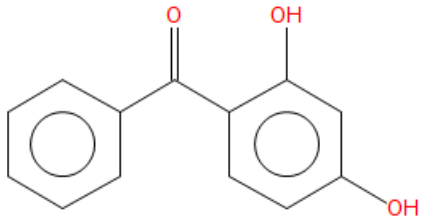
# Thermo Freestyle *Easily* Sends MSMS Spectra to NIST Search




**Uvinul 3000**
**MW 214**
*(UV Absorber/Light Stabilizer )*

Name: Methanone, (2,4-dihydroxyphenyl)phenyl-
Formula: $C_{13}H_{10}O_3$
MW: 214 Exact Mass: 214.062994 CAS#: 131-56-6 NIST#: 492528 ID#: 172010 DB: mainlib

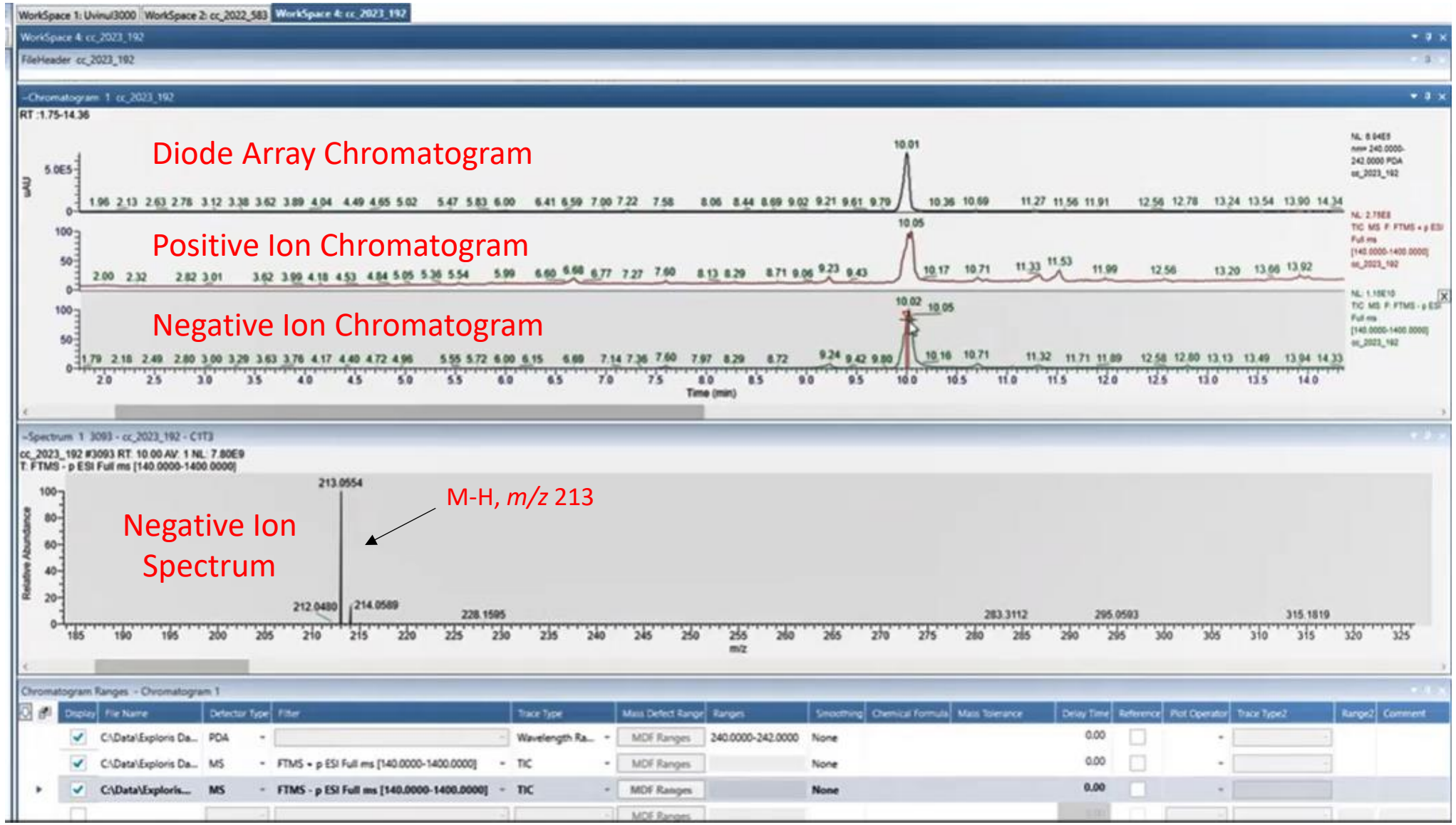
# Summary of Results

- Pos and Neg MSMS Spectra easily sent to NIST Search in accurate mass mode for searching
- Ion polarity imported into NIST search via MSP file
- Shows precursor *m/z* which is very useful
- See typical fields shown in NIST reference spectra below

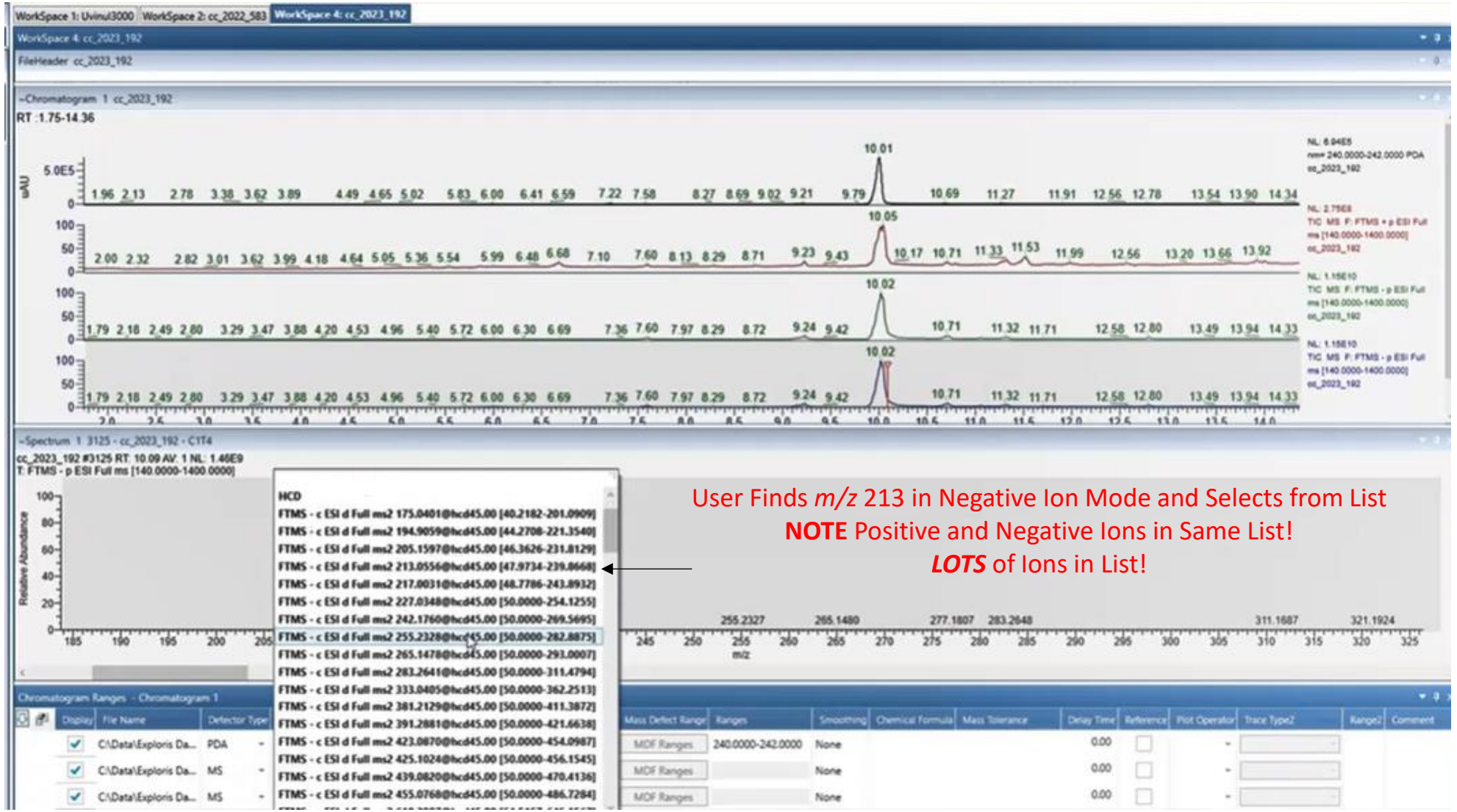
## Approach for Qualitative Analyses in Thermo Orbitrap with Processing in Freestyle

- I really like the Orbitrap approach for qualitative analysis of compounds
- Very easy to use and quickly obtain useful data
- Acquires in Pos/Neg Mode
- Diode Array data
- Automatically determines major ions to fragment
- Collects the MSMS data at several different energies and stores in trap
- Then collects spectrum

# Uvinul 3000 Works Best in Negative Ion Mode Because Phenol



# Instrument Detects Ions and Then Automatically Decides Ones for MSMS Analyses
# User Looks Through List and Picks the One of Interest to Plot Vs. Time

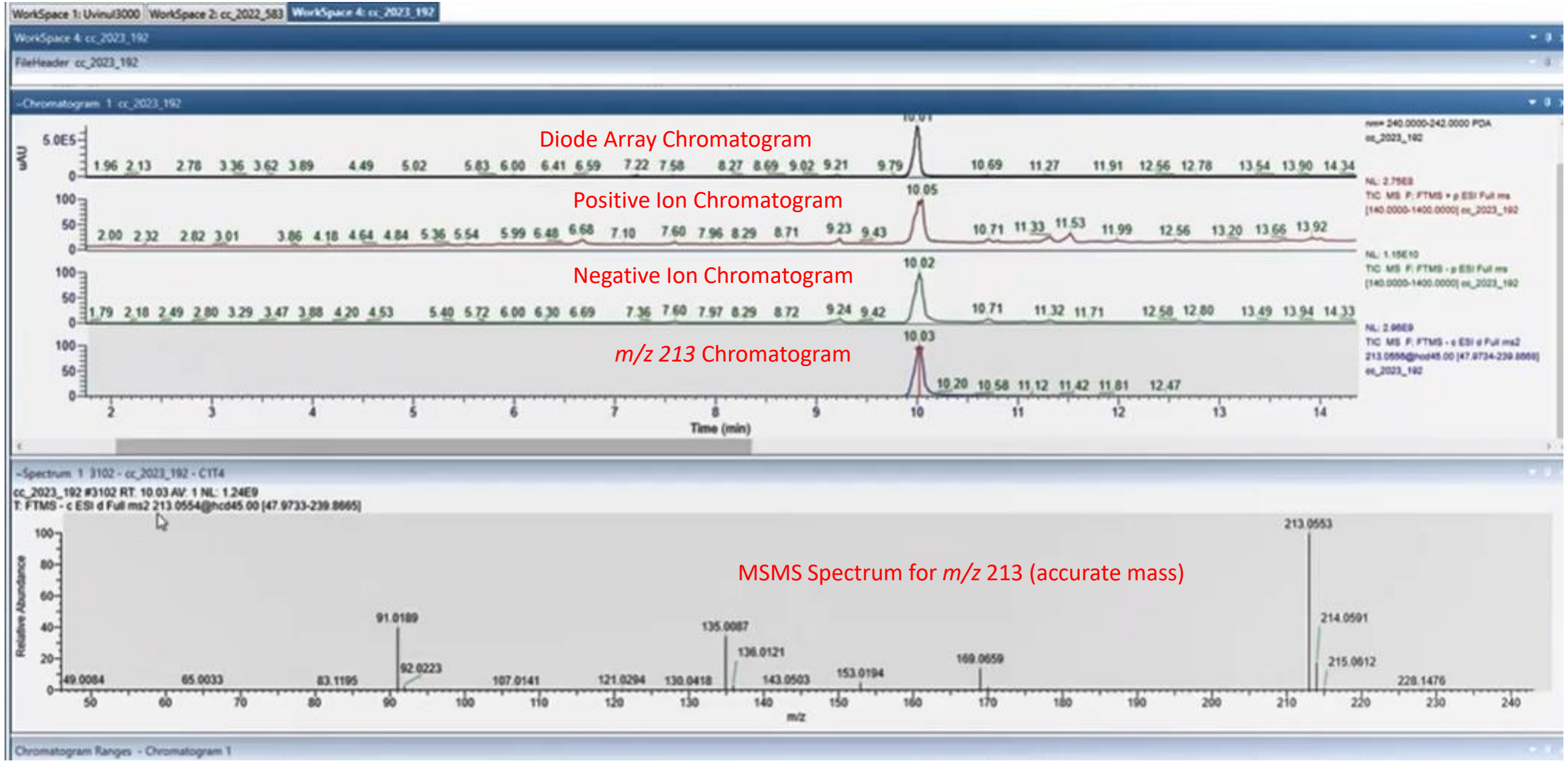



User Finds *m/z* 213 in Negative Ion Mode and Selects from List

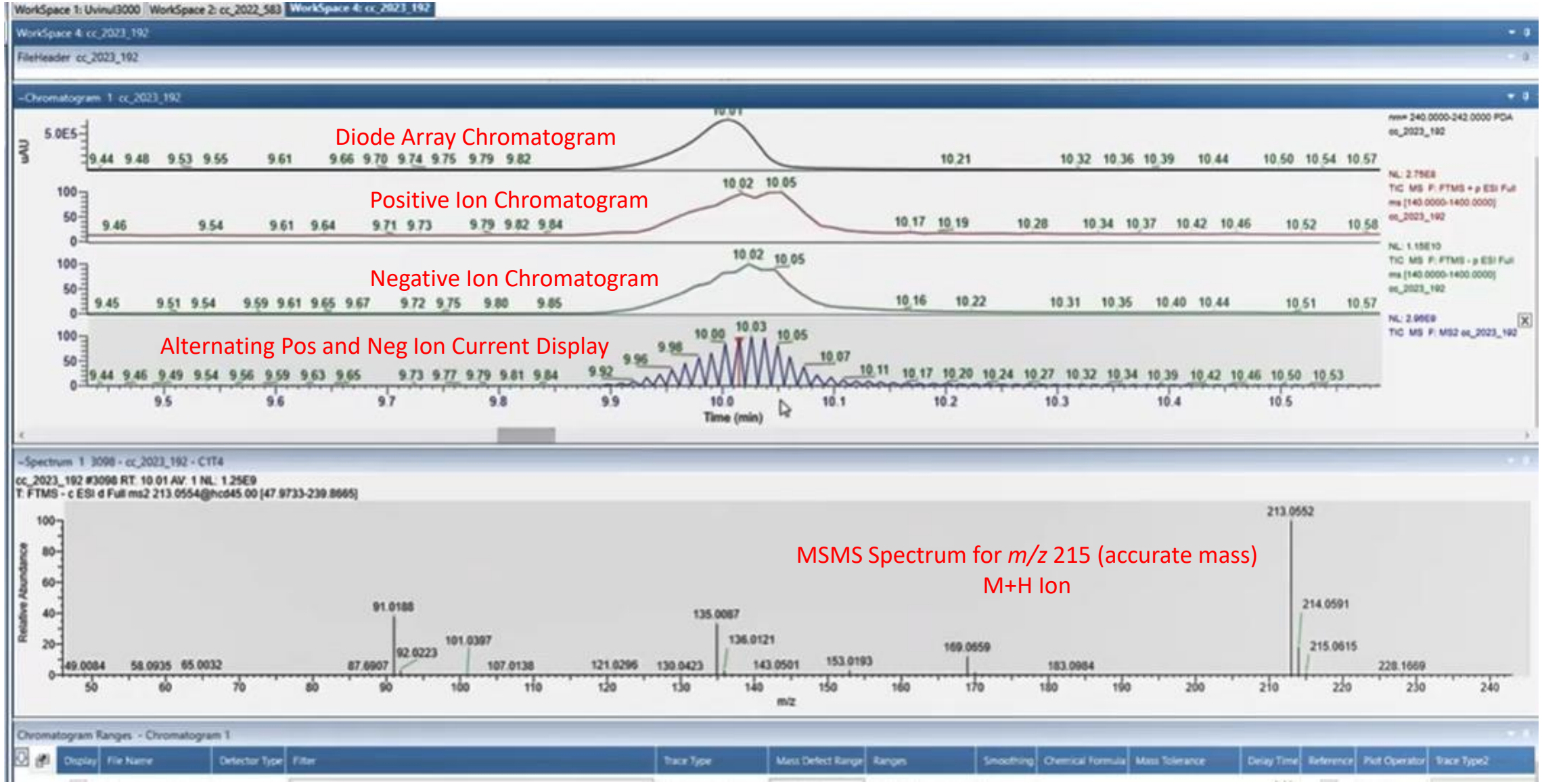
**NOTE** Positive and Negative Ions in Same List!

***LOTS*** of Ions in List!

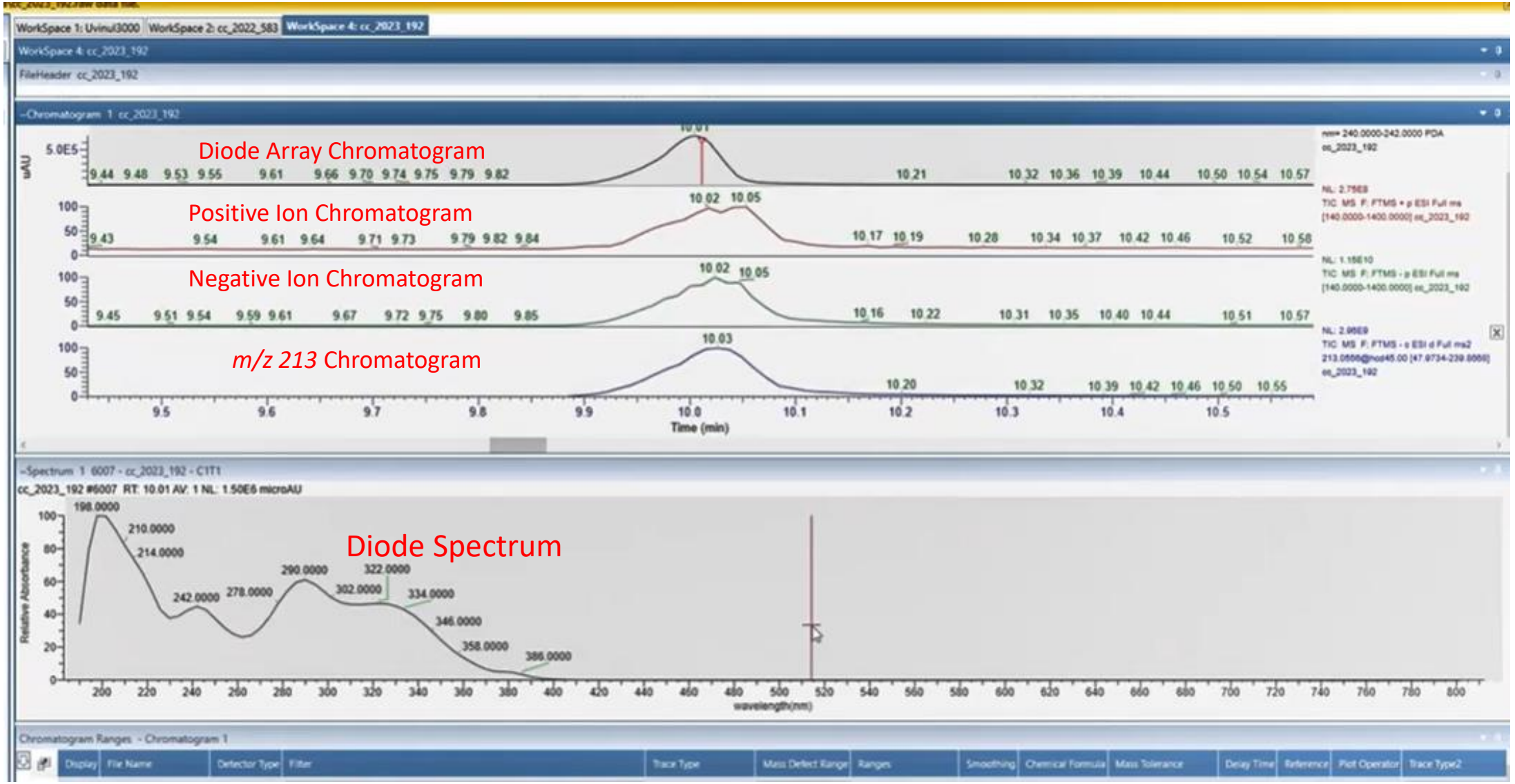
# After User Select, Ion Chromatogram for M-1 Ion at *m/z* 213 Plotted



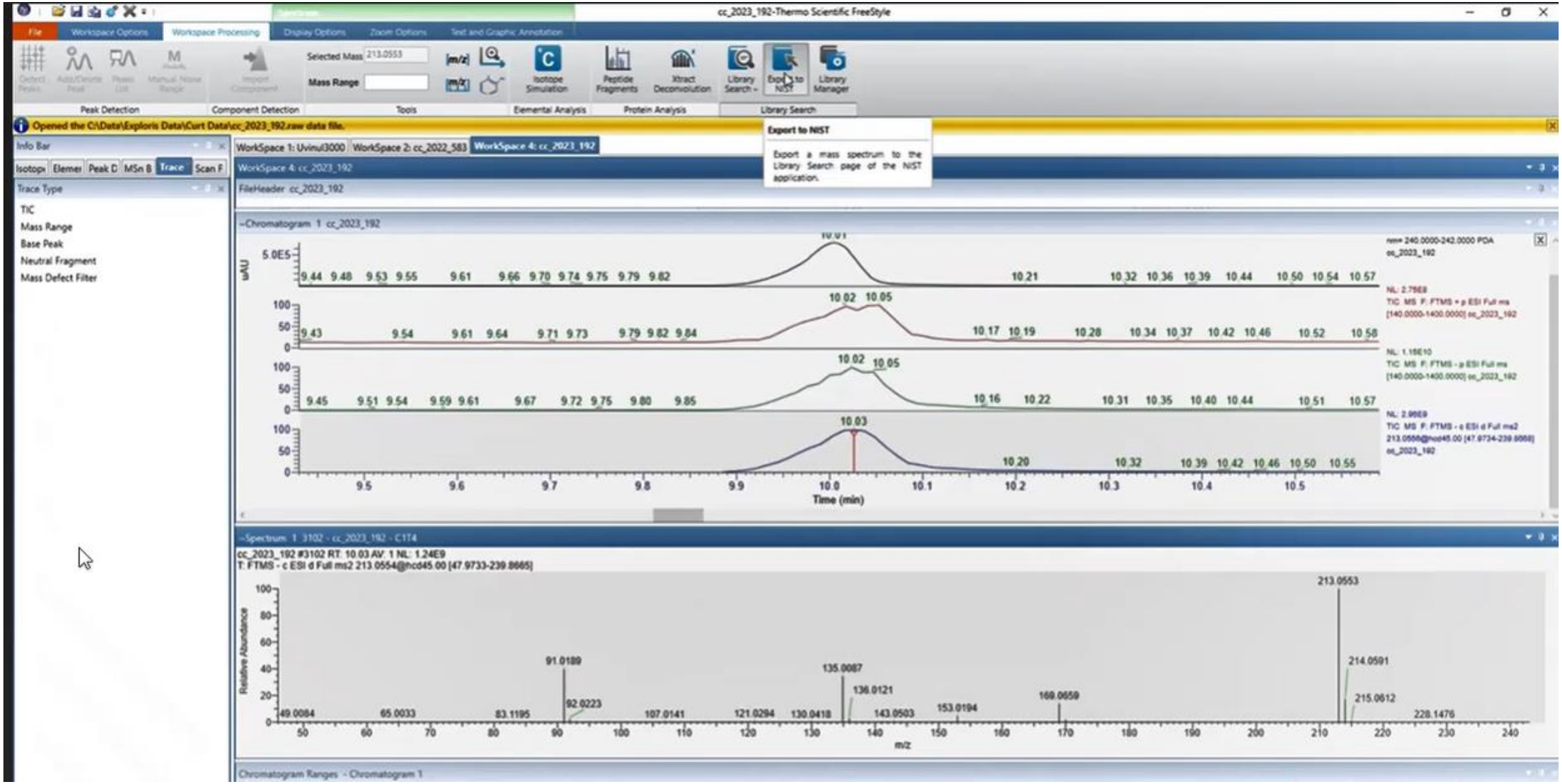
# Can Step Through the Chromatogram in Pos and Negative Chromatogram ("MS2 Mode")
# The Lower Dip Is Positive and the Spike is Negative, Much Stronger Signal in Negative



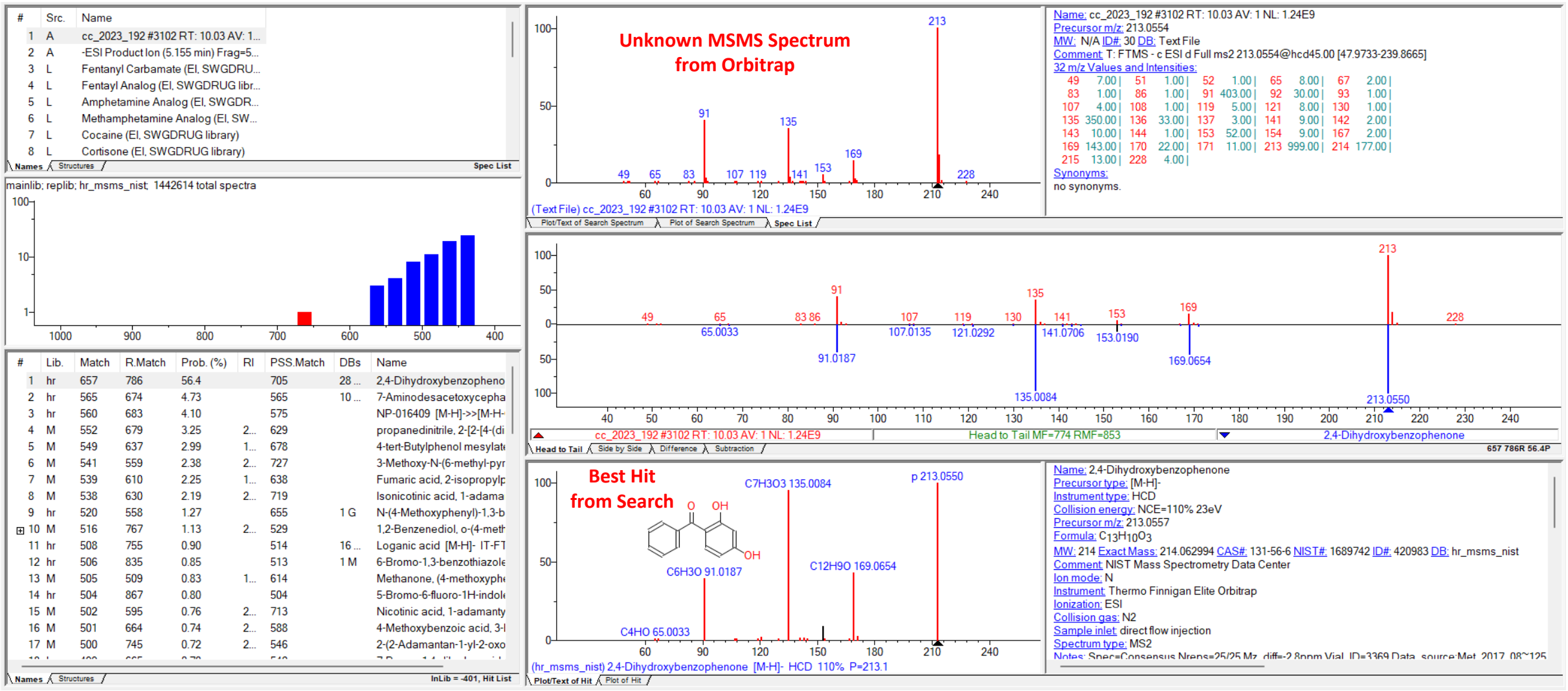
# Can Obtain Diode Array Spectrum Shown on Bottom



# Export to NIST Button
# MSP Format



# Search Results in NIST MS Search of NIST Reference Library




| # | Src. | Name |
|---|---|---|
| 1 | A | cc_2023_192 #3102 RT: 10.03 AV: 1... |
| 2 | A | -ESI Product Ion (5.155 min) Frag=5... |
| 3 | L | Fentanyl Carbamate (EI, SWGDRU... |
| 4 | L | Fentayl Analog (EI, SWGDRUG libr... |
| 5 | L | Amphetamine Analog (EI, SWGDR... |
| 6 | L | Methamphetamine Analog (EI, SW... |
| 7 | L | Cocaine (EI, SWGDRUG library) |
| 8 | L | Cortisone (EI, SWGDRUG library) |

| # | Lib. | Match | R.Match | Prob. (%) | RI | PSS.Match | DBs | Name |
|---|---|---|---|---|---|---|---|---|
| 1 | hr | 657 | 786 | 56.4 | | 705 | 28 ... | 2,4-Dihydroxybenzopheno |
| 2 | hr | 565 | 674 | 4.73 | | 565 | 10 ... | 7-Aminodesacetoxycepha |
| 3 | hr | 560 | 683 | 4.10 | | 575 | | NP-016409 [M-H]->>[M-H- |
| 4 | M | 552 | 679 | 3.25 | 2... | 629 | | propanedinitrile, 2-[2-[4-(di |
| 5 | M | 549 | 637 | 2.99 | 1... | 678 | | 4-tert-Butylphenol mesylate |
| 6 | M | 541 | 559 | 2.38 | 2... | 727 | | 3-Methoxy-N-(6-methyl-pyr |
| 7 | M | 539 | 610 | 2.25 | 1... | 638 | | Fumaric acid, 2-isopropylp |
| 8 | M | 538 | 630 | 2.19 | 2... | 719 | | Isonicotinic acid, 1-adama |
| 9 | hr | 520 | 558 | 1.27 | | 655 | 1 G | N-(4-Methoxyphenyl)-1,3-b |
| 10 | M | 516 | 767 | 1.13 | 2... | 529 | | 1,2-Benzenediol, o-(4-meth |
| 11 | hr | 508 | 755 | 0.90 | | 514 | 16 ... | Loganic acid [M-H]- IT-FT |
| 12 | hr | 506 | 835 | 0.85 | | 513 | 1 M | 6-Bromo-1,3-benzothiazole |
| 13 | M | 505 | 509 | 0.83 | 1... | 614 | | Methanone, (4-methoxyphe |
| 14 | hr | 504 | 867 | 0.80 | | 504 | | 5-Bromo-6-fluoro-1H-indole |
| 15 | M | 502 | 595 | 0.76 | 2... | 713 | | Nicotinic acid, 1-adamanty |
| 16 | M | 501 | 664 | 0.74 | 2... | 588 | | 4-Methoxybenzoic acid, 3-I |
| 17 | M | 500 | 745 | 0.72 | 2... | 546 | | 2-(2-Adamantan-1-yl-2-oxo |

Name: cc_2023_192 #3102 RT: 10.03 AV: 1 NL: 1.24E9
Precursor m/z: 213.0554
MW: N/A ID#: 30 DB: Text File
Comment: T: FTMS - c ESI d Full ms2 213.0554@hcd45.00 [47.9733-239.8665]
32 m/z Values and Intensities:

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 49 | 7.00 | 51 | 1.00 | 52 | 1.00 | 65 | 8.00 | 67 | 2.00 | | |
| 83 | 1.00 | 86 | 1.00 | 91 | 403.00 | 92 | 30.00 | 93 | 1.00 | | |
| 107 | 4.00 | 108 | 1.00 | 119 | 5.00 | 121 | 8.00 | 130 | 1.00 | | |
| 135 | 350.00 | 136 | 33.00 | 137 | 3.00 | 141 | 9.00 | 142 | 2.00 | | |
| 143 | 10.00 | 144 | 1.00 | 153 | 52.00 | 154 | 9.00 | 167 | 2.00 | | |
| 169 | 143.00 | 170 | 22.00 | 171 | 11.00 | 213 | 999.00 | 214 | 177.00 | | |
| 215 | 13.00 | 228 | 4.00 | | | | | | | | |

Synonyms:
no synonyms.

(Text File) cc_2023_192 #3102 RT: 10.03 AV: 1 NL: 1.24E9

cc_2023_192 #3102 RT: 10.03 AV: 1 NL: 1.24E9 | Head to Tail MF=774 RMF=853 | 2,4-Dihydroxybenzophenone

657 786R 56.4P

Name: 2,4-Dihydroxybenzophenone
Precursor type: [M-H]-
Instrument type: HCD
Collision energy: NCE=110% 23eV
Precursor m/z: 213.0557
Formula: $C_{13}H_{10}O_3$
MW: 214 Exact Mass: 214.062994 CAS#: 131-56-6 NIST#: 1689742 ID#: 420983 DB: hr_msms_nist
Comment: NIST Mass Spectrometry Data Center
Ion mode: N
Instrument: Thermo Finnigan Elite Orbitrap
Ionization: ESI
Collision gas: N2
Sample inlet: direct flow injection
Spectrum type: MS2
Notes: Spec=Consensus Nreps=25/25 Mz_diff=-2.8ppm Vial_ID=3369 Data_source:Met_2017_08~125

(hr_msms_nist) 2,4-Dihydroxybenzophenone [M-H]- HCD 110% P=213.1

# Full MSP File Format Exported from Thermo Freestyle to NIST Search

***Note:*** **Includes Precursor m/z Which Is Very Useful in NIST Search Program**

```
Name: cc_2023_192 #3102 RT: 10.03 AV: 1 NL: 1.24E9
PrecursorMZ: 213.0554
DB#: 161
Comments: T: FTMS - c ESI d Full ms2 213.0554@hcd45.00 [47.9733-239.8665]
Num Peaks: 32
49 7.00
51 1.00
52 1.00
65 8.00
67 2.00
83 1.00
86 1.00
91 403.00
92 30.00
93 1.00
107 4.00
108 1.00
119 5.00
121 8.00
130 1.00
135 350.00
136 33.00
137 3.00
141 9.00
142 2.00
143 10.00
144 1.00
153 52.00
154 9.00
167 2.00
169 143.00
170 22.00
171 11.00
213 999.00
214 177.00
215 13.00
228 4.00
```

# MS Interpreter Will Interpret Fragments and Show the Mass Error, *e.g. m/z* 137, 0.1 ppm error!