LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

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-BF122419.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 | 4.416 | 392 | 396 | 408 | rBV | 39925 | 59025 | 2.03% | 0.209% |
| 2 | 5.045 | 499 | 503 | 518 | rVB | 394861 | 466920 | 16.09% | 1.654% |
| 3 | 5.457 | 570 | 573 | 593 | rBV | 2141898 | 2154554 | 74.25% | 7.634% |
| 4 | 6.481 | 743 | 747 | 762 | rBV | 2594365 | 2364763 | 81.49% | 8.378% |
| 5 | 6.616 | 766 | 770 | 774 | rBV | 2880756 | 2499889 | 86.15% | 8.857% |
| 6 | 6.845 | 806 | 809 | 816 | rBV | 676324 | 620363 | 21.38% | 2.198% |
| 7 | 7.004 | 832 | 836 | 846 | rBV | 2453853 | 1945901 | 67.06% | 6.894% |
| 8 | 7.410 | 901 | 905 | 925 | rBV | 1424209 | 1448925 | 49.93% | 5.134% |
| 9 | 8.134 | 1025 | 1028 | 1048 | rVB | 925059 | 832735 | 28.70% | 2.950% |
| 10 | 9.210 | 1208 | 1211 | 1215 | rBV | 3261343 | 2901899 | 100.00% | 10.282% |
| 11 | 9.610 | 1276 | 1279 | 1287 | rVB | 99817 | 89242 | 3.08% | 0.316% |
| 12 | 9.892 | 1324 | 1327 | 1331 | rBV | 1059236 | 976651 | 33.66% | 3.460% |
| 13 | 9.928 | 1331 | 1333 | 1337 | rVB | 38050 | 32101 | 1.11% | 0.114% |
| 14 | 10.686 | 1458 | 1462 | 1474 | rBV | 2225998 | 2021678 | 69.67% | 7.163% |
| 15 | 11.286 | 1559 | 1564 | 1568 | rVB3 | 21415 | 33542 | 1.16% | 0.119% |
| 16 | 11.386 | 1578 | 1581 | 1583 | rBV | 1220811 | 986111 | 33.98% | 3.494% |
| 17 | 11.410 | 1583 | 1585 | 1590 | rVV | 395652 | 323207 | 11.14% | 1.145% |
| 18 | 11.463 | 1590 | 1594 | 1597 | rVB | 75964 | 87106 | 3.00% | 0.309% |
| 19 | 11.622 | 1617 | 1621 | 1624 | rBV2 | 24674 | 36708 | 1.26% | 0.130% |
| 20 | 11.892 | 1664 | 1667 | 1668 | rBV | 53320 | 48272 | 1.66% | 0.171% |
| 21 | 11.910 | 1668 | 1670 | 1678 | rVV4 | 272049 | 349230 | 12.03% | 1.237% |
| 22 | 12.004 | 1682 | 1686 | 1688 | rVV2 | 75359 | 89303 | 3.08% | 0.316% |
| 23 | 12.027 | 1688 | 1690 | 1694 | rVB | 38660 | 38265 | 1.32% | 0.136% |
| 24 | 12.186 | 1714 | 1717 | 1720 | rBV | 38669 | 35561 | 1.23% | 0.126% |
| 25 | 12.339 | 1737 | 1743 | 1745 | rBV6 | 18689 | 32273 | 1.11% | 0.114% |
| 26 | 12.439 | 1756 | 1760 | 1763 | rBV | 49804 | 54474 | 1.88% | 0.193% |
| 27 | 12.474 | 1763 | 1766 | 1769 | rVV4 | 34301 | 44800 | 1.54% | 0.159% |
| 28 | 12.533 | 1773 | 1776 | 1780 | rVV2 | 27405 | 33243 | 1.15% | 0.118% |
| 29 | 12.604 | 1785 | 1788 | 1794 | rBV | 434169 | 393285 | 13.55% | 1.393% |
| 30 | 12.704 | 1801 | 1805 | 1810 | rBV3 | 54085 | 77531 | 2.67% | 0.275% |
| 31 | 12.833 | 1822 | 1827 | 1833 | rBV2 | 318705 | 406093 | 13.99% | 1.439% |
| 32 | 12.974 | 1847 | 1851 | 1855 | rBV | 3104097 | 2854148 | 98.35% | 10.112% |
| 33 | 13.057 | 1860 | 1865 | 1869 | rBV4 | 29446 | 56456 | 1.95% | 0.200% |
| 34 | 13.163 | 1881 | 1883 | 1886 | rVB | 42865 | 39990 | 1.38% | 0.142% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.268 | 1897 | 1901 | 1905 | rBV2 | 37615 | 49019 | 1.69% | 0.174% |
| 36 | 13.545 | 1945 | 1948 | 1951 | rBV3 | 38203 | 48436 | 1.67% | 0.172% |
| 37 | 13.868 | 2000 | 2003 | 2014 | rVB3 | 277332 | 462741 | 15.95% | 1.640% |
| 38 | 14.039 | 2025 | 2032 | 2035 | rBV2 | 999249 | 1090216 | 37.57% | 3.863% |
| 39 | 14.063 | 2035 | 2036 | 2042 | rVB | 175395 | 133965 | 4.62% | 0.475% |
| 40 | 14.192 | 2055 | 2058 | 2061 | rBV3 | 56735 | 65134 | 2.24% | 0.231% |
| 41 | 14.498 | 2108 | 2110 | 2112 | rBV2 | 78365 | 67305 | 2.32% | 0.238% |
| 42 | 15.092 | 2207 | 2211 | 2217 | rBV | 153923 | 306455 | 10.56% | 1.086% |
| 43 | 15.462 | 2271 | 2274 | 2280 | rVB | 131489 | 170858 | 5.89% | 0.605% |
| 44 | 15.527 | 2281 | 2285 | 2293 | rBV | 730798 | 953344 | 32.85% | 3.378% |
| 45 | 15.980 | 2359 | 2362 | 2366 | rVB3 | 90116 | 121832 | 4.20% | 0.432% |
| 46 | 16.227 | 2401 | 2404 | 2413 | rVB2 | 187540 | 320760 | 11.05% | 1.136% |

Sum of corrected areas: 28224309

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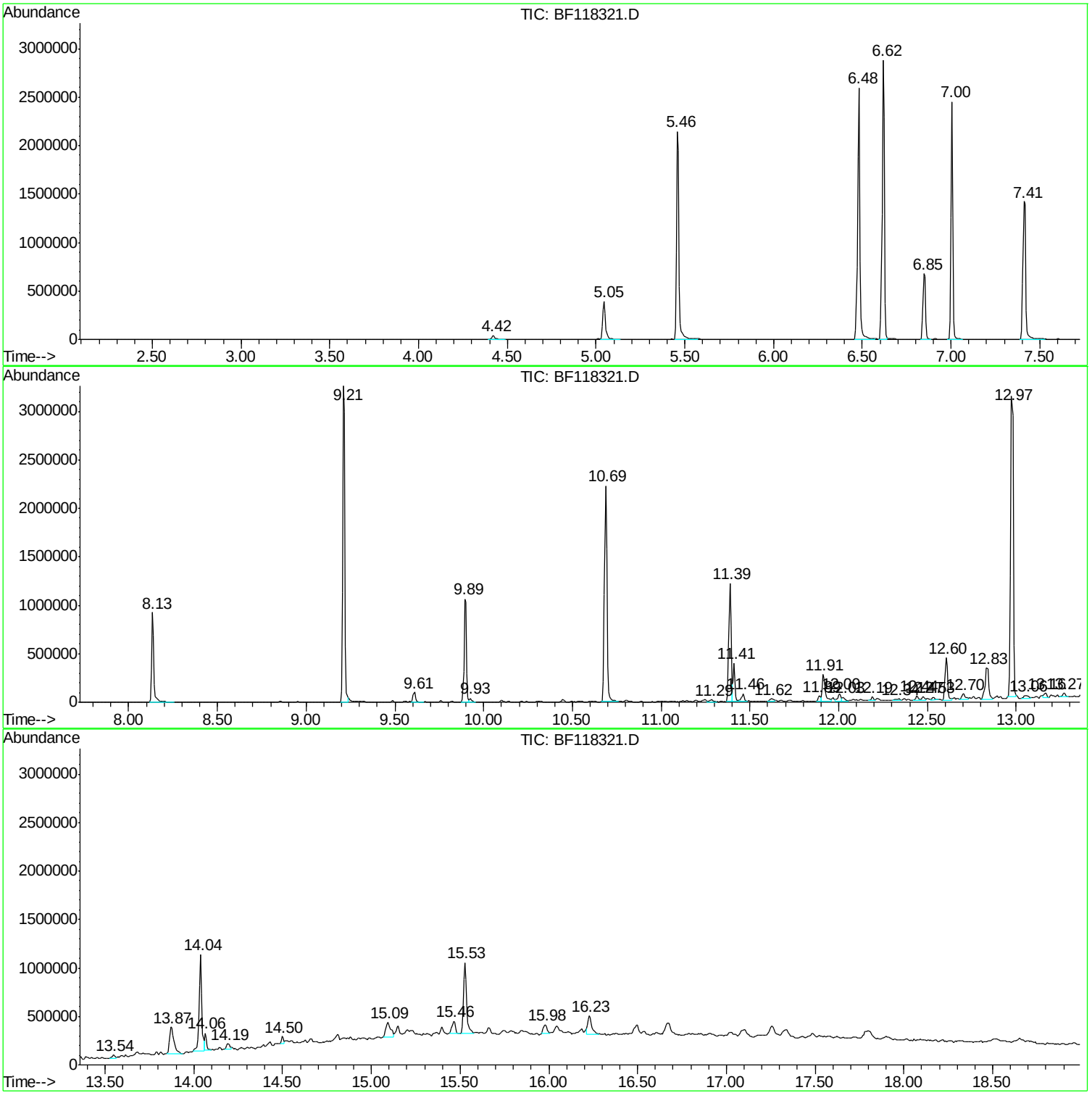
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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 F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

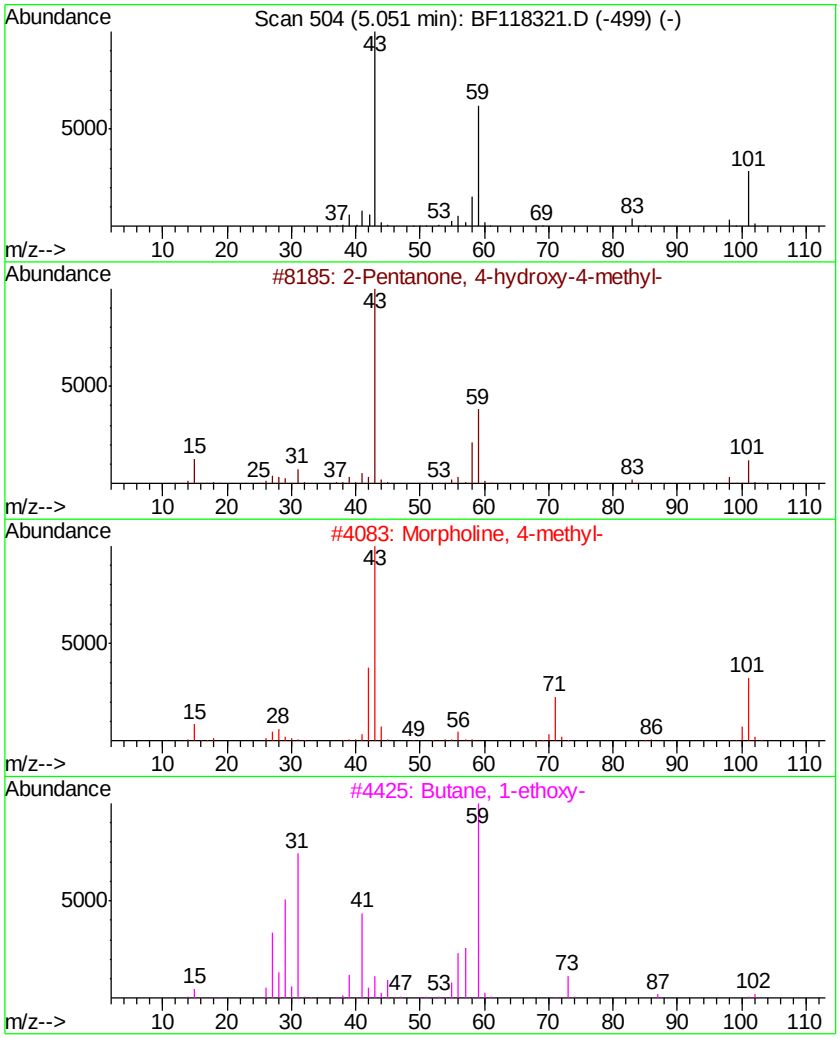
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

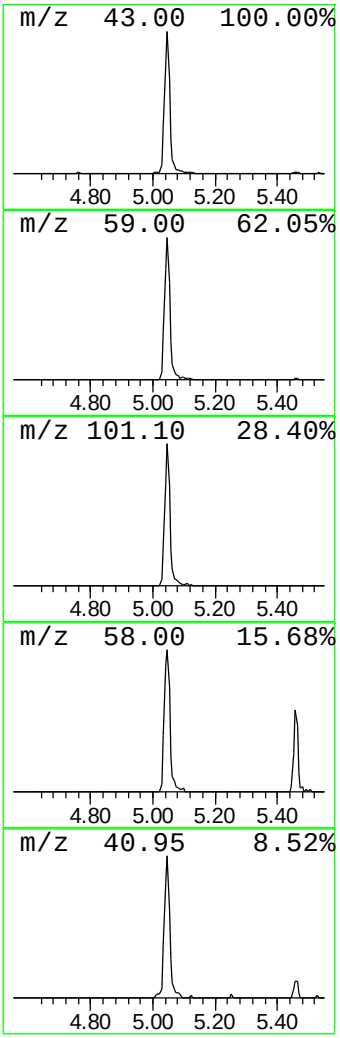
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.05 | 15.05 ng | 466920 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 3 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

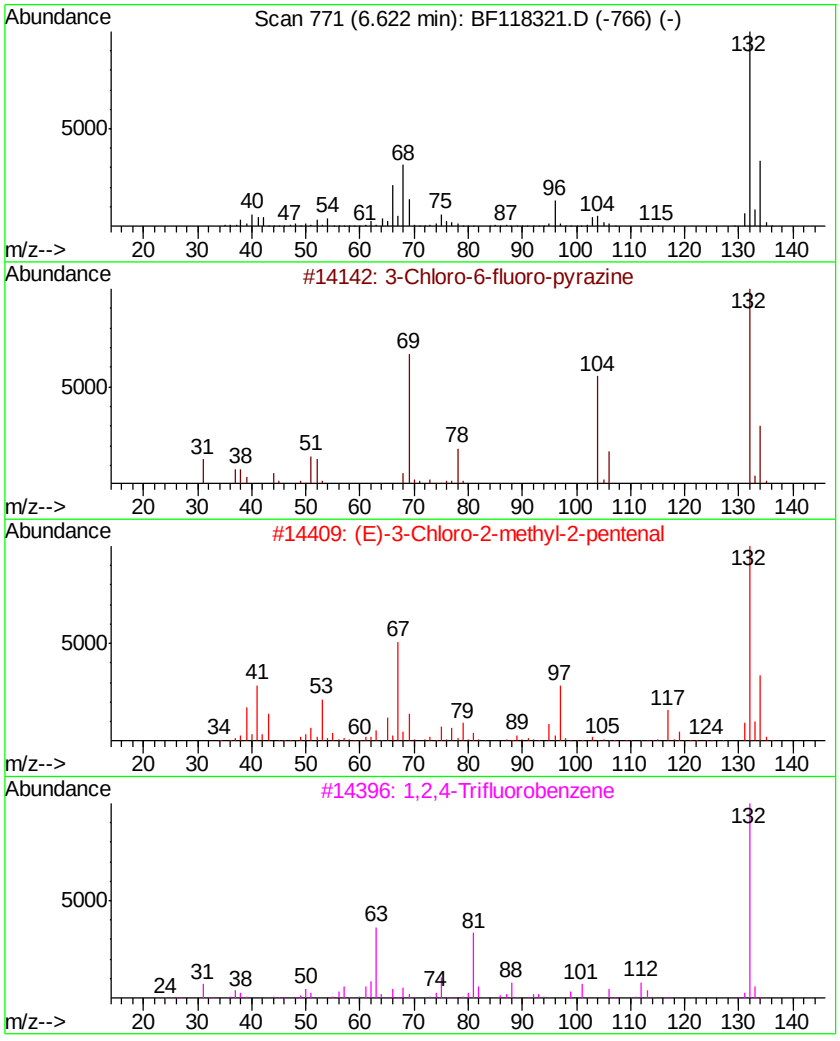
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

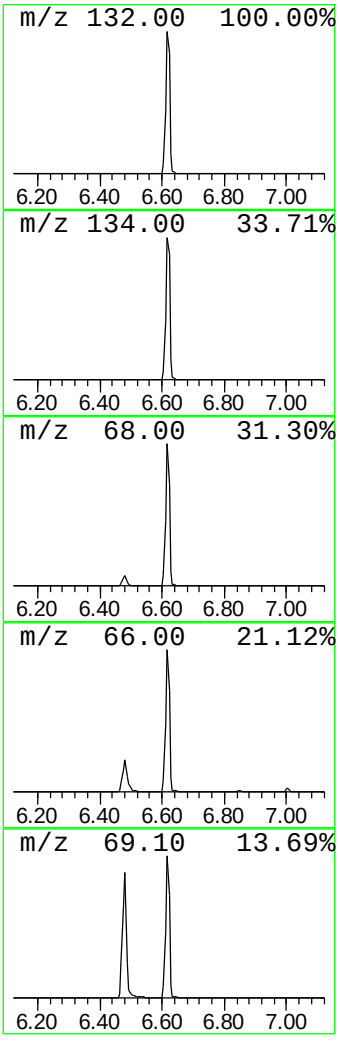
**********

Peak Number 2 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 80.59 ng | 2499890 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

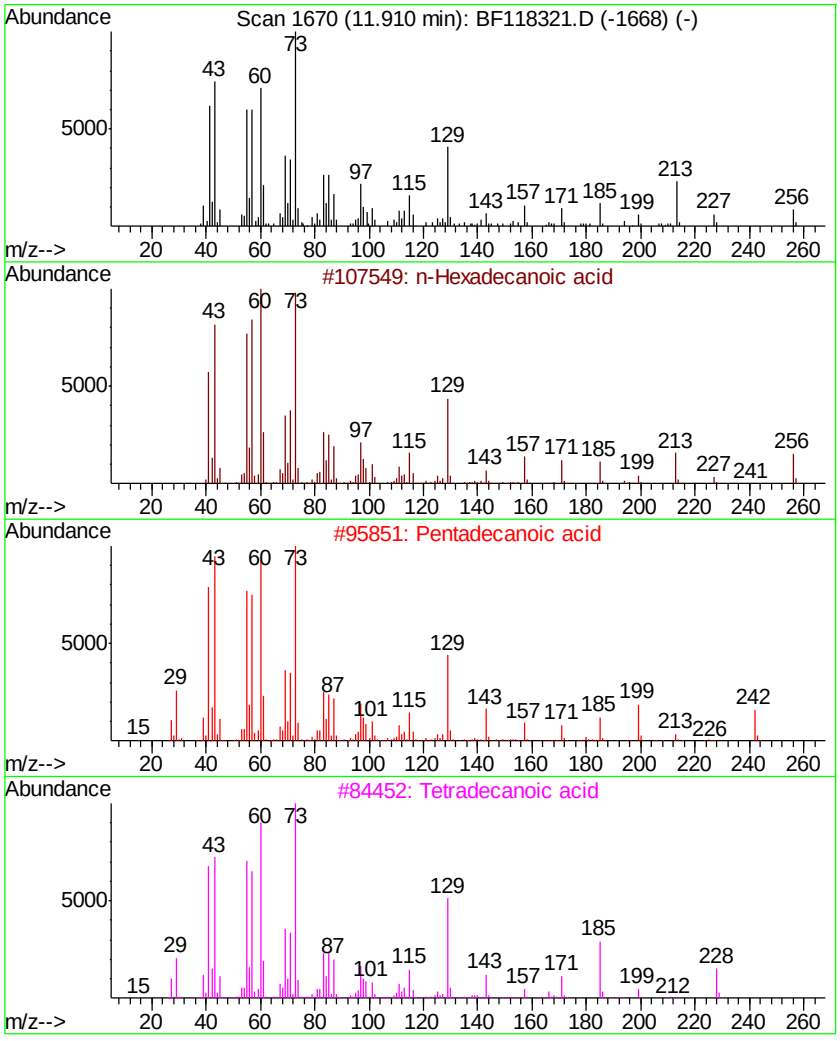
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

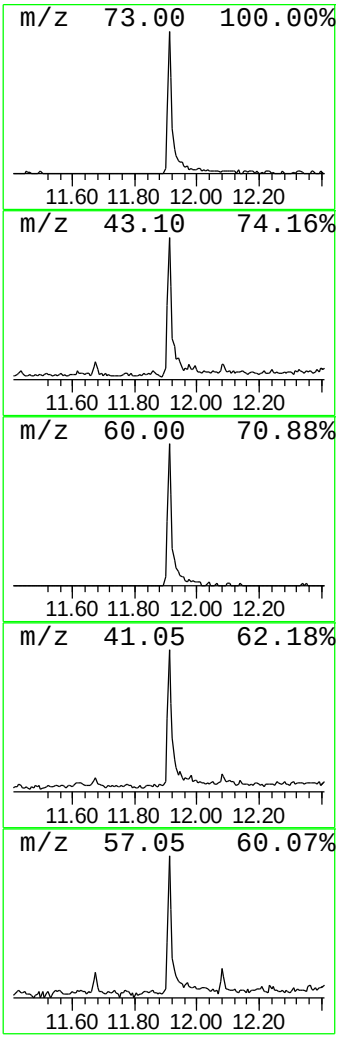
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.91 | 7.08 ng | 349230 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 52 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 46 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

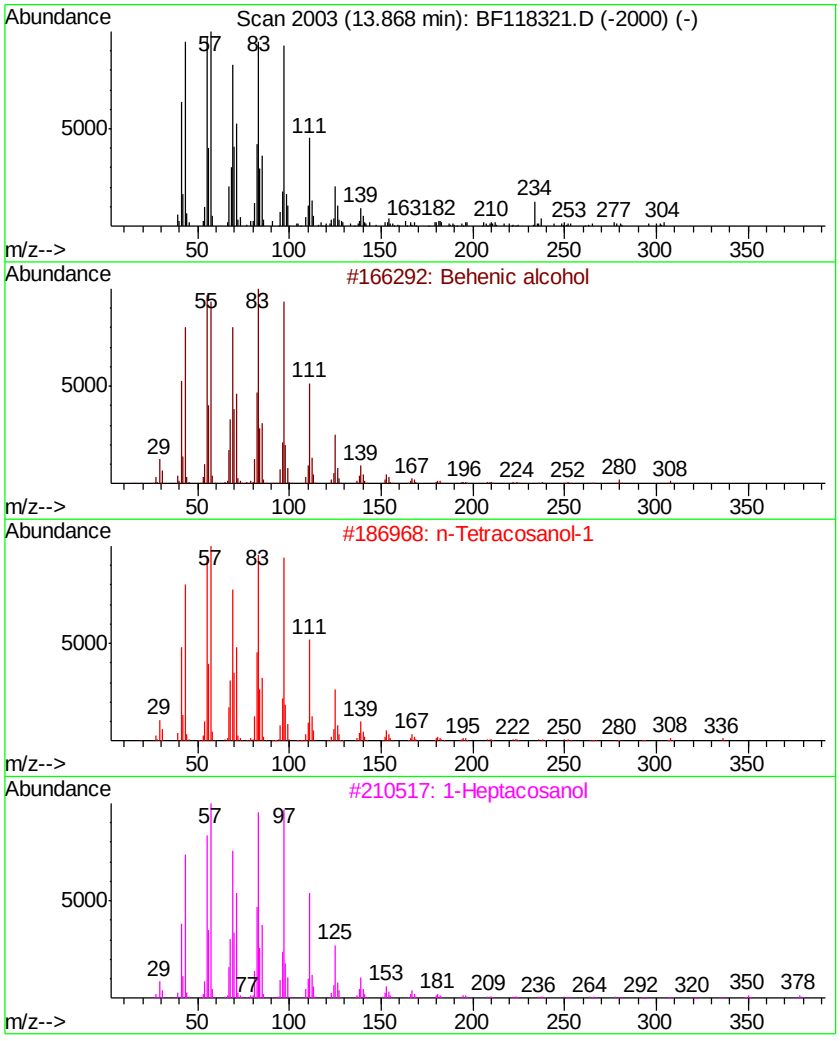
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

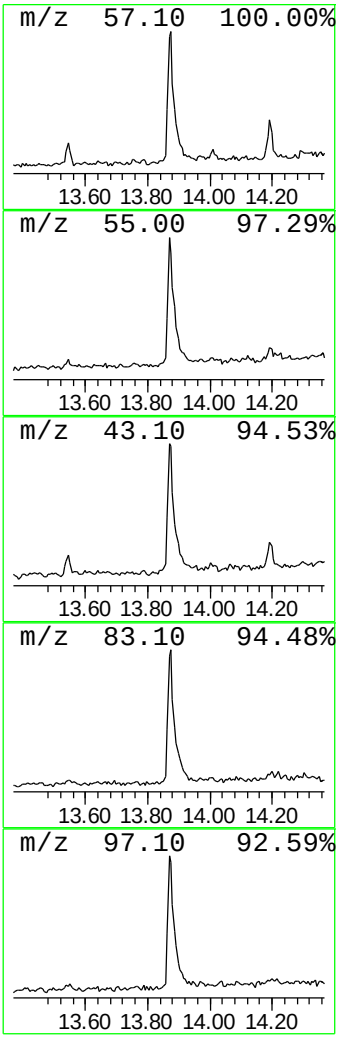
**********

Peak Number 5 Behenic alcohol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.87 | 8.49 ng | 462741 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 95 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 94 |
| 4 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

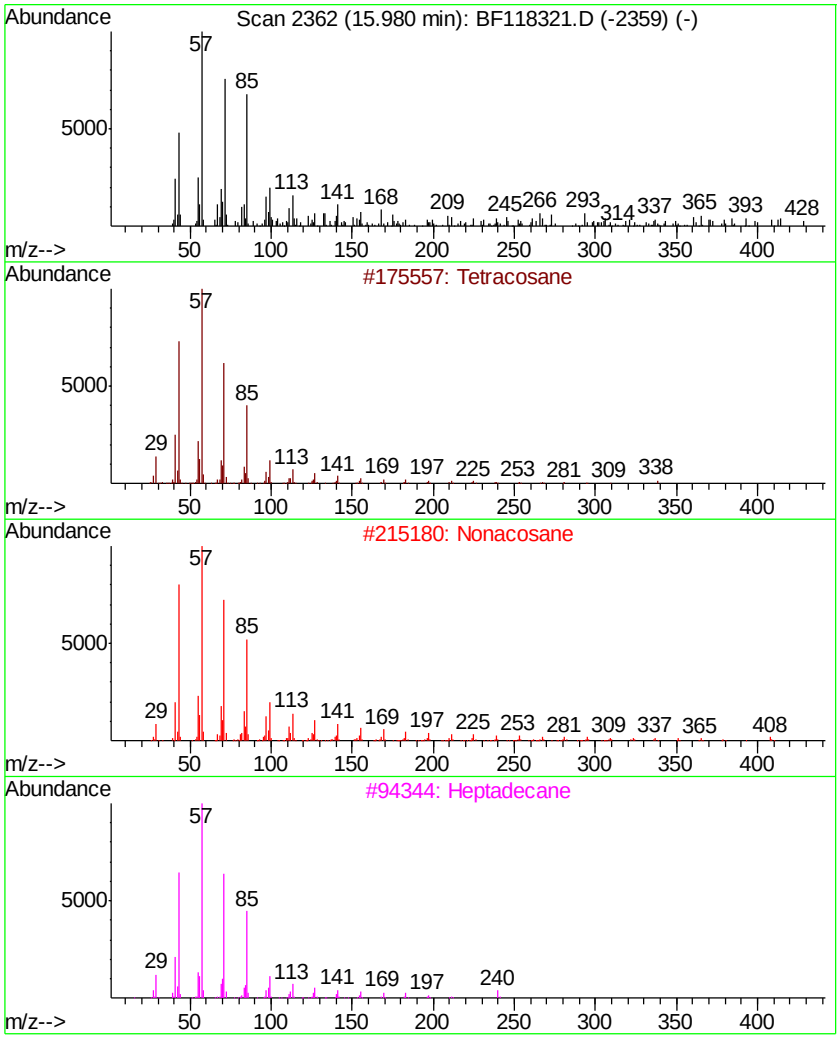
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

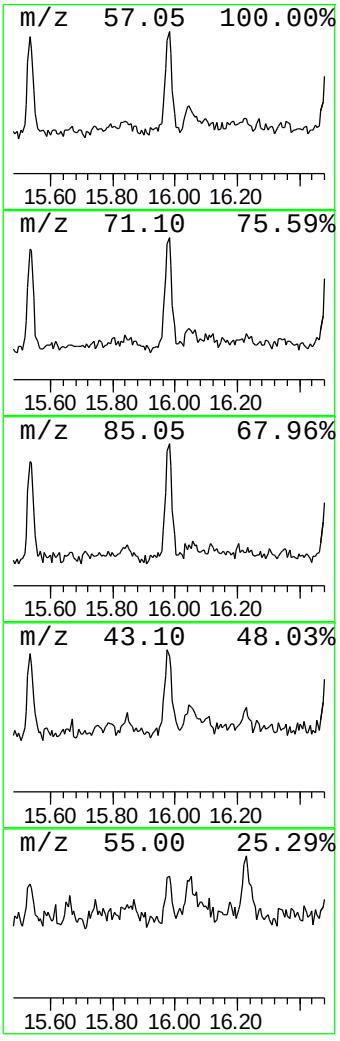
**********

Peak Number 6 Tetracosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.98 | 2.56 ng | 121832 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 2 | Nonacosane | 408 | C29H60 | 000630-03-5 | 87 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 76 |
| 4 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 74 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 74 |



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Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

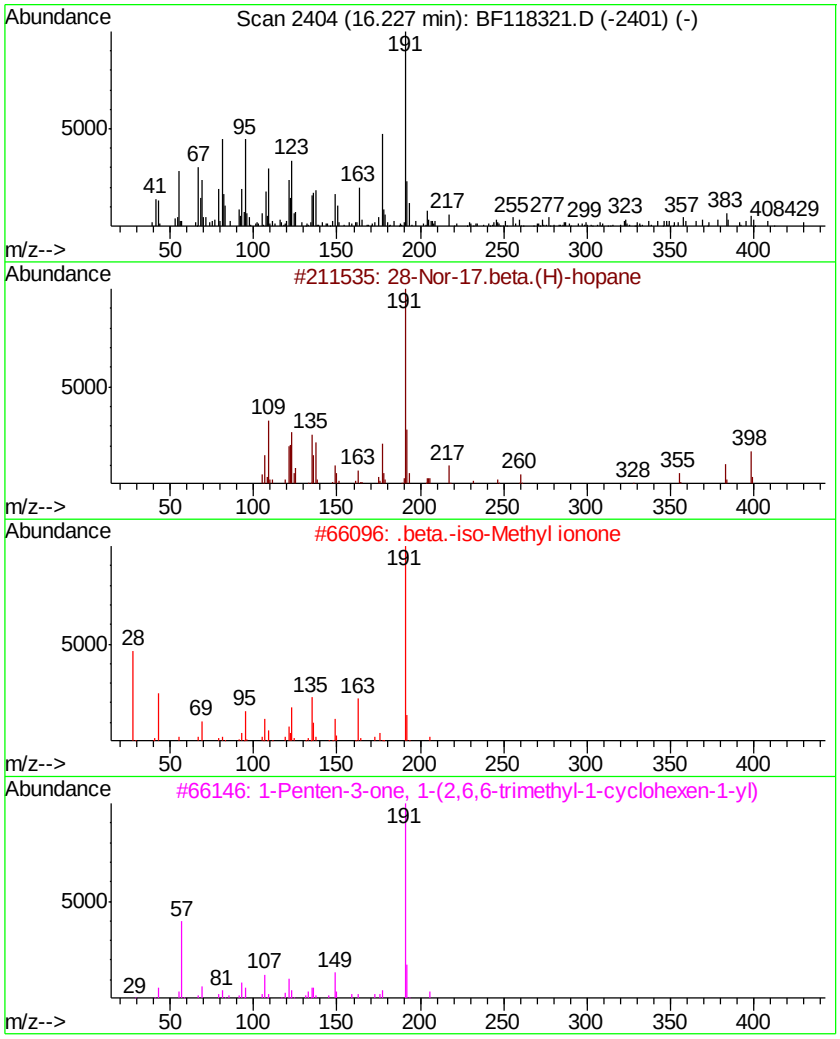
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

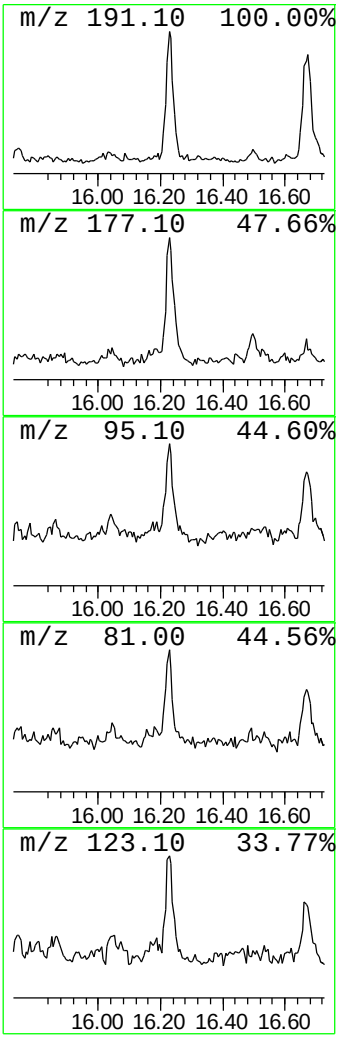
**********

Peak Number 7 unknown16.23 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.23 | 6.73 ng | 320760 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 28-Nor-17.beta.(H)-hopane | 398 | C29H50 | 036728-72-0 | 46 |
| 2 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 43 |
| 3 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 35 |
| 4 | 5-Fluoro-2-trifluoromethylbenzoi... | 352 | C14H6Cl2F4O2 | 1000357-63-5 | 30 |
| 5 | 5-Fluoro-2-trifluoromethylbenzoi... | 352 | C14H6Cl2F4O2 | 1000331-60-9 | 30 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122619\
Data File : BF118321.D
Acq On : 26 Dec 2019 17:27
Operator : JU
Sample : K6437-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** GP-3-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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... | 5.05 | 15.1 | ng | 466920 | 1 | 6.85 | 620363 | 20.0 |
| unknown6.62 | 6.62 | 80.6 | ng | 2499890 | 1 | 6.85 | 620363 | 20.0 |
| n-Hexadecanoic acid | 11.91 | 7.1 | ng | 349230 | 4 | 11.39 | 986111 | 20.0 |
| Behenic alcohol | 13.87 | 8.5 | ng | 462741 | 5 | 14.04 | 1090220 | 20.0 |
| Tetracosane | 15.98 | 2.6 | ng | 121832 | 6 | 15.53 | 953344 | 20.0 |
| unknown16.23 | 16.23 | 6.7 | ng | 320760 | 6 | 15.53 | 953344 | 20.0 |