

Slide 2. Spectrum from the Kuster dataset validating the *OR5K5* olfactory receptor.

Spectrum for peptide SSAAMAK

Slide 3. Spectrum from the Kuster dataset validating the *OR52I1* olfactory receptor.

Spectrum for peptide AVFDLSSK

Slide 4. Spectrum from the Kuster dataset validating the *OR52P1* olfactory receptor.

Spectrum for peptide VFQSGQGMGIK

Slide 5. Spectrum from the Kuster dataset validating the *OR52N1* olfactory receptor.

Spectrum for peptide QIQEGVIK

Slide 6. Spectrum from the Kuster dataset validating the *OR6B3* olfactory receptor.

Spectrum for peptide EFKNALK

Slide 7. Spectrum from the Kuster dataset validating the *OR3A3* olfactory receptor.

Spectrum for peptide NTDVQGALCQLLVGKR

| Sequence | -log q-... | -log PEP | Search Engr... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|-----------------------------------|------------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|---------------|--------------|------------|--------------|
| MS² K.SSAAMAK.A | 2.0898 | -99 | Mascot | 26.98 | 4.39 | 2 | 736.4728 | 736.4657 | -9.62 | Dimethyl:2... | | Munoz_M... | IPS_Singa... |
| MS² K.SSAAMAK.A | 2.0898 | -99 | Mascot | 26.98 | 4.39 | 2 | 736.4728 | 736.4657 | -9.62 | Dimethyl:2... | | Munoz_M... | IPS_Singa... |
| MS² K.SSAAMAK.A | 2.0898 | -99 | Mascot | 26.98 | 4.39 | 2 | 736.4728 | 736.4657 | -9.62 | Dimethyl:2... | | Munoz_M... | IPS_Singa... |

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

Neutral loss:

CH4O NH3 C3H6S

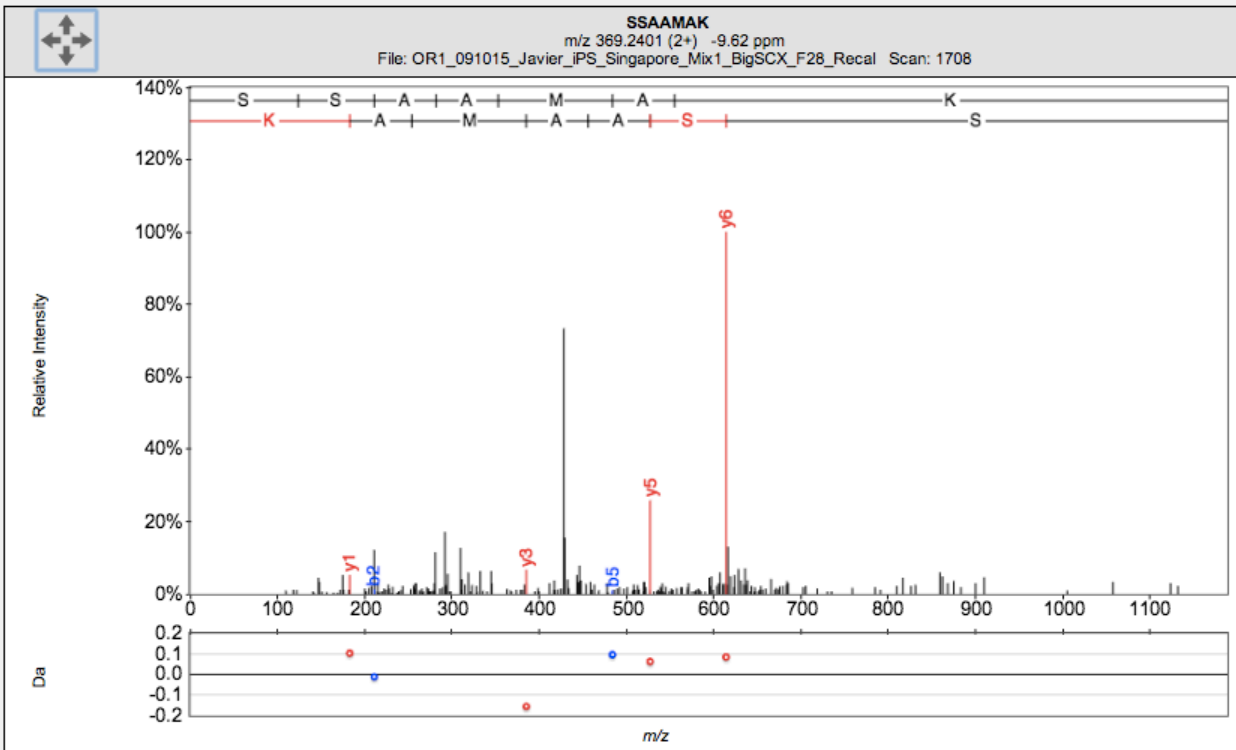
C2H4S H2O CO

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



| b1+ | # | Seq # | y1+ |
|-----------------|---|-------|-------------------|
| 124.115 | 1 | S | 7 |
| 211.147 | 2 | S | 6 614.3723 |
| 282.1841 | 3 | A | 5 527.3403 |
| 353.2212 | 4 | A | 4 456.3032 |
| 484.2617 | 5 | M | 3 385.2661 |
| 555.2988 | 6 | A | 2 254.2256 |
| | 7 | K | 1 183.1885 |

| Sequence | -log q... | -log PEP | Search Engl... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|------------------------------------|-----------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|--------------|--------------|-------------|----------------|
| MS² R.AVFDLSSK.T | 2.3667 | 1.56 | Andromeda | 63.49 | 11.49 | 2 | 873.4687 | 865.4545 | -9175.15 | Label:13C... | | Geiger_C... | HMELonza |
| MS² R.AVFDLSSK.T | 2.3667 | 1.56 | Andromeda | 63.49 | 11.49 | 2 | 873.4687 | 865.4545 | -9175.15 | Label:13C... | | Geiger_C... | HMELonza |
| MS² R.AVFDLSSK.T | 2.0768 | 1.43 | Andromeda | 98.52 | 29.33 | 2 | 865.4545 | 865.4545 | -0.01 | | | Joshi_MS... | Label-free ... |
| MS² R.AVFDLSSK.T | 2.0755 | 1.43 | Andromeda | 82.45 | 6.42 | 2 | 865.4545 | 865.4545 | -0.01 | | | CPTAC_C... | Clinical_pr... |
| MS² R.AVFDLSSK.T | 2.4811 | 1.41 | Andromeda | 60.59 | 18.48 | 2 | 873.4687 | 865.4545 | -9175.15 | Label:13C... | | Geiger_C... | HCC1937 |

< 1 2 >

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

Neutral loss:

H2O NH3 C2O

C4H9N CH4O C3H9N

CO C4H8 C2H5N

C5H11N C4H11N C3H6

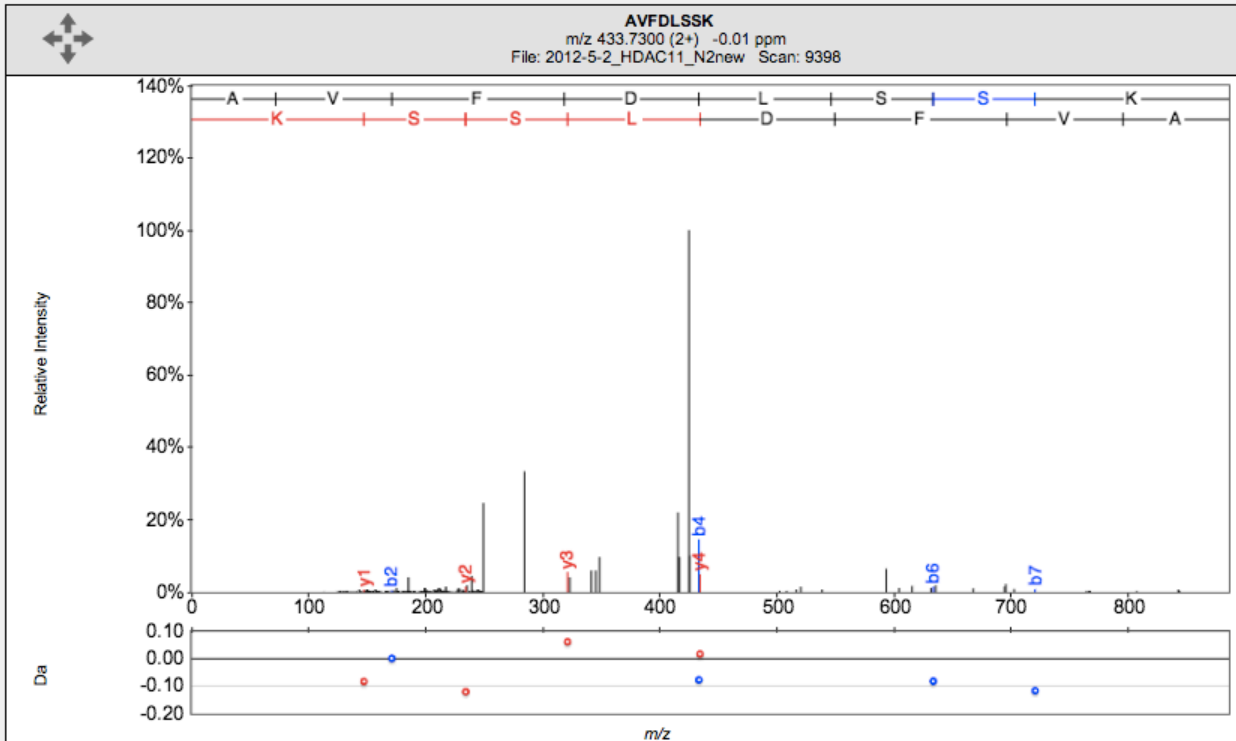
C2H4O2

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



| b1+ | # | Seq | # | y1+ |
|----------|---|-----|---|----------|
| 72.0444 | 1 | A | 8 | |
| 171.1128 | 2 | V | 7 | 795.4247 |
| 318.1812 | 3 | F | 6 | 696.3563 |
| 433.2082 | 4 | D | 5 | 549.2879 |
| 546.2922 | 5 | L | 4 | 434.2609 |
| 633.3243 | 6 | S | 3 | 321.1769 |
| 720.3563 | 7 | S | 2 | 234.1448 |
| | 8 | K | 1 | 147.1128 |

| Sequence | -log q-... | -log PEP | Search Engl... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|---------------------------------------|------------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|-------------|--------------|------------|--------------|
| MS² R.VFQSGQGGMGIKA | 2.07 | 0.21 | Mascot | 29.98 | 10.36 | 3 | 1222.6380 | 1222.6315 | -5.34 | Dimethyl... | Oxidation... | Munoz_E... | Comparis... |
| MS² R.VFQSGQGGMGIKA | 2.07 | 0.21 | Mascot | 29.98 | 10.36 | 3 | 1222.6380 | 1222.6315 | -5.34 | Dimethyl... | Oxidation... | Munoz_E... | Compariso... |

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

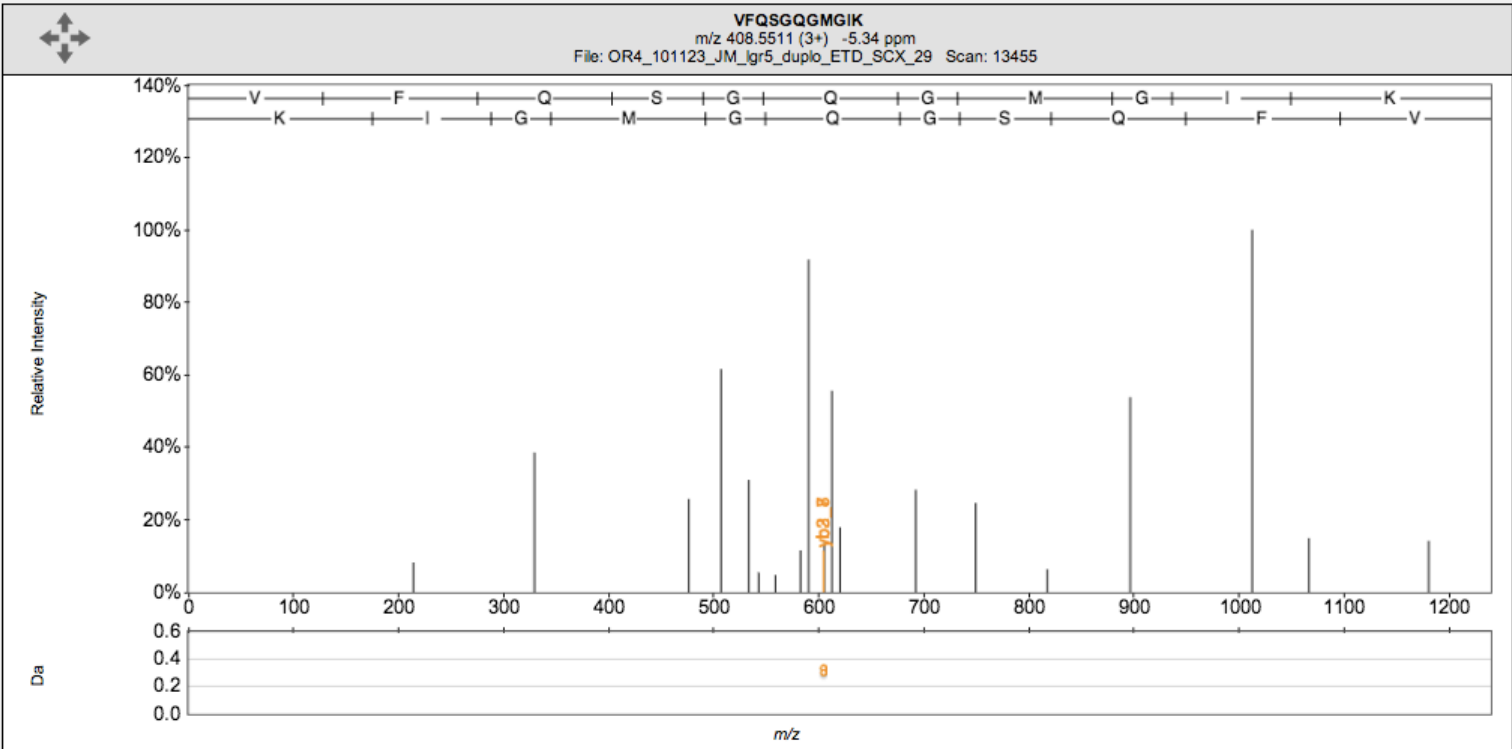
Neutral loss:

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



Fragment Ion Table

| Sequence | -log q... | -log PEP | Search Engl... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|------------------------------------|-----------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|-------------|--------------|-------------|---------------|
| MS² K.QIQEGVIK.F | 2.346 | 1.88 | Andromeda | 93.43 | 2.36 | 2 | 913.5233 | 913.5233 | 0.01 | | | Maier_MC... | tissue_pro... |
| MS² K.QIQEGVIK.F | 5 | 1 | Mascot | 38.48 | 1.72 | 2 | 913.5233 | 914.5187 | 1089.7 | | | Nagaraj_... | Deep prot... |
| MS² K.QIQEGVIK.F | 3.0218 | 0.39 | Mascot | 49.95 | 2.07 | 2 | 913.5233 | 914.5184 | 1089.31 | | | Human_b... | Proteome ... |
| MS² K.QIQEGVIK.F | 3.0687 | 0.31 | Mascot | 51.09 | 2.27 | 2 | 913.5233 | 914.5179 | 1088.74 | | | Human_b... | Proteome ... |
| MS² K.QIQEGVIK.F | 2.0583 | 0.15 | Mascot | 24.22 | 7.65 | 2 | 913.5233 | 913.5237 | 0.51 | | | Human_b... | Proteome ... |

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

Neutral loss:

H2O C3H6 NH3

C2H5NO C2H5N C5H11N

C3H9N C3H5NO CH3NO

C2H4 C4H9N C4H11N

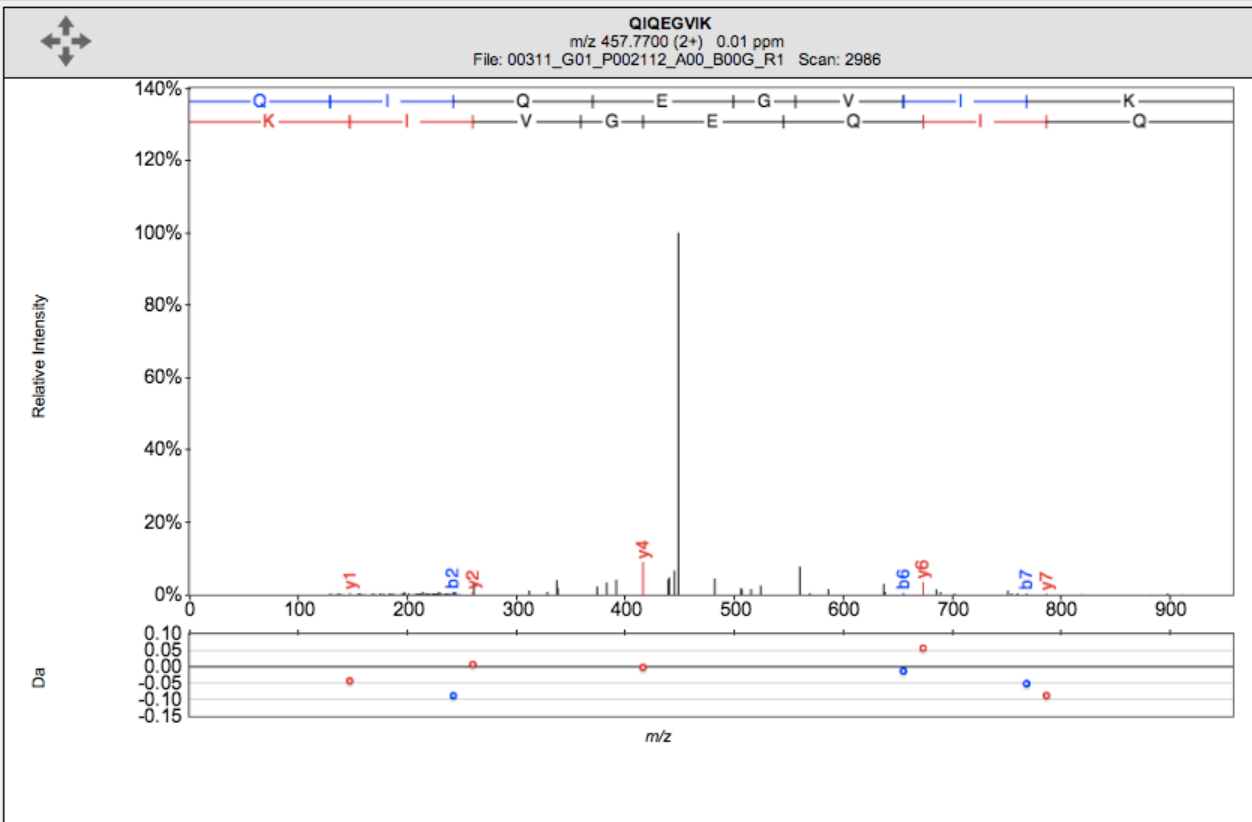
CO

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



| b1+ | # | Seq # | y1+ |
|----------|---|-------|-------------------|
| 129.0659 | 1 | Q | 8 |
| 242.1499 | 2 | I | 7 786.472 |
| 370.2085 | 3 | Q | 6 673.3879 |
| 499.2511 | 4 | E | 5 545.3293 |
| 556.2726 | 5 | G | 4 416.2867 |
| 655.341 | 6 | V | 3 359.2653 |
| 768.425 | 7 | I | 2 260.1969 |
| | 8 | K | 1 147.1128 |

| Sequence | -log q-... | -log PEP | Search Engi... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|-----------------------------------|------------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|-------------|--------------|--------------|----------------|
| MS² K.EFKNALK.K | 2.6669 | 1.16 | Andromeda | 97.07 | 10.2 | 2 | 848.4756 | 848.4756 | 0 | | | Cutler_Pe... | Roche_hu... |
| MS² K.EFKNALK.K | 2.6711 | 0.93 | Andromeda | 94.26 | 24.26 | 2 | 848.4756 | 848.4756 | 0 | | | Cutler_Pe... | Roche_hu... |
| MS² K.EFKNALK.K | 2.2728 | 0.6 | Andromeda | 76.85 | 6.85 | 2 | 848.4756 | 848.4756 | 0 | | | IEC_prote... | colon |
| MS² K.EFKNALK.K | 2.0411 | 0.66 | Andromeda | 76.85 | 5.5 | 2 | 848.4756 | 848.4756 | 0 | | | Moghadda... | full proteo... |
| MS² K.EFKNALK.K | 2.3445 | 0.58 | Andromeda | 76.04 | 6.65 | 2 | 848.4756 | 848.4756 | 0 | | | Cutler_Pe... | Roche_hu... |

< 1 2 3 >

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

Neutral loss:

C5H11N NH3 C4H8

H2O C2H5N C4H9N

C3H6 C4H11N C3H9N

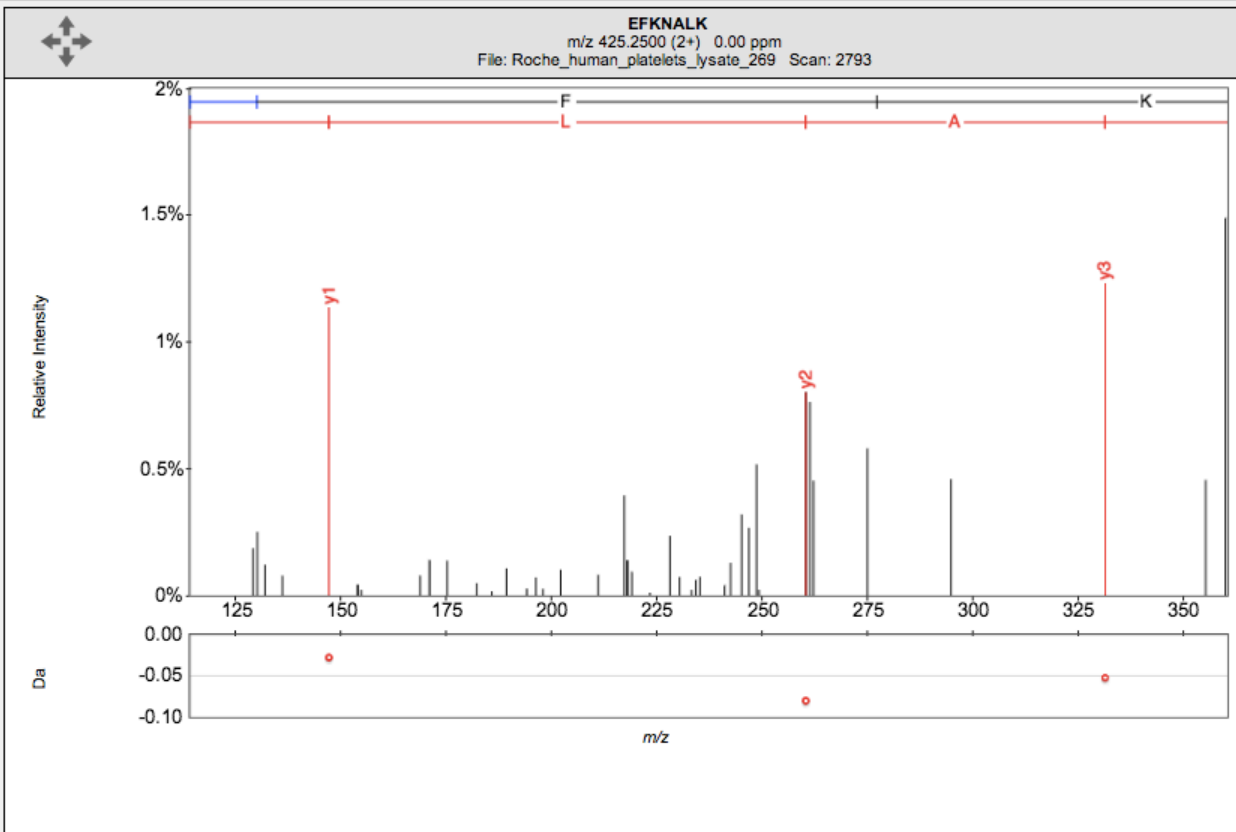
C2H4O2

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



| b1+ | # | Seq # | y1+ |
|----------|---|-------|----------|
| 130.0499 | 1 | E 7 | |
| 277.1183 | 2 | F 6 | 720.4403 |
| 405.2132 | 3 | K 5 | 573.3719 |
| 519.2562 | 4 | N 4 | 445.2769 |
| 590.2933 | 5 | A 3 | 331.234 |
| 703.3774 | 6 | L 2 | 260.1969 |
| | 7 | K 1 | 147.1128 |

| Sequence | -log q-... | -log PEP | Search Engi... | Score | Delta Score | z | Theoretic... | Measured... | Mass Err... | Fixed Mo... | Variable ... | Project | Experiment |
|--|------------|----------|----------------|-------|-------------|---|--------------|-------------|-------------|-------------|--------------|------------|--------------|
| MS² R.NTDVQGALCQLLVGKR.S | 2.2539 | 0.53 | Andromeda | 81.45 | 4.86 | 3 | 1827.0037 | 1770.9411 | -30685.54 | Carbamid... | | Munoz_M... | 4Skin_Mix... |
| MS² R.NTDVQGALCQLLVGKR.S | 2.2539 | 0.53 | Andromeda | 81.45 | 4.86 | 3 | 1827.0037 | 1770.9411 | -30685.54 | Carbamid... | | Munoz_M... | 4Skin_Mix... |
| MS² R.NTDVQGALCQLLVGKR.S | 2.2539 | 0.53 | Andromeda | 81.45 | 4.86 | 3 | 1827.0037 | 1770.9411 | -30685.54 | Carbamid... | | Munoz_M... | 4Skin_Mix... |

[Click for peptide details](#)

> Reference spectrum

> Fragments

Select All Deselect All

a: 1+ 2+ 3+

b: 1+ 2+ 3+

c: 1+ 2+ 3+

x: 1+ 2+ 3+

y: 1+ 2+ 3+

z: 1+ 2+ 3+

yb:

IM:

M[H]:

Neutral loss:

CH3NO C2H4O CO2

NH3 CH2N2 C3H6

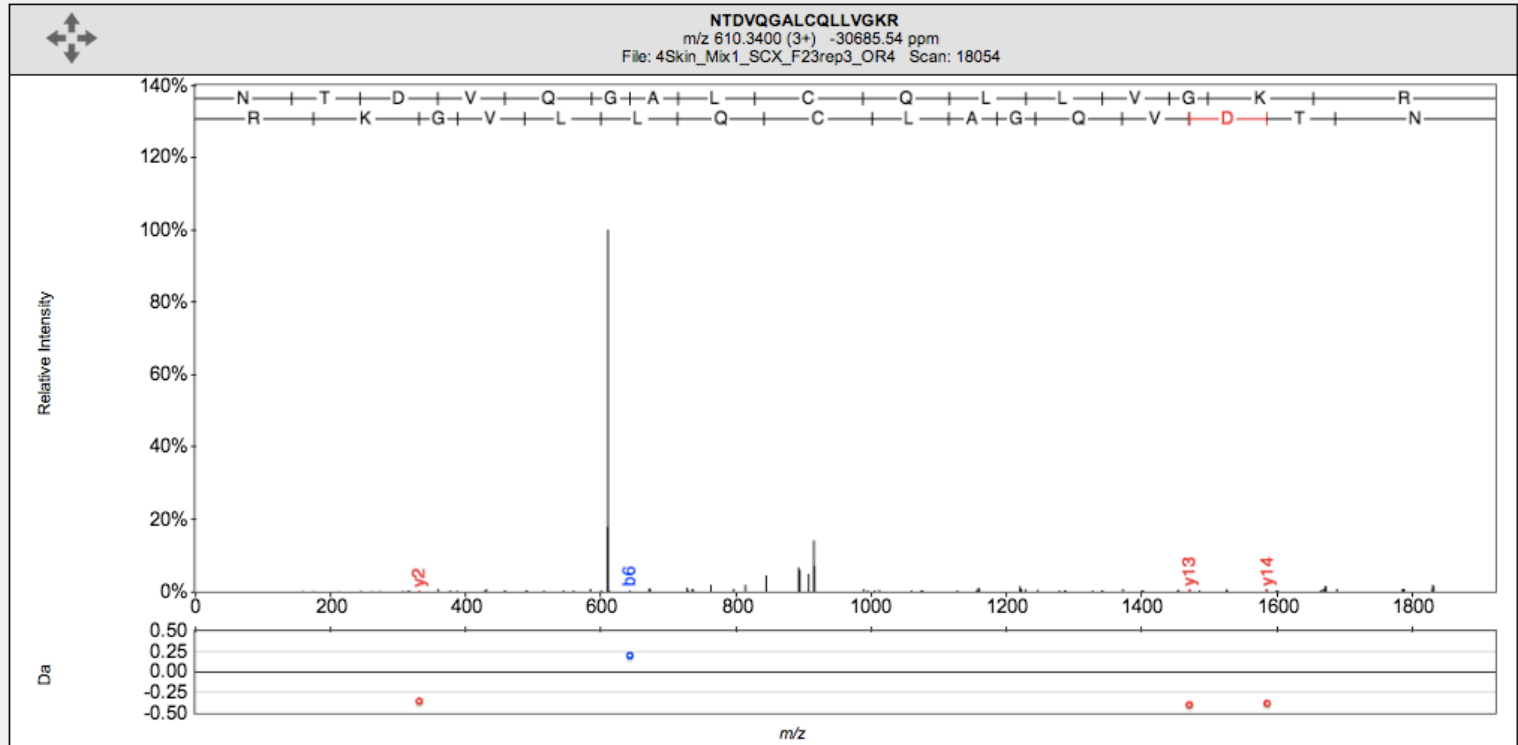
C2H5NO C3H9N3

Max neutral loss count: 3

Mass tolerance: 0.4 Da

Expert Mode: on off

> Configuration



Fragment Ion Table