LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

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_P\METHODS\8270-BP112719.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 | 5.616 | 595 | 600 | 611 | rVB | 286409 | 442698 | 17.43% | 1.990% |
| 2 | 6.216 | 695 | 702 | 712 | rBV | 1709176 | 2133328 | 84.01% | 9.591% |
| 3 | 7.758 | 957 | 964 | 973 | rBV | 1839697 | 2303524 | 90.71% | 10.357% |
| 4 | 7.946 | 990 | 996 | 1001 | rBV | 1889469 | 2250386 | 88.62% | 10.118% |
| 5 | 8.305 | 1052 | 1057 | 1064 | rVB | 498889 | 553575 | 21.80% | 2.489% |
| 6 | 8.546 | 1092 | 1098 | 1103 | rBV | 1489922 | 1725111 | 67.93% | 7.756% |
| 7 | 9.187 | 1200 | 1207 | 1211 | rBV | 1262897 | 1450151 | 57.11% | 6.520% |
| 8 | 10.340 | 1391 | 1403 | 1408 | rBV | 612066 | 690235 | 27.18% | 3.103% |
| 9 | 12.116 | 1699 | 1705 | 1710 | rBV | 2119896 | 2539431 | 100.00% | 11.417% |
| 10 | 12.787 | 1814 | 1819 | 1825 | rVB | 197096 | 224647 | 8.85% | 1.010% |
| 11 | 13.198 | 1883 | 1889 | 1894 | rBV | 700752 | 805744 | 31.73% | 3.623% |
| 12 | 14.492 | 2103 | 2109 | 2121 | rBV | 1453359 | 1802864 | 70.99% | 8.106% |
| 13 | 15.592 | 2291 | 2296 | 2300 | rBV | 686071 | 793748 | 31.26% | 3.569% |
| 14 | 15.628 | 2300 | 2302 | 2308 | rVB | 37924 | 41947 | 1.65% | 0.189% |
| 15 | 16.481 | 2443 | 2447 | 2454 | rBV | 179531 | 260006 | 10.24% | 1.169% |
| 16 | 17.339 | 2590 | 2593 | 2597 | rVB | 56911 | 62390 | 2.46% | 0.281% |
| 17 | 17.569 | 2629 | 2632 | 2636 | rBV2 | 62610 | 74475 | 2.93% | 0.335% |
| 18 | 17.645 | 2642 | 2645 | 2648 | rVB | 42717 | 49080 | 1.93% | 0.221% |
| 19 | 17.881 | 2680 | 2685 | 2689 | rBV | 2269261 | 2469160 | 97.23% | 11.101% |
| 20 | 19.116 | 2892 | 2895 | 2900 | rVB2 | 138165 | 176195 | 6.94% | 0.792% |
| 21 | 19.233 | 2911 | 2915 | 2919 | rBV | 620667 | 723284 | 28.48% | 3.252% |
| 22 | 21.010 | 3214 | 3217 | 3225 | rVB | 488373 | 670114 | 26.39% | 3.013% |

Sum of corrected areas: 22242093

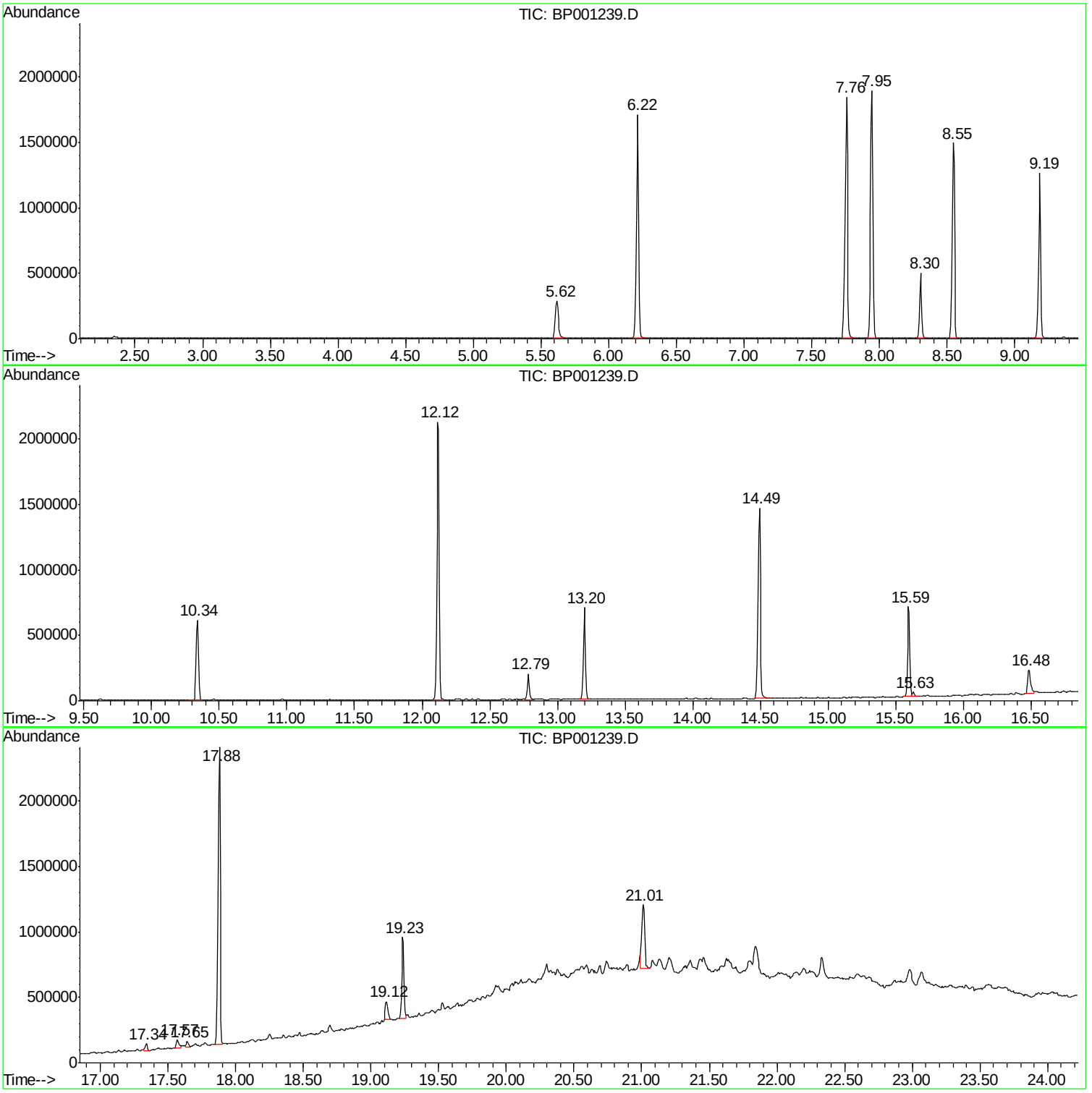
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

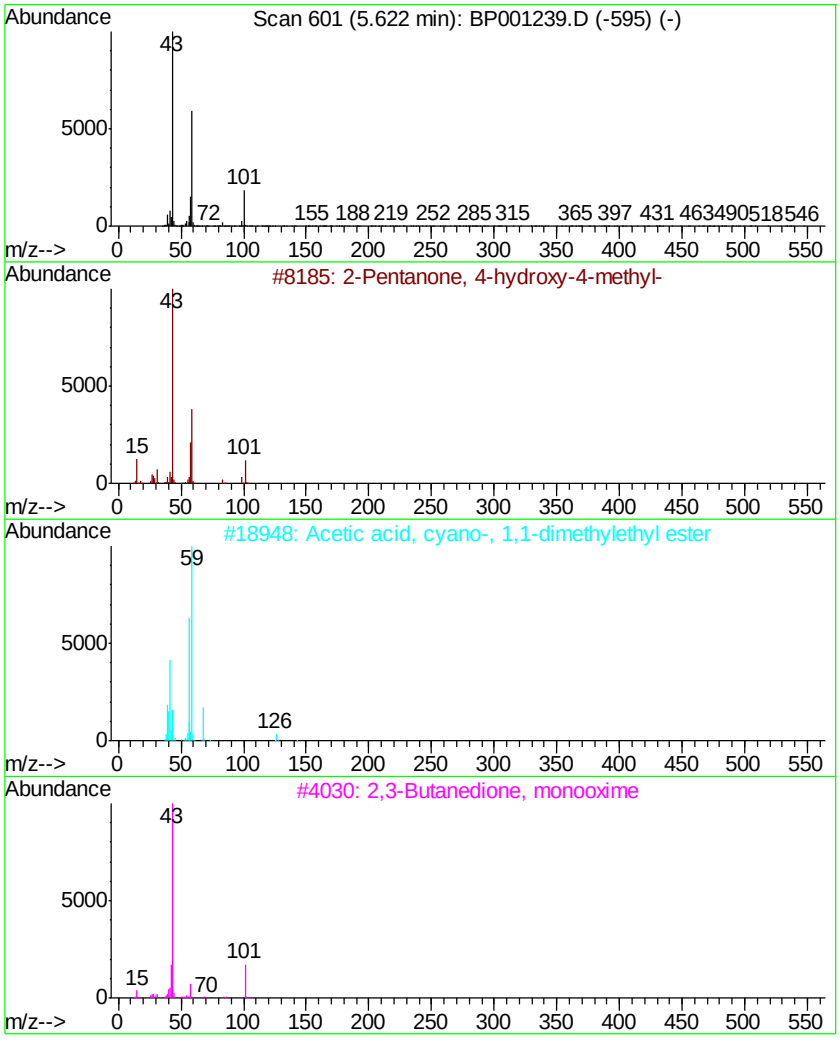
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

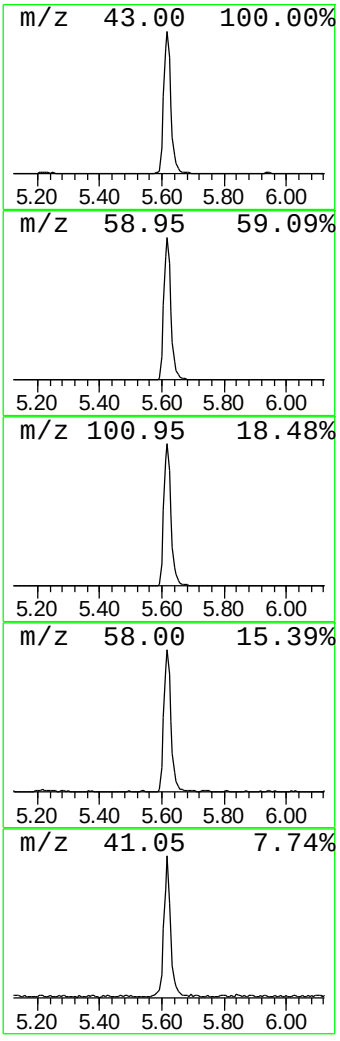
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.62 | 15.99 ng | 442698 | 1,4-Dichlorobenzene-d4 | 8.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 10 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 5 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

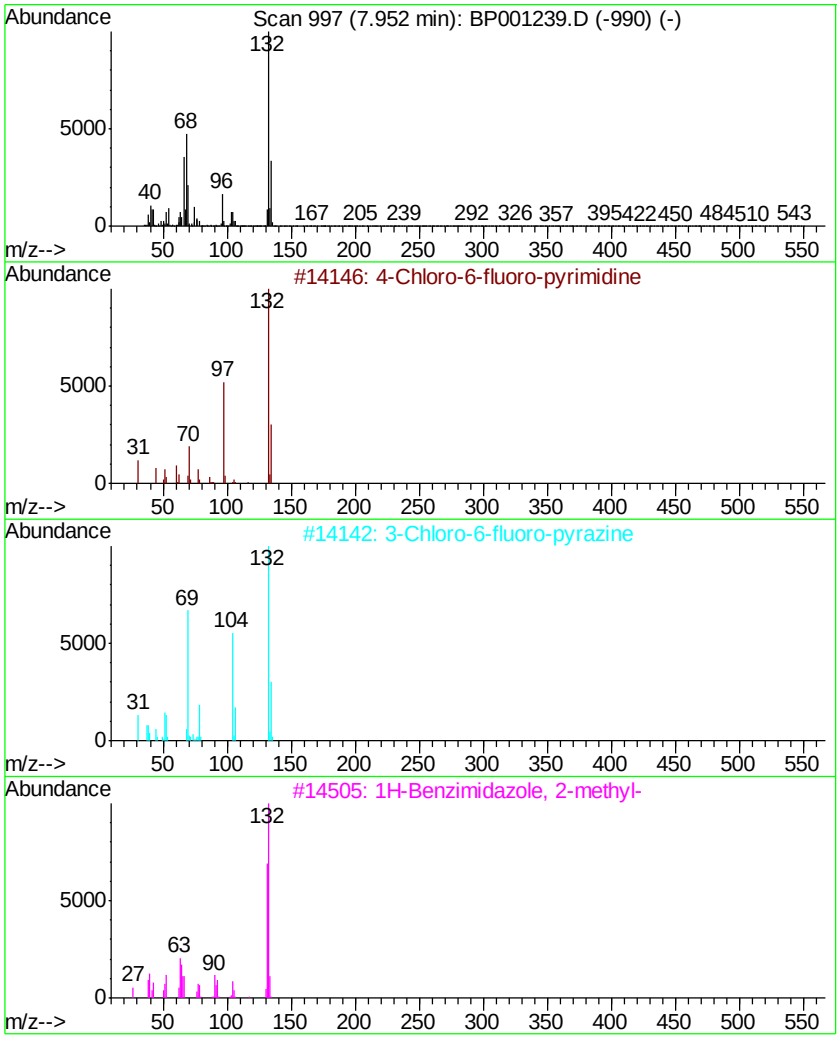
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

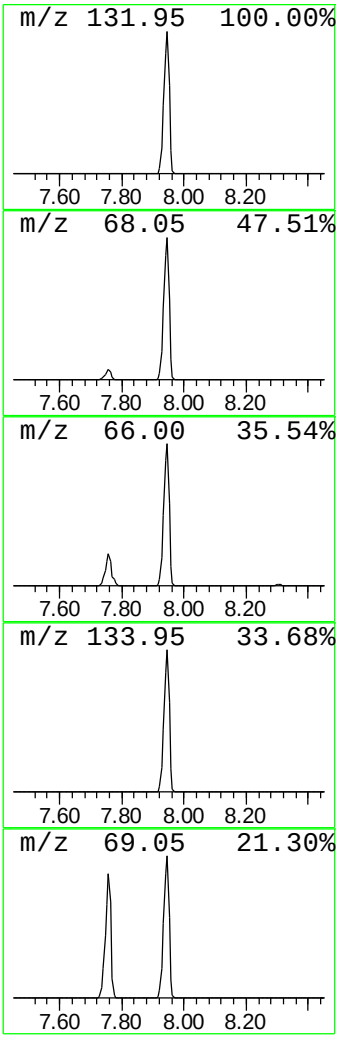
**********

Peak Number 2 unknown7.95 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.95 | 81.30 ng | 2250390 | 1,4-Dichlorobenzene-d4 | 8.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 14 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 10 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 10 |
| 5 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 10 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

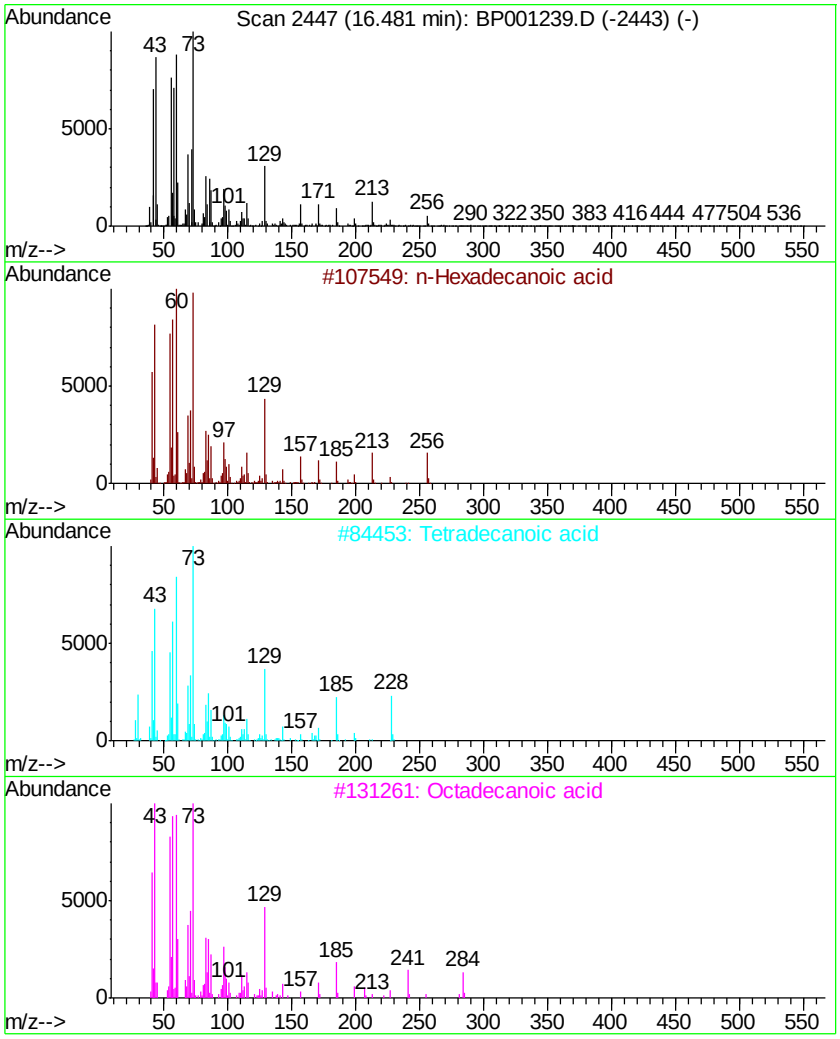
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

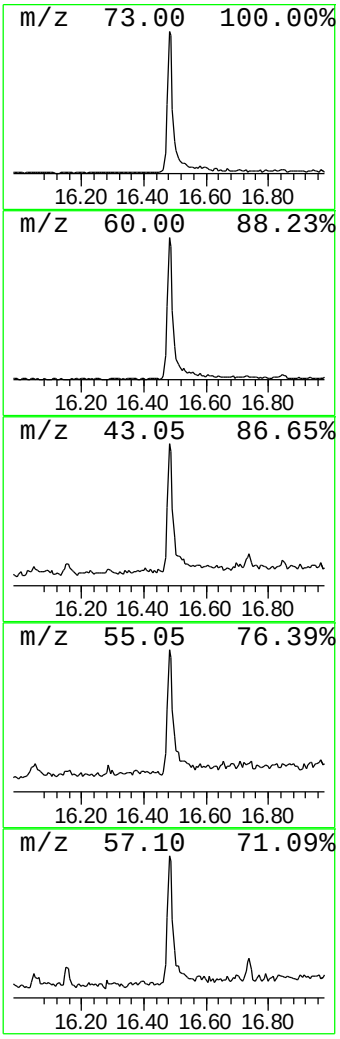
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.48 | 6.55 ng | 260006 | Phenanthrene-d10 | 15.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 90 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 81 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

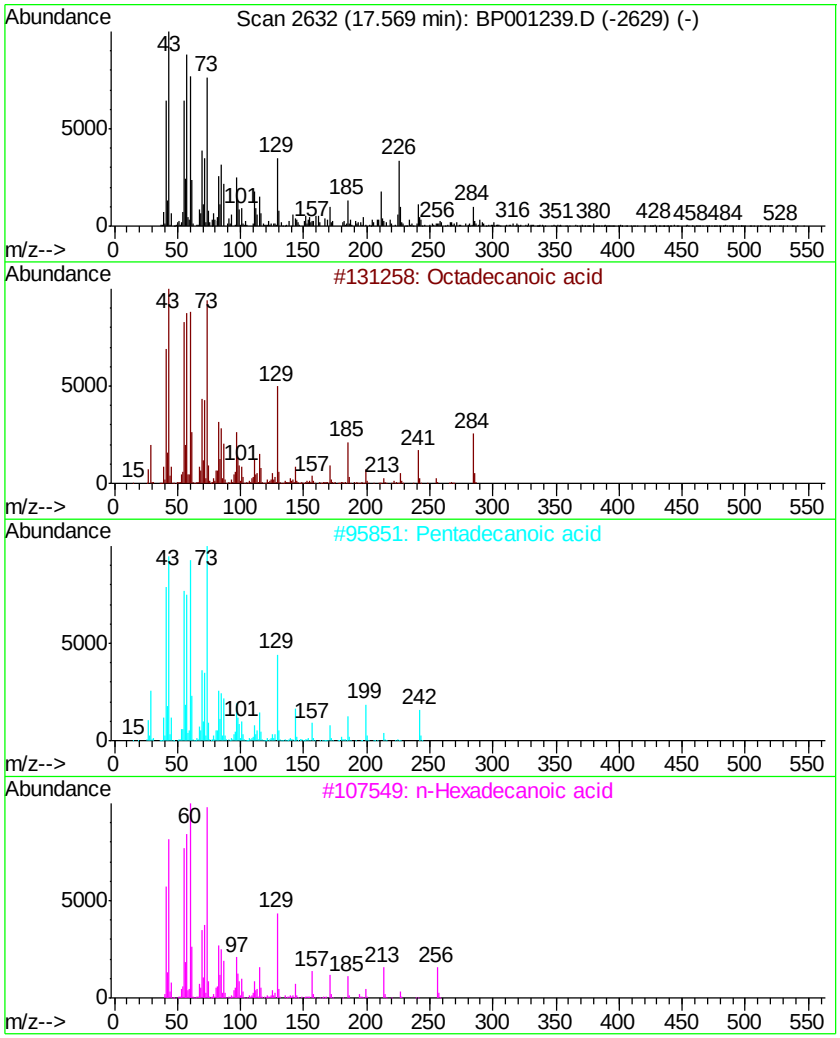
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

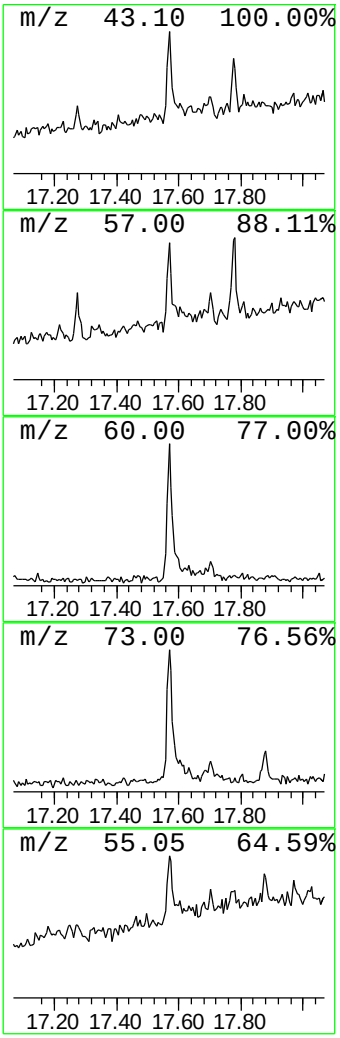
**********

Peak Number 5 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.57 | 2.06 ng | 74475 | Chrysene-d12 | 19.23 |

| 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 | 93 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90 |
| 4 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 81 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



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Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

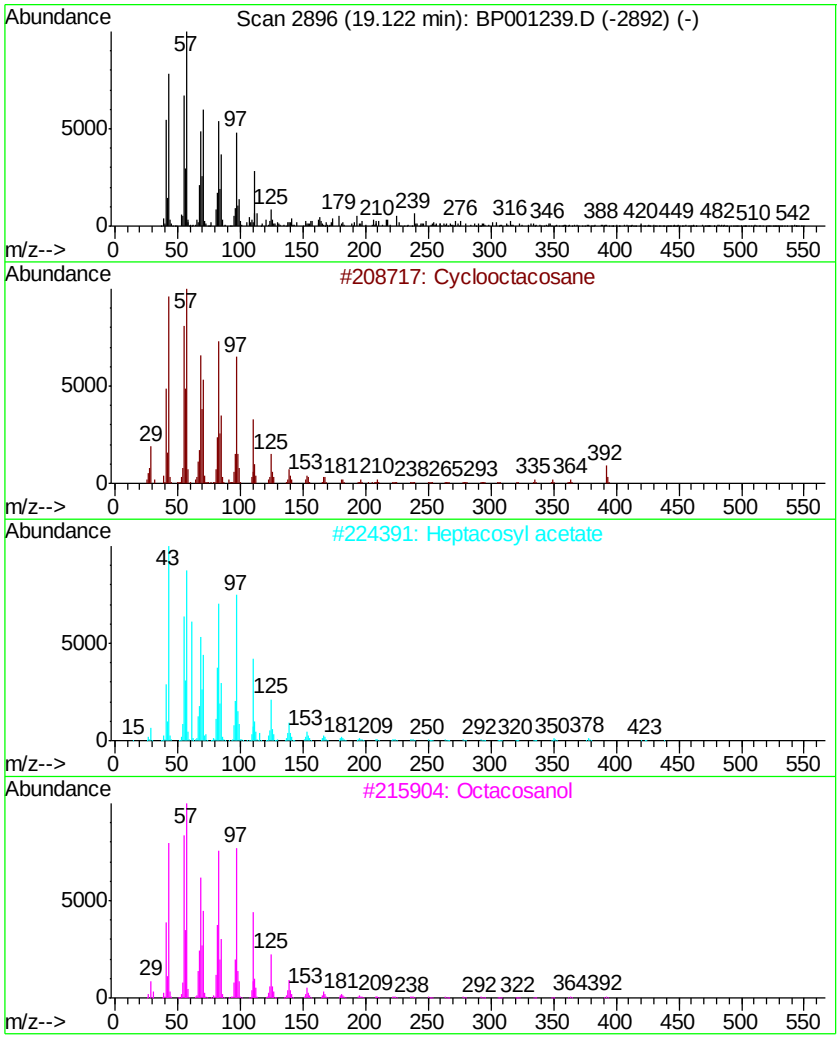
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

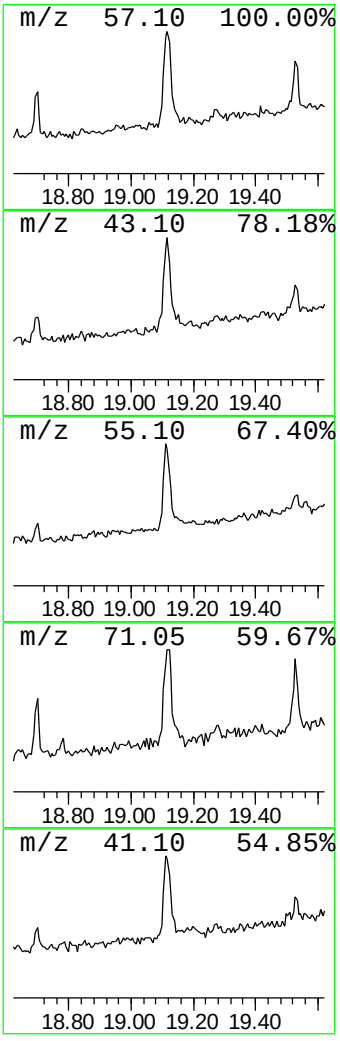
**********

Peak Number 6 Cyclooctacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.12 | 4.87 ng | 176195 | Chrysene-d12 | 19.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclooctacosane | 392 | C28H56 | 000297-24-5 | 94 |
| 2 | Heptacosyl acetate | 438 | C29H58O2 | 1000351-78-2 | 93 |
| 3 | Octacosanol | 410 | C28H58O | 000557-61-9 | 91 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 5 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP120619\
Data File : BP001239.D
Acq On : 06 Dec 2019 19:52
Operator : JU
Sample : K6119-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SB-6-(7-9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.62 | 16.0 | ng | 442698 | 1 | 8.30 | 553575 | 20.0 |
| unknown7.95 | 7.95 | 81.3 | ng | 2250390 | 1 | 8.30 | 553575 | 20.0 |
| n-Hexadecanoic acid | 16.48 | 6.5 | ng | 260006 | 4 | 15.59 | 793748 | 20.0 |
| Octadecanoic acid | 17.57 | 2.1 | ng | 74475 | 5 | 19.23 | 723284 | 20.0 |
| Cyclooctacosane | 19.12 | 4.9 | ng | 176195 | 5 | 19.23 | 723284 | 20.0 |