# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117913.D
Acq On : 21 Nov 2019 15:40
Operator : JU
Sample : K5933-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC-COMP-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.152 | 6 | 11 | 29 | rVB | 659621 | 970466 | 21.80% | 2.832% |
| 2 | 5.122 | 509 | 516 | 523 | rBV | 439838 | 518632 | 11.65% | 1.514% |
| 3 | 5.522 | 579 | 584 | 588 | rBV | 2592378 | 2666349 | 59.89% | 7.781% |
| 4 | 6.534 | 751 | 756 | 759 | rBV | 2758754 | 2868726 | 64.43% | 8.372% |
| 5 | 6.681 | 777 | 781 | 784 | rBV | 3360104 | 2986471 | 67.08% | 8.715% |
| 6 | 6.916 | 817 | 821 | 824 | rBV | 894834 | 743003 | 16.69% | 2.168% |
| 7 | 7.075 | 844 | 848 | 851 | rBV | 2592083 | 2330594 | 52.35% | 6.801% |
| 8 | 7.475 | 912 | 916 | 919 | rBV | 2070305 | 1809917 | 40.65% | 5.282% |
| 9 | 8.204 | 1036 | 1040 | 1043 | rBV | 1064770 | 949707 | 21.33% | 2.772% |
| 10 | 9.281 | 1219 | 1223 | 1226 | rBV | 4567414 | 3638692 | 81.73% | 10.619% |
| 11 | 9.675 | 1286 | 1290 | 1299 | rBV | 681883 | 600253 | 13.48% | 1.752% |
| 12 | 9.963 | 1336 | 1339 | 1350 | rVB | 1359643 | 1183214 | 26.58% | 3.453% |
| 13 | 10.757 | 1470 | 1474 | 1477 | rBV | 2564113 | 2266213 | 50.90% | 6.614% |
| 14 | 11.457 | 1589 | 1593 | 1600 | rBV | 1555116 | 1297971 | 29.15% | 3.788% |
| 15 | 11.974 | 1678 | 1681 | 1693 | rBV | 241175 | 287987 | 6.47% | 0.840% |
| 16 | 12.769 | 1812 | 1816 | 1827 | rBV | 266418 | 346455 | 7.78% | 1.011% |
| 17 | 12.863 | 1828 | 1832 | 1836 | rVB2 | 43921 | 50668 | 1.14% | 0.148% |
| 18 | 13.051 | 1859 | 1864 | 1867 | rBV | 4792752 | 4452279 | 100.00% | 12.993% |
| 19 | 13.951 | 2013 | 2017 | 2031 | rBV2 | 210667 | 450424 | 10.12% | 1.314% |
| 20 | 14.104 | 2039 | 2043 | 2047 | rBV | 1556071 | 1432163 | 32.17% | 4.180% |
| 21 | 14.568 | 2118 | 2122 | 2125 | rBV | 65791 | 76577 | 1.72% | 0.223% |
| 22 | 14.863 | 2169 | 2172 | 2181 | rBV2 | 349285 | 500837 | 11.25% | 1.462% |
| 23 | 15.239 | 2233 | 2236 | 2241 | rVB | 104479 | 119658 | 2.69% | 0.349% |
| 24 | 15.615 | 2294 | 2300 | 2303 | rBV | 1113934 | 1421099 | 31.92% | 4.147% |
| 25 | 16.104 | 2378 | 2383 | 2388 | rBV | 80159 | 127561 | 2.87% | 0.372% |
| 26 | 16.627 | 2470 | 2472 | 2478 | rVB3 | 49675 | 78403 | 1.76% | 0.229% |
| 27 | 17.503 | 2616 | 2621 | 2627 | rBV9 | 34567 | 91958 | 2.07% | 0.268% |

Sum of corrected areas: 34266277

LSC Report - Integrated Chromatogram

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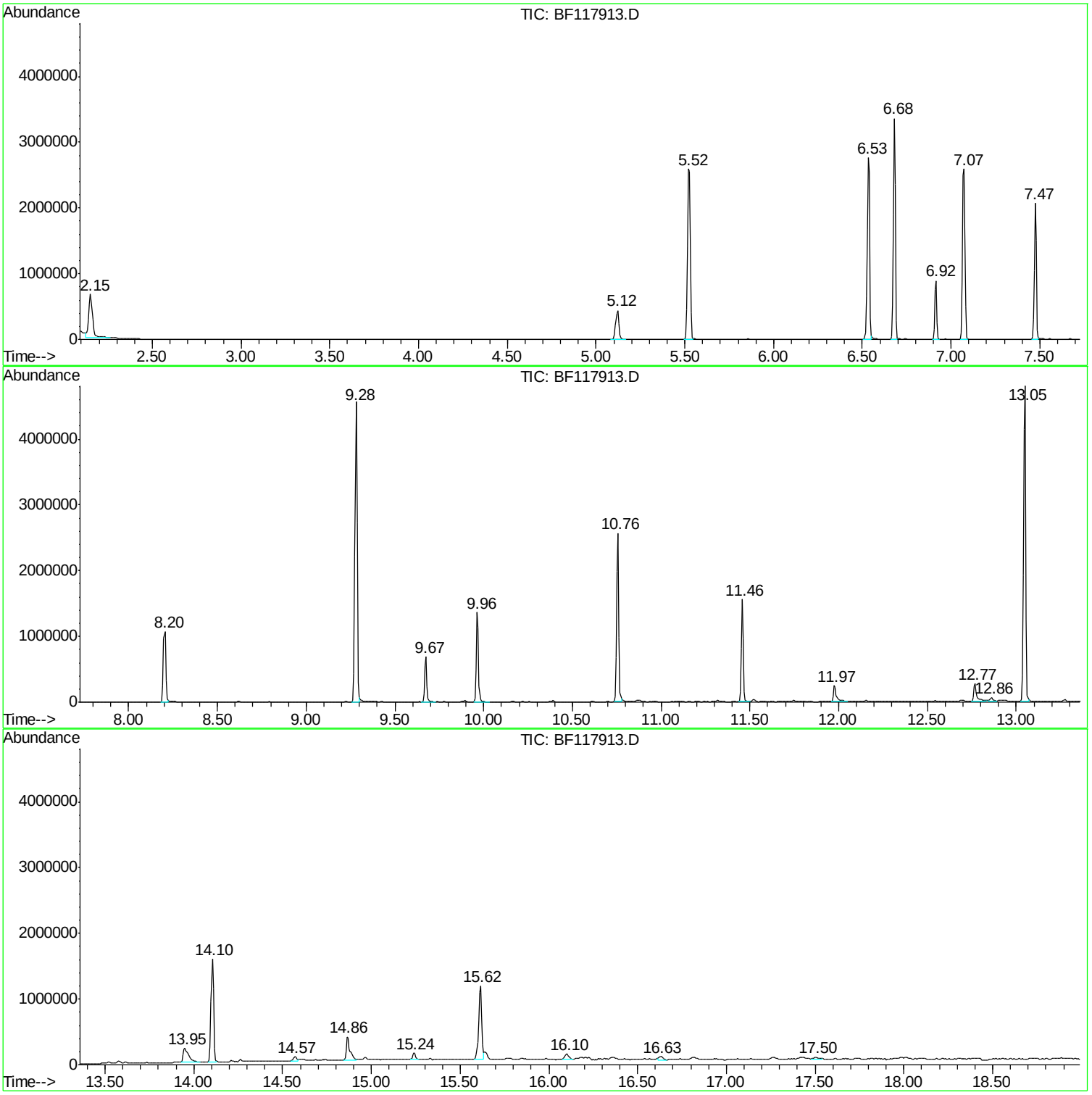
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
WC-COMP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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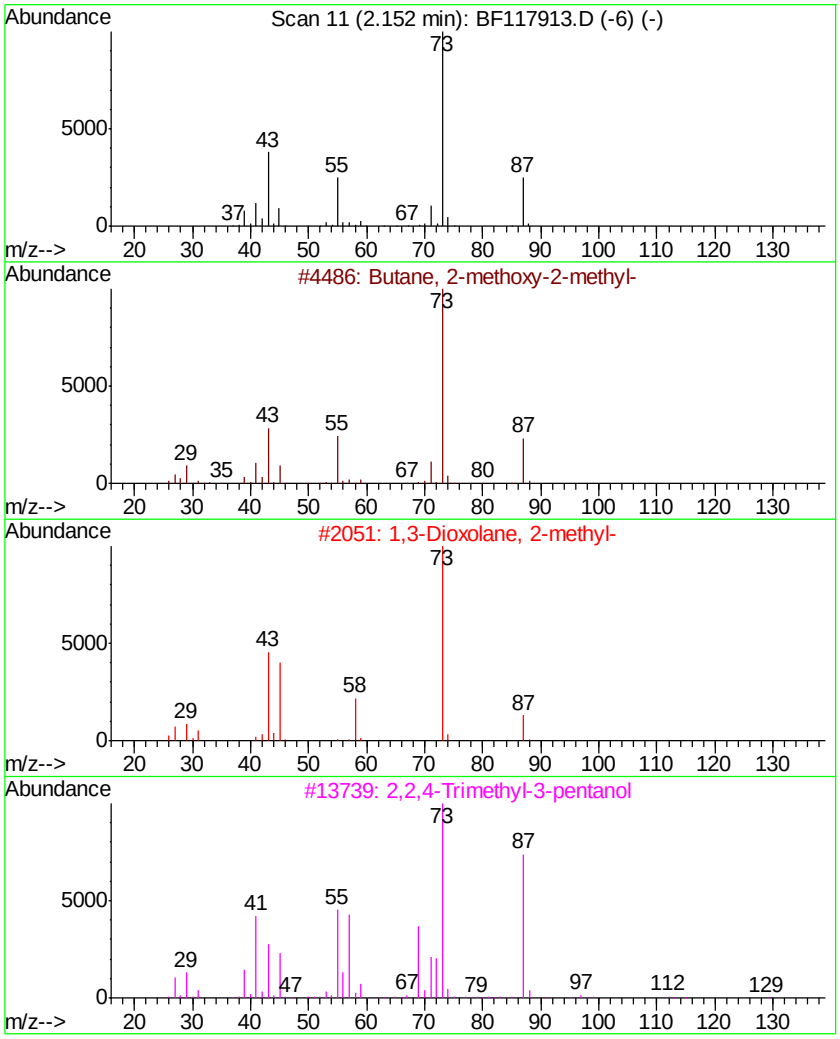
TIC Integration Parameters: LSCINT.P

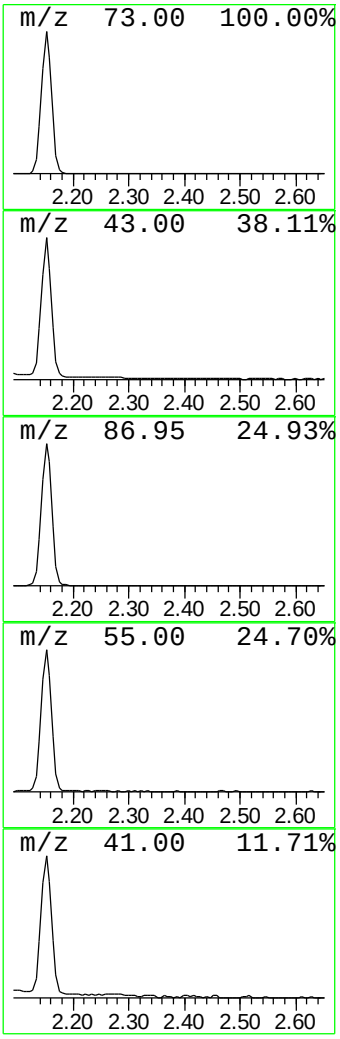
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.15 | 26.12 ng | 970466 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 38 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 38 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 27 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |



# Library Search Compound Report

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Sample : K5933-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC-COMP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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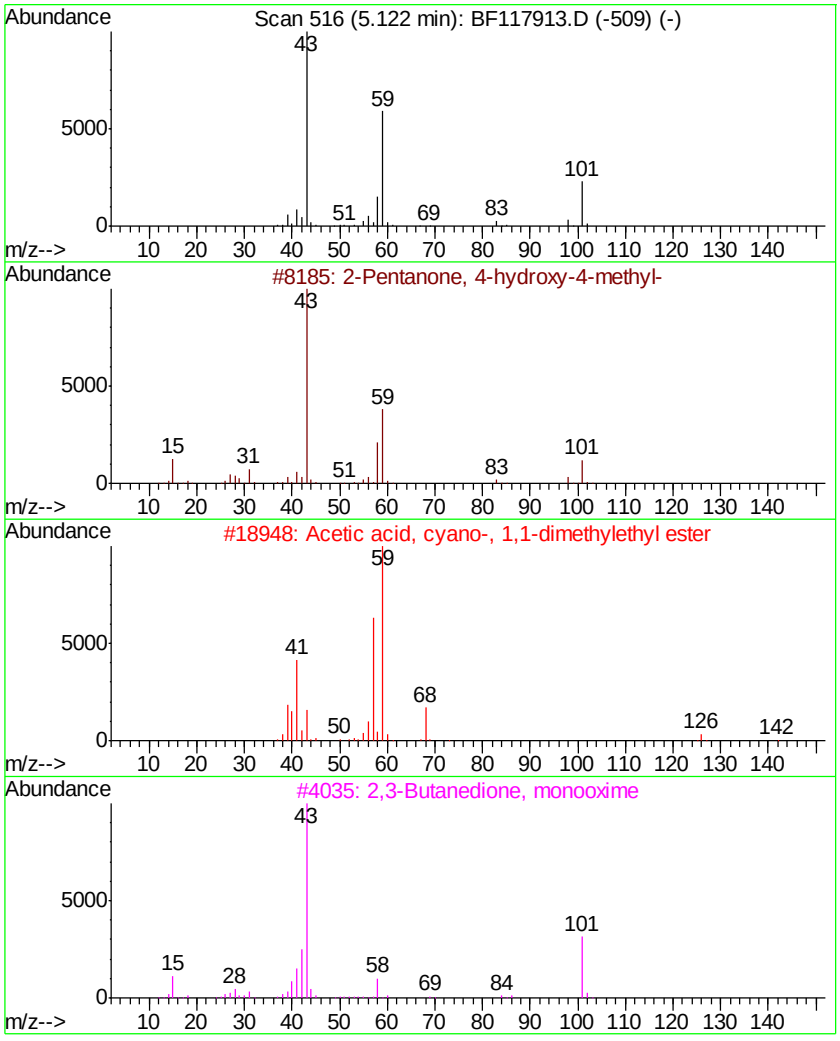
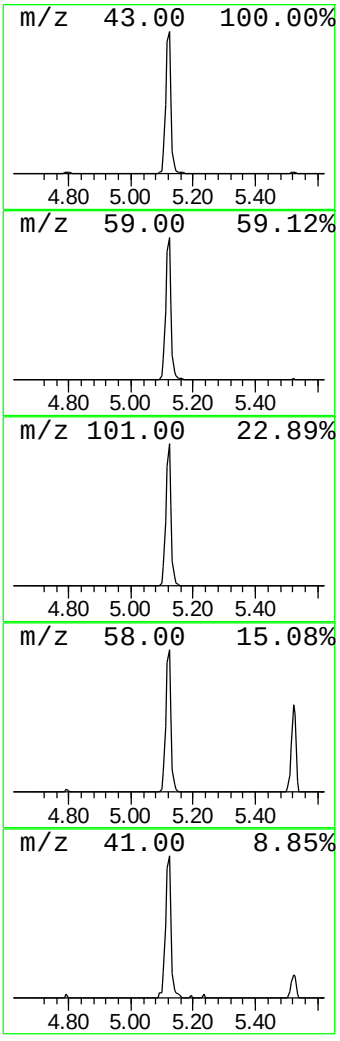
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 13.96 ng | 518632 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



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Operator : JU
Sample : K5933-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC-COMP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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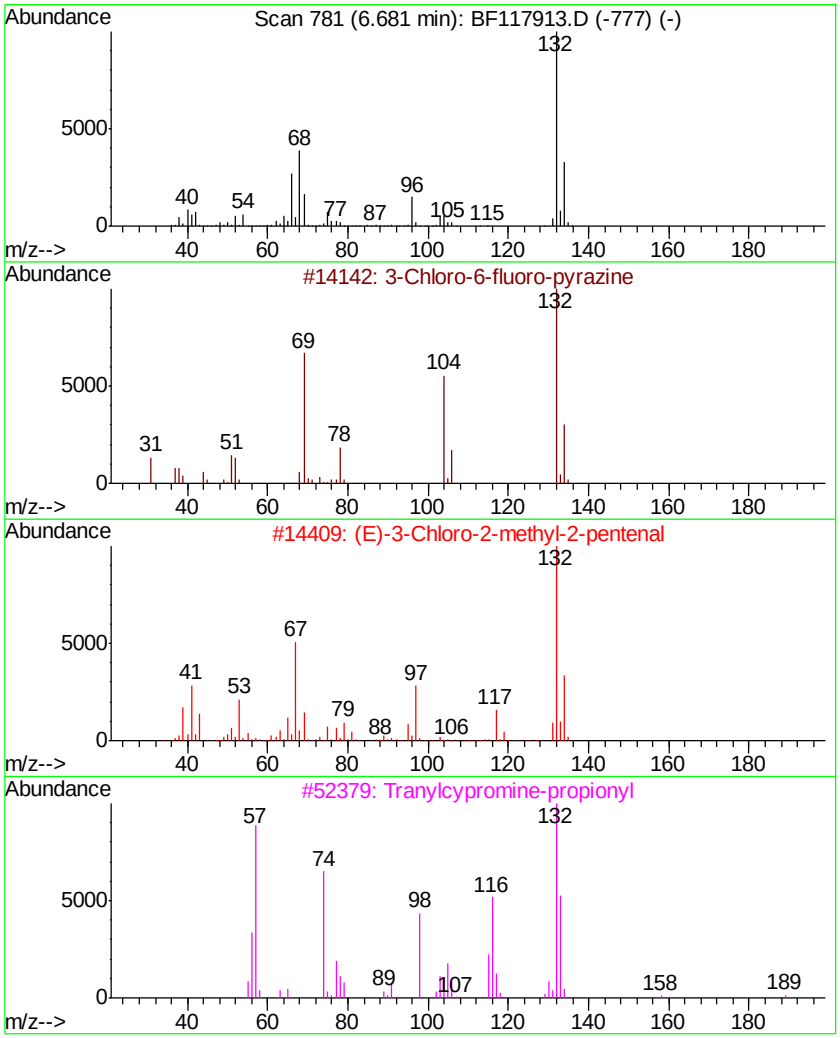
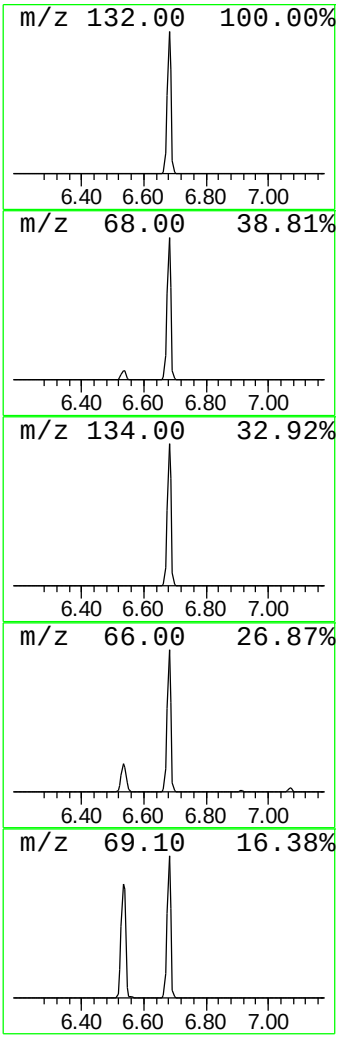
Peak Number 3 unknown6.68 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.68 | 80.39 ng | 2986470 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



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ALS Vial : 15 Sample Multiplier: 1

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TIC Integration Parameters: LSCINT.P

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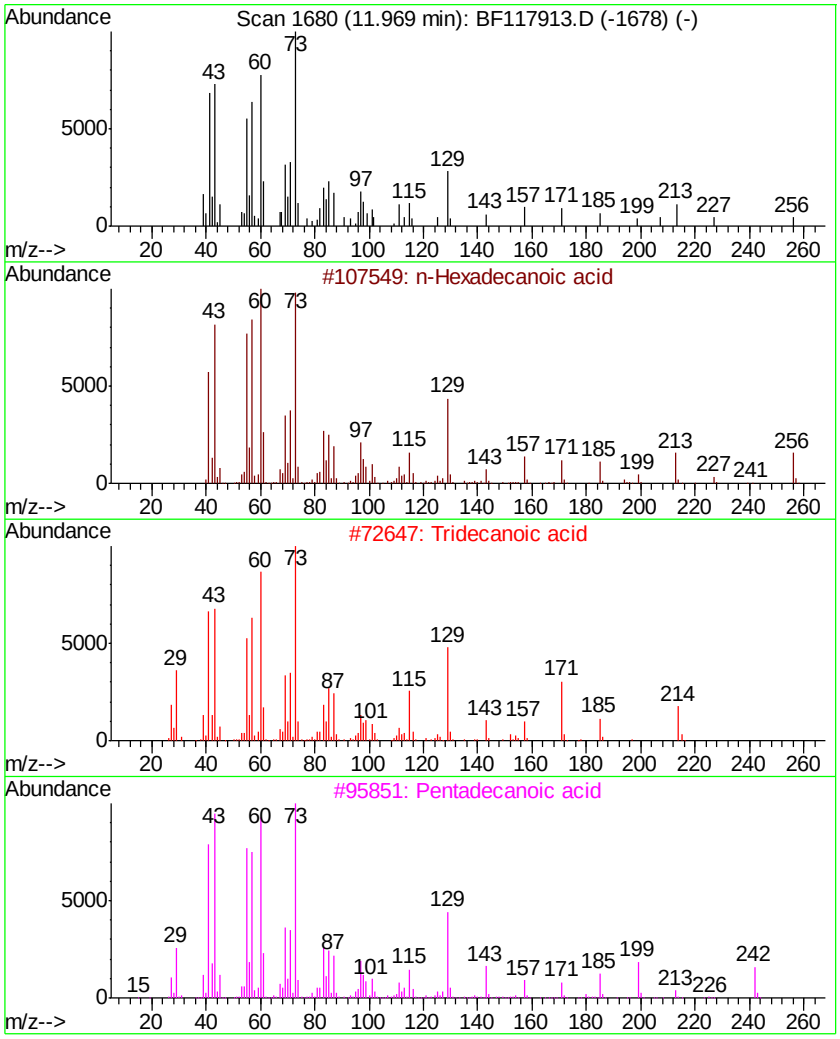
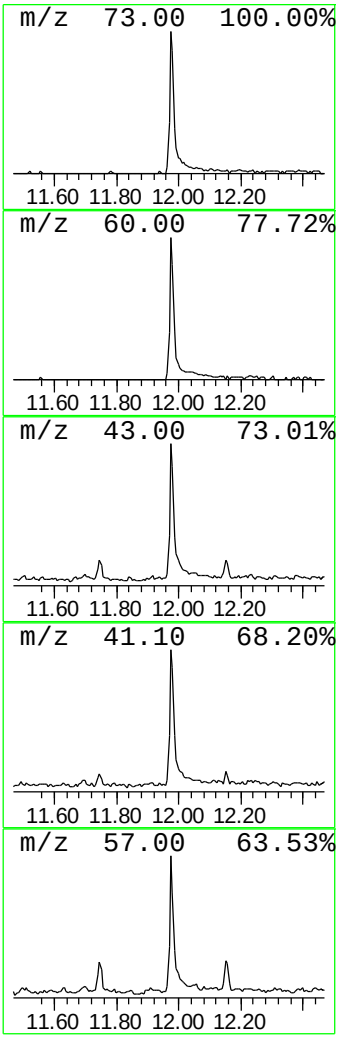
Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.97 | 4.44 ng | 287987 | Phenanthrene-d10 | 11.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 5 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 38 |



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Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** WC-COMP-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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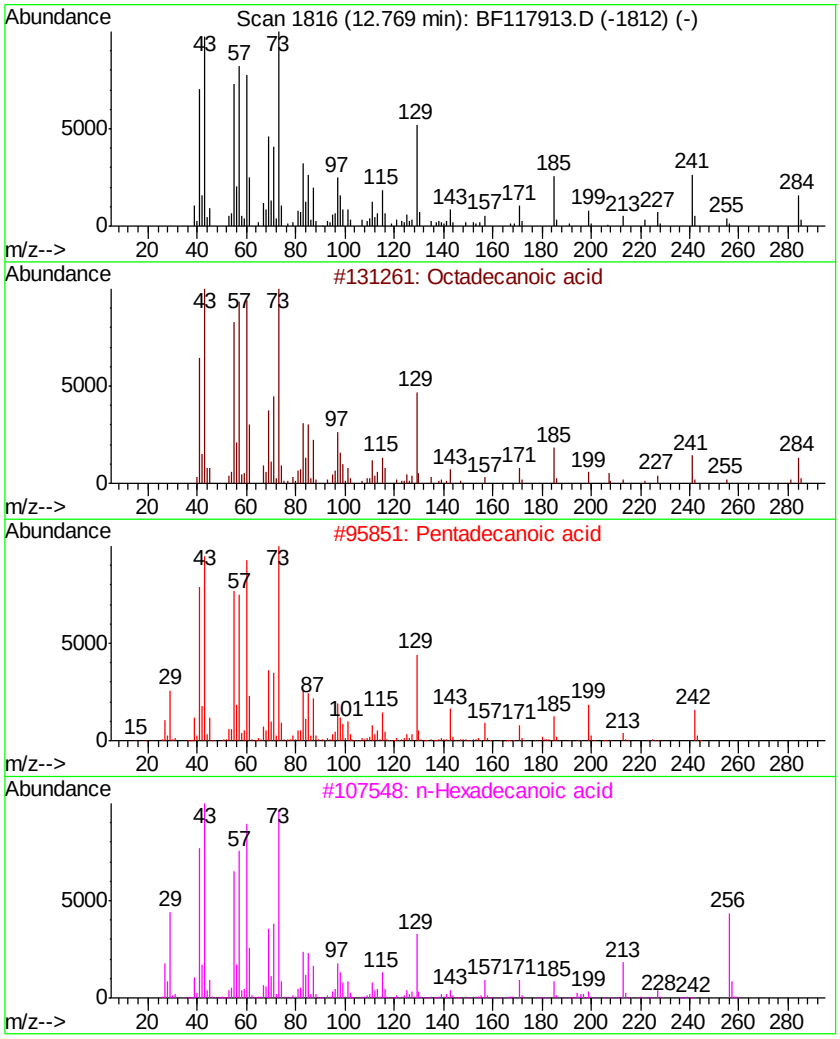
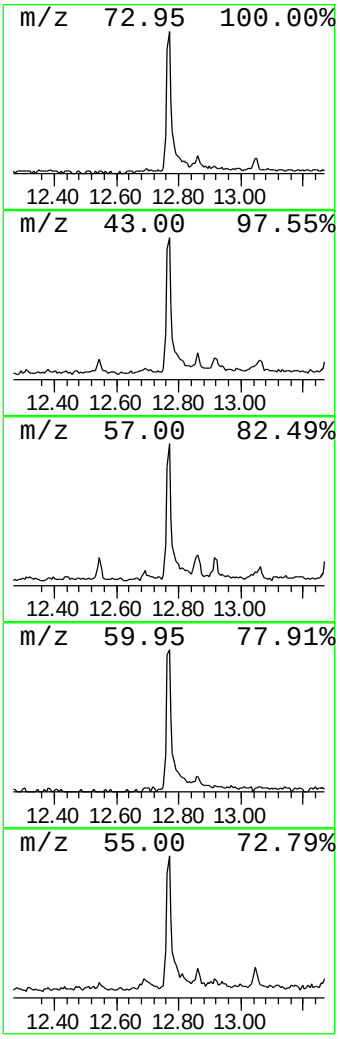
Peak Number 6 Octadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.77 | 5.34 ng | 346455 | Phenanthrene-d10 | 11.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 89 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 5 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 72 |



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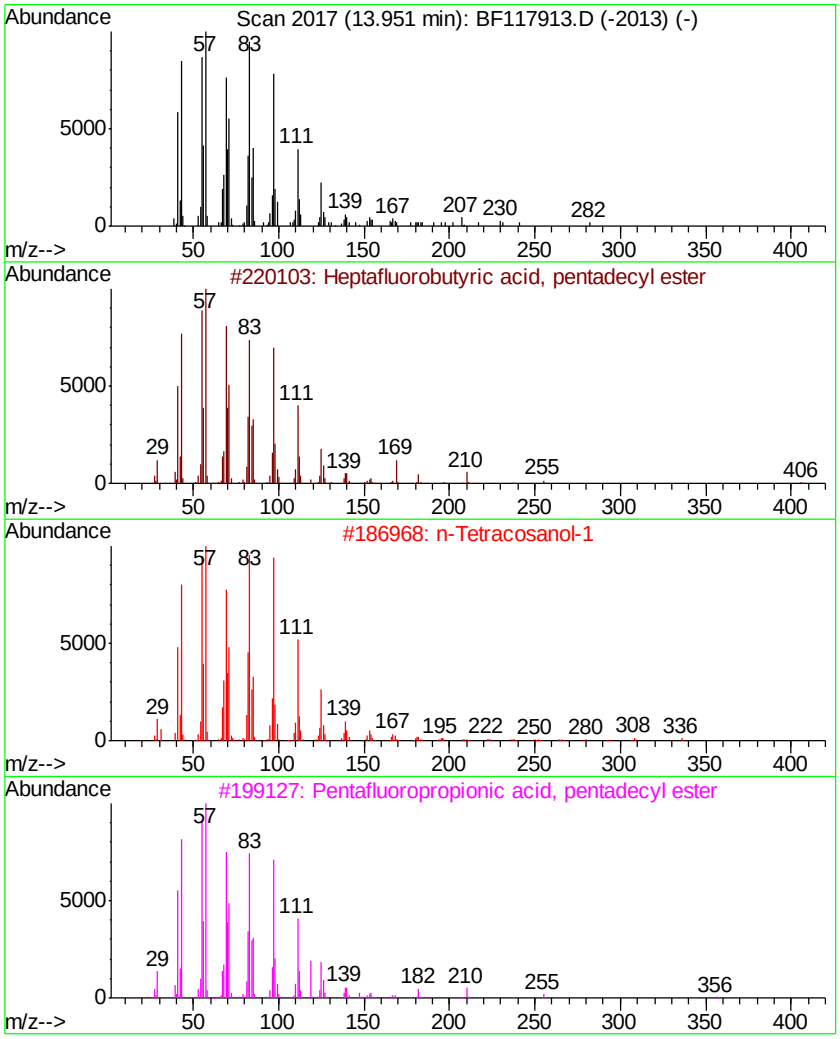
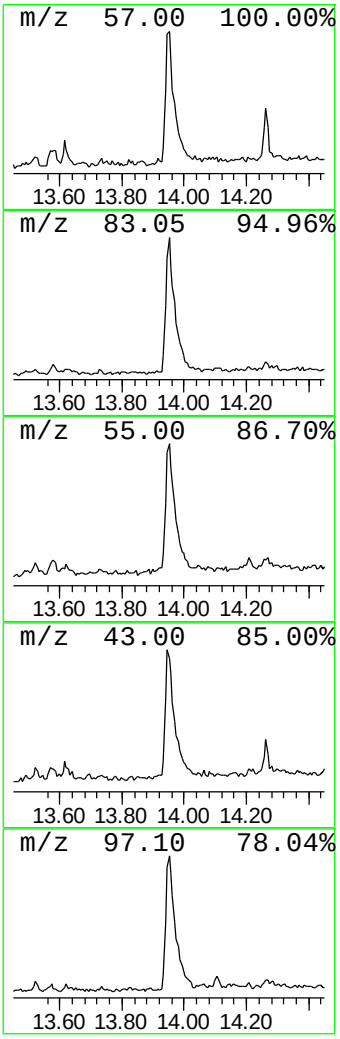
**********

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.95 | 6.29 ng | 450424 | Chrysene-d12 | 14.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 3 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 4 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |



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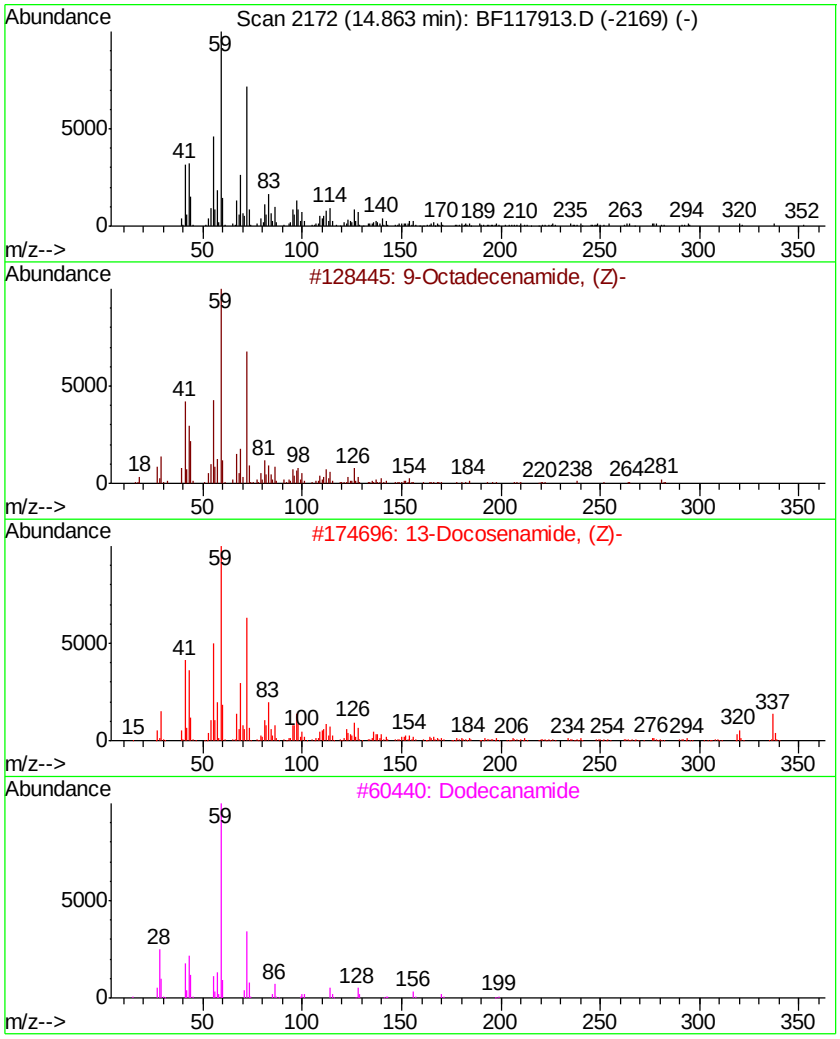
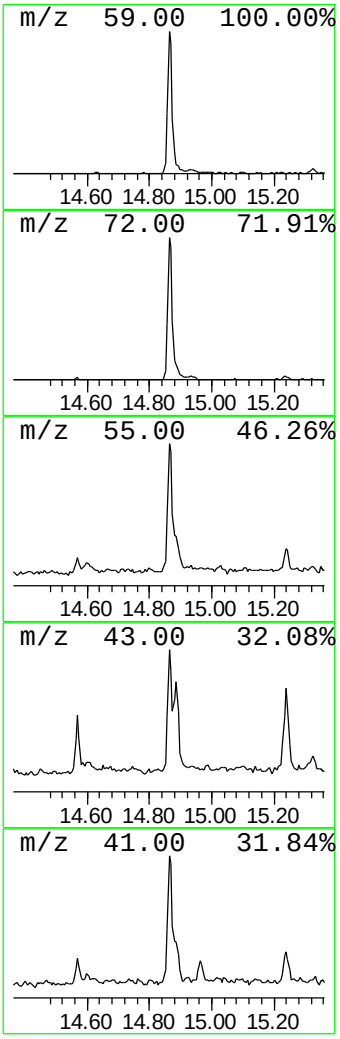
**********

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.86 | 7.05 ng | 500837 | Perylene-d12 | 15.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 99 |
| 2 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 94 |
| 3 | Dodecanamide | 199 | C12H25NO | 001120-16-7 | 64 |
| 4 | Decanamide- | 171 | C10H21NO | 002319-29-1 | 59 |
| 5 | Heptanamide, 4-ethyl-5-methyl- | 171 | C10H21NO | 054789-40-1 | 59 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 2.15 | 26.1 | ng | 970466 | 1 | 6.92 | 743003 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 14.0 | ng | 518632 | 1 | 6.92 | 743003 | 20.0 |
| unknown6.68 | 6.68 | 80.4 | ng | 2986470 | 1 | 6.92 | 743003 | 20.0 |
| n-Hexadecanoic acid | 11.97 | 4.4 | ng | 287987 | 4 | 11.46 | 1297970 | 20.0 |
| Octadecanoic acid | 12.77 | 5.3 | ng | 346455 | 4 | 11.46 | 1297970 | 20.0 |
| Heptafluorobutyri... | 13.95 | 6.3 | ng | 450424 | 5 | 14.10 | 1432160 | 20.0 |
| 9-Octadecenamide,... | 14.86 | 7.0 | ng | 500837 | 6 | 15.62 | 1421100 | 20.0 |