that the toxin *Ricinus communis* is contained in the sample.

About this data

- ▶ Output from PEAKS DeNovo assembly software
- ▶ Sample contains *Ricinus communis* (castor bean)
- ▶ Peptide column contains Amino Acid Sequence of Peptides
- ▶ 5798 rows indicate 5798 peptides

Slide with R Output

```
peaks <- read.csv( "/home/danvogel/R/Capstone/poster/denovo.ricin.555510.csv")  
#summary( peaks )  
head( peaks )
```

##	Fraction	Source.File	Feature	Peptide	Scan
## 1	1	555510-DeNovo.raw	17632	HQLQEC(+57.02)C(+57.02)NELK	3199
## 2	1	555510-DeNovo.raw	6866	C(+57.02)GMEPLEC(+57.02)K	3827
## 3	1	555510-DeNovo.raw	2376	AFGMELLR	11020
## 4	1	555510-DeNovo.raw	5054	LTVAEFTDR	7616
## 5	1	555510-DeNovo.raw	-	HQLQEC(+57.02)C(+57.02)NELK	3540
## 6	1	555510-DeNovo.raw	22925	THLDDELYNQLVEK	9959

##	Tag.Length	Denovo.Score	ALC....	length	m.z	z	RT	Predict	RT	Ar
## 1	11	97	97	11	729.8253	2	8.25	-	6682900	
## 2	9	97	97	9	562.2323	2	9.42	-	110430	
## 3	8	97	97	8	468.7523	2	20.59	-	94512	
## 4	9	97	97	9	526.2742	2	15.20	-	127040	
## 5	11	97	97	11	729.8248	2	8.73	-		
## 6	14	96	96	14	858.9246	2	18.75	-	10508	

##	Mass	ppm	PTM	local.confidence.
## 1	1457.6392	-2.1	Carbamidomethylation	91 93 100 98 100 100 99 95 99 99
## 2	1122.4507	-0.6	Carbamidomethylation	93 93 99 100 99 100 100 97
## 3	935.4899	0.2		95 97 99 98 99 98 98
## 4	1050.5344	-0.6		98 98 100 100 100 97 92 93
## 5	1457.6392	-2.9	Carbamidomethylation	85 93 100 98 100 100 99 97 100 98
## 6	1715.8367	-1.2		88 90 99 99 98 99 99 99 96 98 99 95 95

##	tag	0	made
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