LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

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-BF121918.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 | 2.193 | 14 | 18 | 22 | rVB | 48942 | 65468 | 2.17% | 0.216% |
| 2 | 3.422 | 224 | 227 | 240 | rBV | 20924 | 46753 | 1.55% | 0.154% |
| 3 | 5.110 | 510 | 514 | 520 | rBV | 127658 | 149137 | 4.93% | 0.492% |
| 4 | 5.528 | 581 | 585 | 589 | rBV | 2546843 | 2408066 | 79.65% | 7.943% |
| 5 | 6.534 | 751 | 756 | 761 | rBV | 2852348 | 2758544 | 91.24% | 9.099% |
| 6 | 6.675 | 776 | 780 | 783 | rBV | 3037140 | 2599777 | 85.99% | 8.575% |
| 7 | 6.898 | 815 | 818 | 822 | rVB | 1163179 | 946100 | 31.29% | 3.121% |
| 8 | 7.057 | 841 | 845 | 849 | rBV | 2457524 | 2028080 | 67.08% | 6.689% |
| 9 | 7.457 | 908 | 913 | 916 | rBV | 1941209 | 1623195 | 53.69% | 5.354% |
| 10 | 8.181 | 1032 | 1036 | 1040 | rBV | 1452163 | 1212664 | 40.11% | 4.000% |
| 11 | 9.257 | 1215 | 1219 | 1222 | rBV | 3583061 | 3023357 | 100.00% | 9.972% |
| 12 | 9.645 | 1281 | 1285 | 1290 | rVB | 396098 | 336902 | 11.14% | 1.111% |
| 13 | 9.934 | 1331 | 1334 | 1338 | rBV | 1462959 | 1377302 | 45.56% | 4.543% |
| 14 | 9.969 | 1338 | 1340 | 1343 | rVB | 104463 | 78955 | 2.61% | 0.260% |
| 15 | 10.257 | 1381 | 1389 | 1392 | rBV3 | 69860 | 207359 | 6.86% | 0.684% |
| 16 | 10.369 | 1406 | 1408 | 1412 | rVB2 | 49595 | 38894 | 1.29% | 0.128% |
| 17 | 10.722 | 1464 | 1468 | 1472 | rBV | 2243236 | 1968872 | 65.12% | 6.494% |
| 18 | 10.839 | 1486 | 1488 | 1489 | rBV | 59837 | 44978 | 1.49% | 0.148% |
| 19 | 10.857 | 1489 | 1491 | 1497 | rVB | 54451 | 54151 | 1.79% | 0.179% |
| 20 | 11.286 | 1560 | 1564 | 1567 | rBV3 | 50605 | 55522 | 1.84% | 0.183% |
| 21 | 11.322 | 1567 | 1570 | 1574 | rVB | 43140 | 47515 | 1.57% | 0.157% |
| 22 | 11.422 | 1583 | 1587 | 1590 | rBV | 1697657 | 1389105 | 45.95% | 4.582% |
| 23 | 11.445 | 1590 | 1591 | 1594 | rVB | 96565 | 52646 | 1.74% | 0.174% |
| 24 | 11.716 | 1634 | 1637 | 1640 | rBV | 53243 | 40595 | 1.34% | 0.134% |
| 25 | 11.945 | 1673 | 1676 | 1680 | rVB2 | 100635 | 91052 | 3.01% | 0.300% |
| 26 | 12.033 | 1688 | 1691 | 1694 | rBV | 38194 | 41378 | 1.37% | 0.136% |
| 27 | 12.122 | 1704 | 1706 | 1712 | rBV2 | 43639 | 55031 | 1.82% | 0.182% |
| 28 | 12.175 | 1712 | 1715 | 1719 | rVV2 | 80136 | 73684 | 2.44% | 0.243% |
| 29 | 12.280 | 1730 | 1733 | 1738 | rBV6 | 40247 | 46719 | 1.55% | 0.154% |
| 30 | 12.510 | 1770 | 1772 | 1776 | rBV2 | 40717 | 36004 | 1.19% | 0.119% |
| 31 | 12.645 | 1791 | 1795 | 1797 | rBV | 264305 | 248972 | 8.23% | 0.821% |
| 32 | 12.680 | 1797 | 1801 | 1804 | rVV | 659770 | 560744 | 18.55% | 1.850% |
| 33 | 12.863 | 1827 | 1832 | 1834 | rBV | 249448 | 253287 | 8.38% | 0.835% |
| 34 | 13.004 | 1852 | 1856 | 1860 | rBV | 3309600 | 2868321 | 94.87% | 9.461% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

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-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.239 | 1893 | 1896 | 1897 | rBV | 44504 | 37179 | 1.23% | 0.123% |
| 36 | 13.486 | 1935 | 1938 | 1941 | rBV2 | 80791 | 107941 | 3.57% | 0.356% |
| 37 | 13.580 | 1952 | 1954 | 1960 | rVB | 56128 | 53015 | 1.75% | 0.175% |
| 38 | 13.898 | 2004 | 2008 | 2015 | rVB2 | 243016 | 292000 | 9.66% | 0.963% |
| 39 | 14.057 | 2031 | 2035 | 2038 | rBV | 1213869 | 1263239 | 41.78% | 4.167% |
| 40 | 14.086 | 2038 | 2040 | 2043 | rVB | 86568 | 72363 | 2.39% | 0.239% |
| 41 | 14.163 | 2051 | 2053 | 2057 | rVV2 | 46967 | 42630 | 1.41% | 0.141% |
| 42 | 14.221 | 2061 | 2063 | 2069 | rVB2 | 85920 | 91636 | 3.03% | 0.302% |
| 43 | 14.533 | 2113 | 2116 | 2120 | rVB | 121853 | 128729 | 4.26% | 0.425% |
| 44 | 14.839 | 2165 | 2168 | 2172 | rBV | 79235 | 82341 | 2.72% | 0.272% |
| 45 | 15.104 | 2211 | 2213 | 2216 | rBV | 60049 | 75518 | 2.50% | 0.249% |
| 46 | 15.186 | 2224 | 2227 | 2230 | rBV | 92718 | 107291 | 3.55% | 0.354% |
| 47 | 15.474 | 2273 | 2276 | 2280 | rVB | 72068 | 79098 | 2.62% | 0.261% |
| 48 | 15.545 | 2283 | 2288 | 2291 | rBV | 840003 | 1055851 | 34.92% | 3.483% |

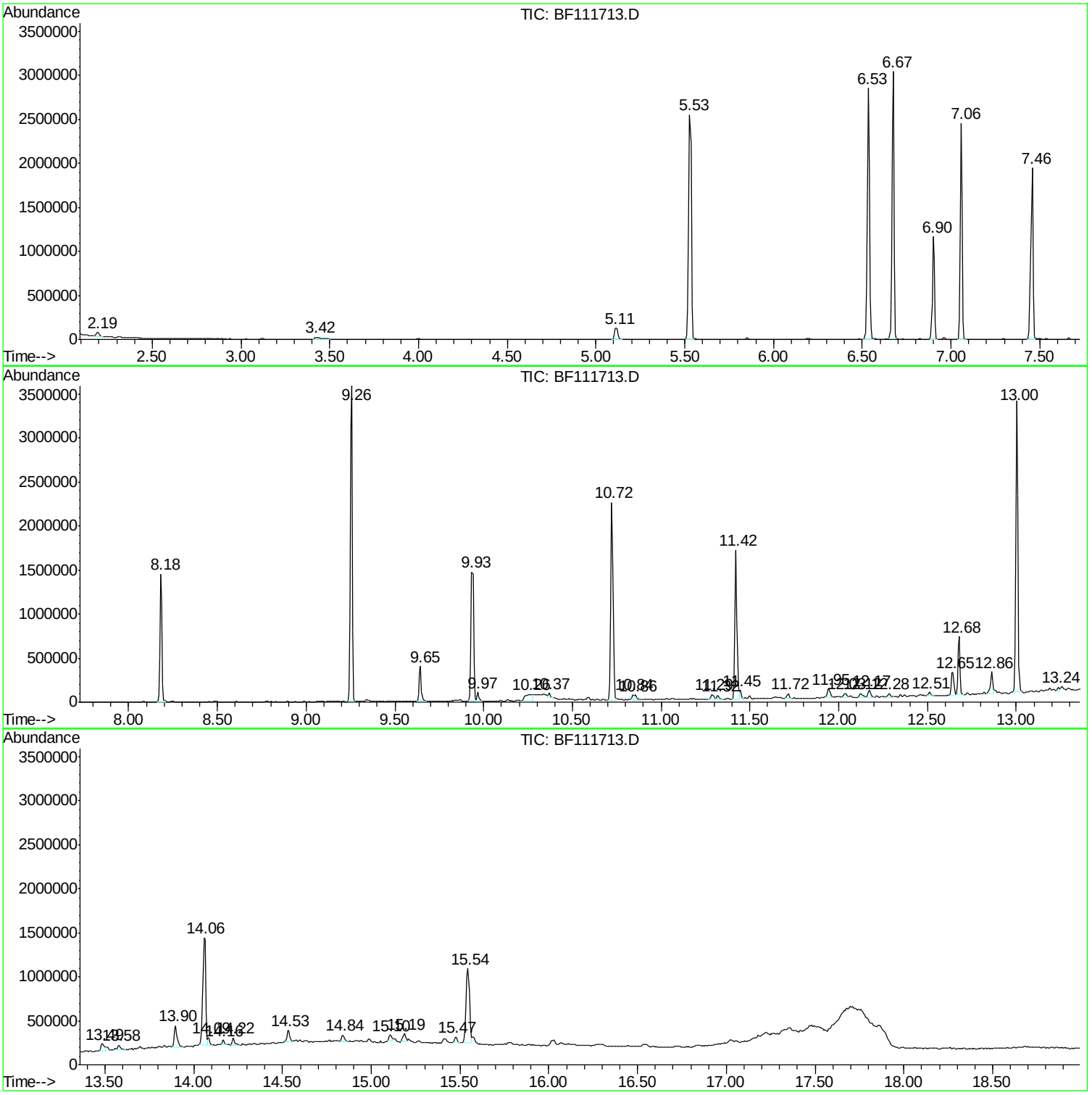
Sum of corrected areas: 30317960

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

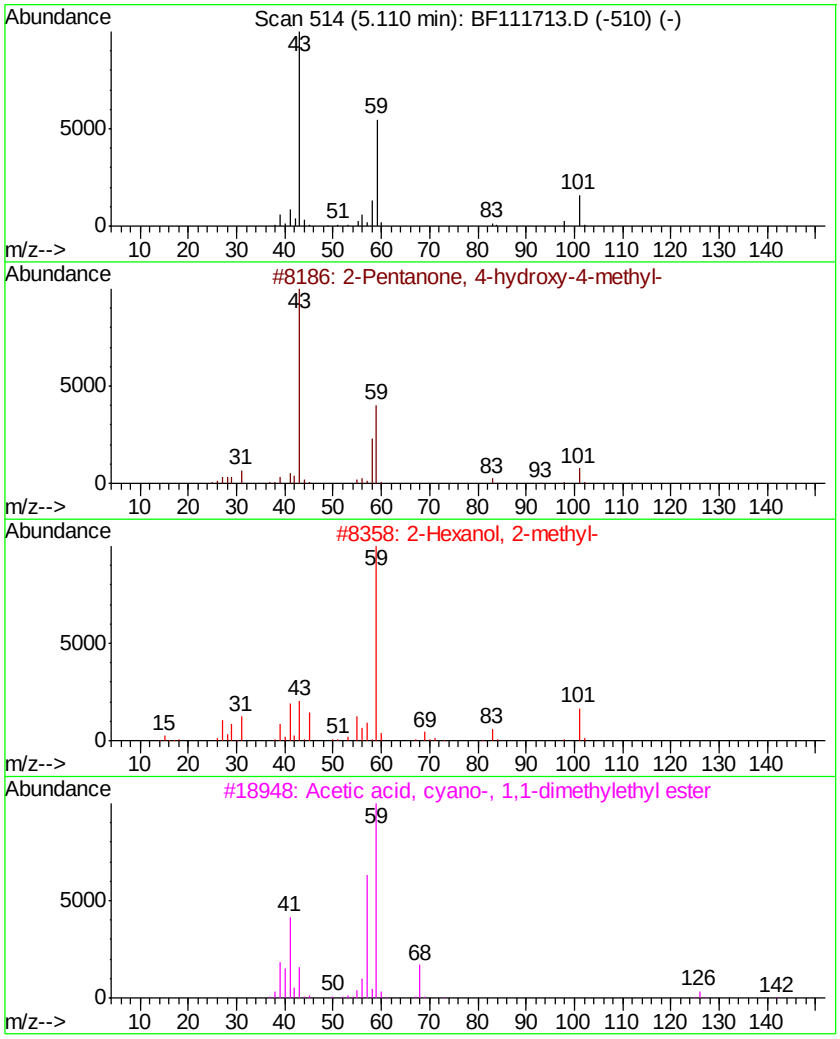
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

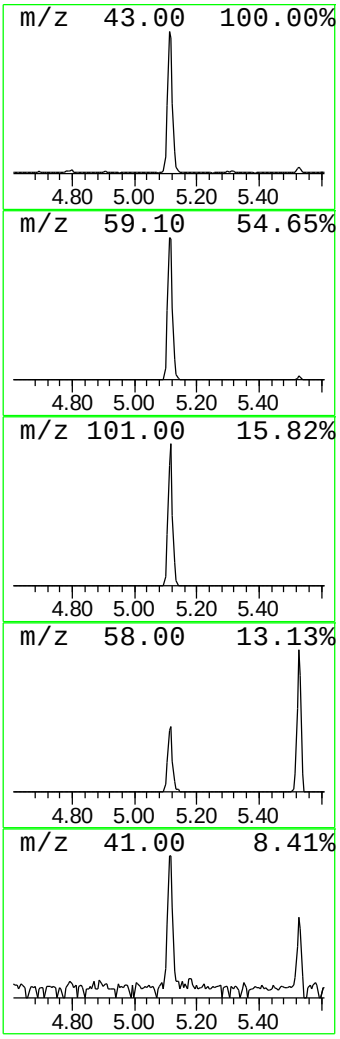
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 3.15 ng | 149137 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 17 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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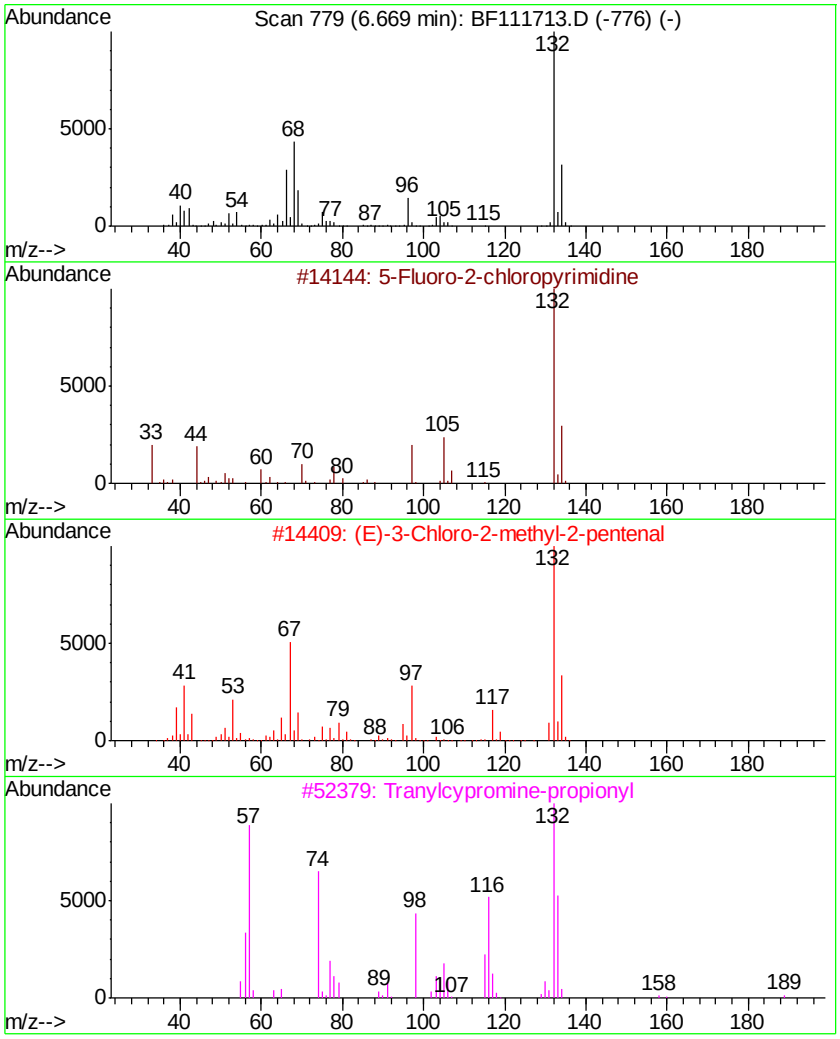
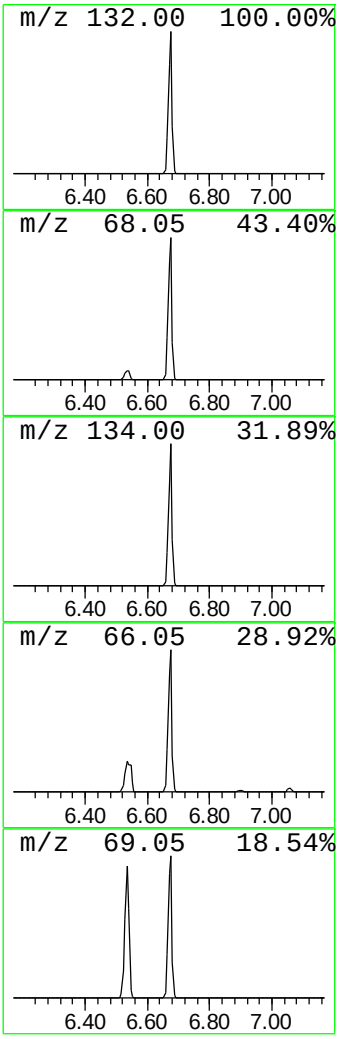
Peak Number 2 unknown6.67 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 54.96 ng | 2599780 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 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 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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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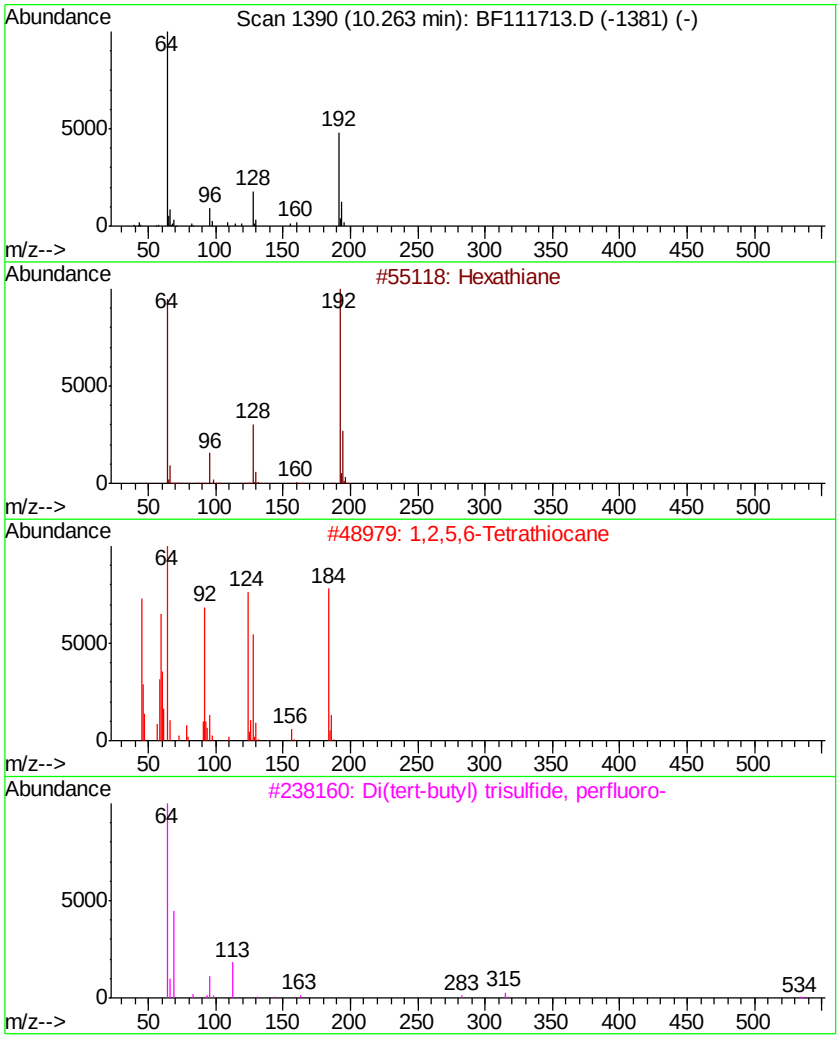
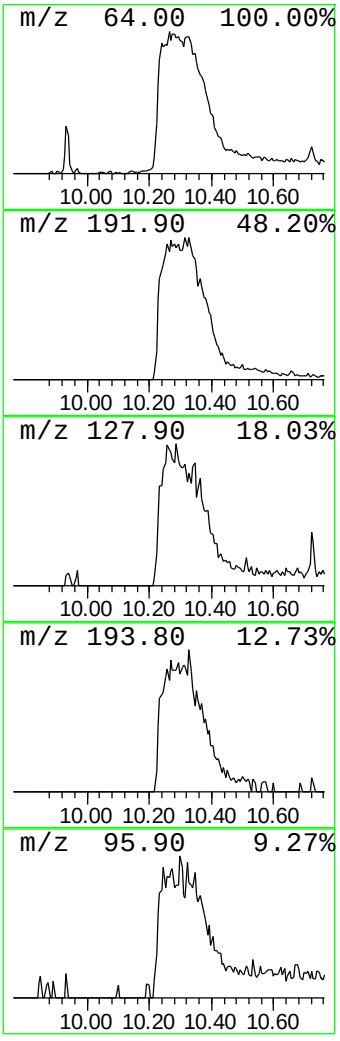
Peak Number 4 Hexathiane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.26 | 3.01 ng | 207359 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexathiane | 192 | S6 | 013798-23-7 | 91 |
| 2 | 1,2,5,6-Tetrathiocane | 184 | C4H8S4 | 001940-01-8 | 39 |
| 3 | Di(tert-butyl) trisulfide, perfl... | 534 | C8F18S3 | 016005-64-4 | 9 |
| 4 | Tetrazolo[1,5-b]pyridazine, 6-ch... | 155 | C4H2ClN5 | 021413-15-0 | 7 |
| 5 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 4 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

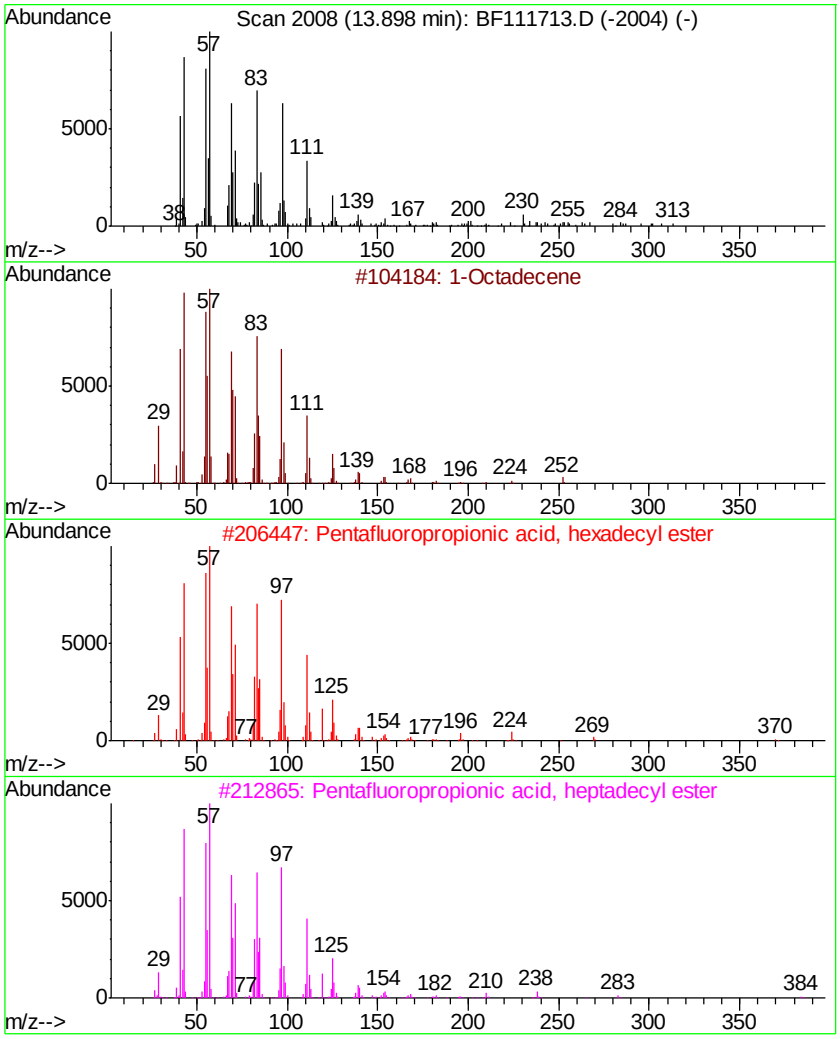
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

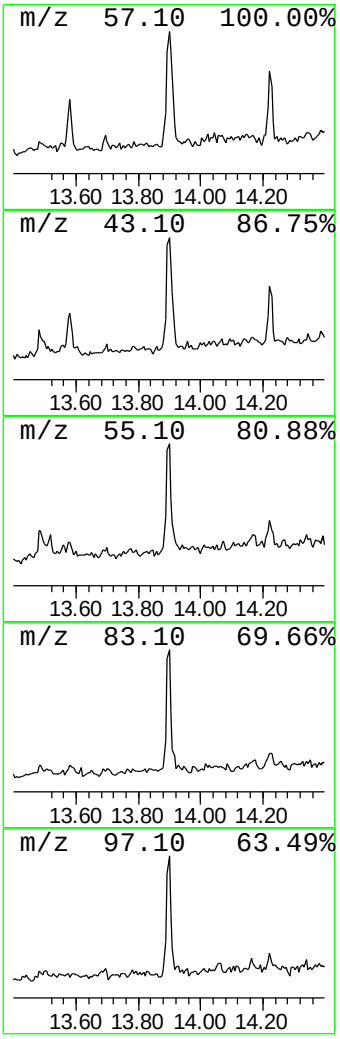
**********

Peak Number 5 1-Octadecene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.90 | 4.62 ng | 292000 | Chrysene-d12 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 92 |
| 2 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 91 |
| 3 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91 |
| 4 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 91 |
| 5 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

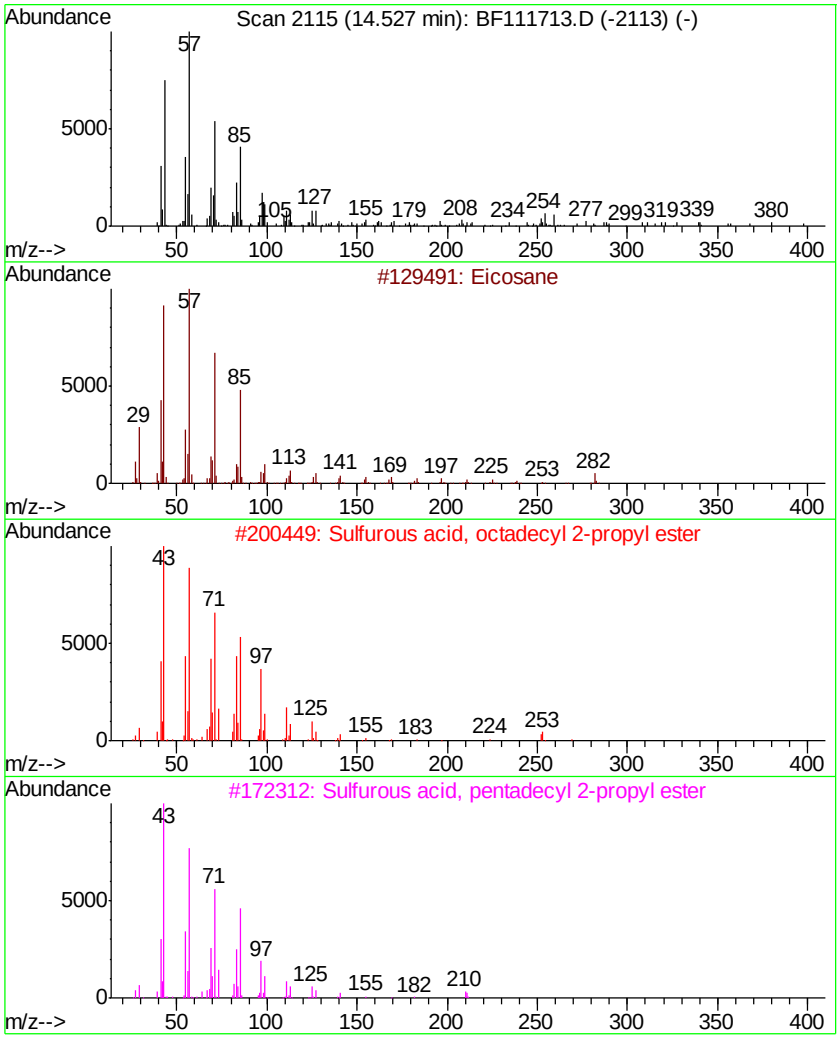
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

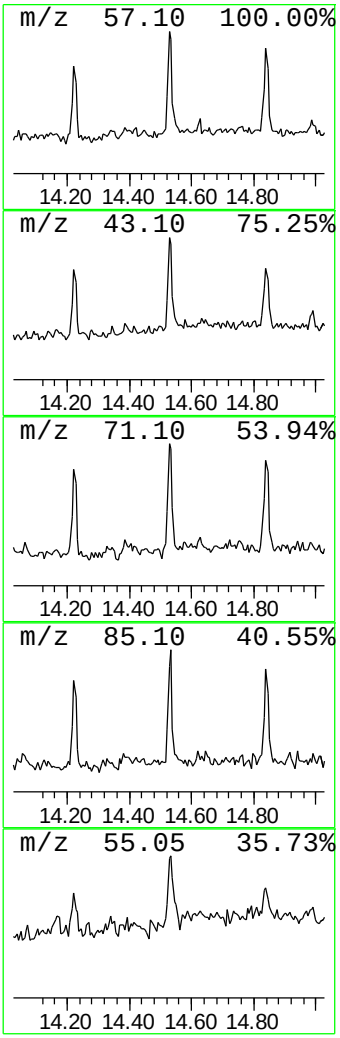
**********

Peak Number 6 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.53 | 2.04 ng | 128729 | Chrysene-d12 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 2 | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 74 |
| 3 | Sulfurous acid, pentadecyl 2-pro... | 334 | C18H38O3S | 1000309-12-6 | 72 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 70 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

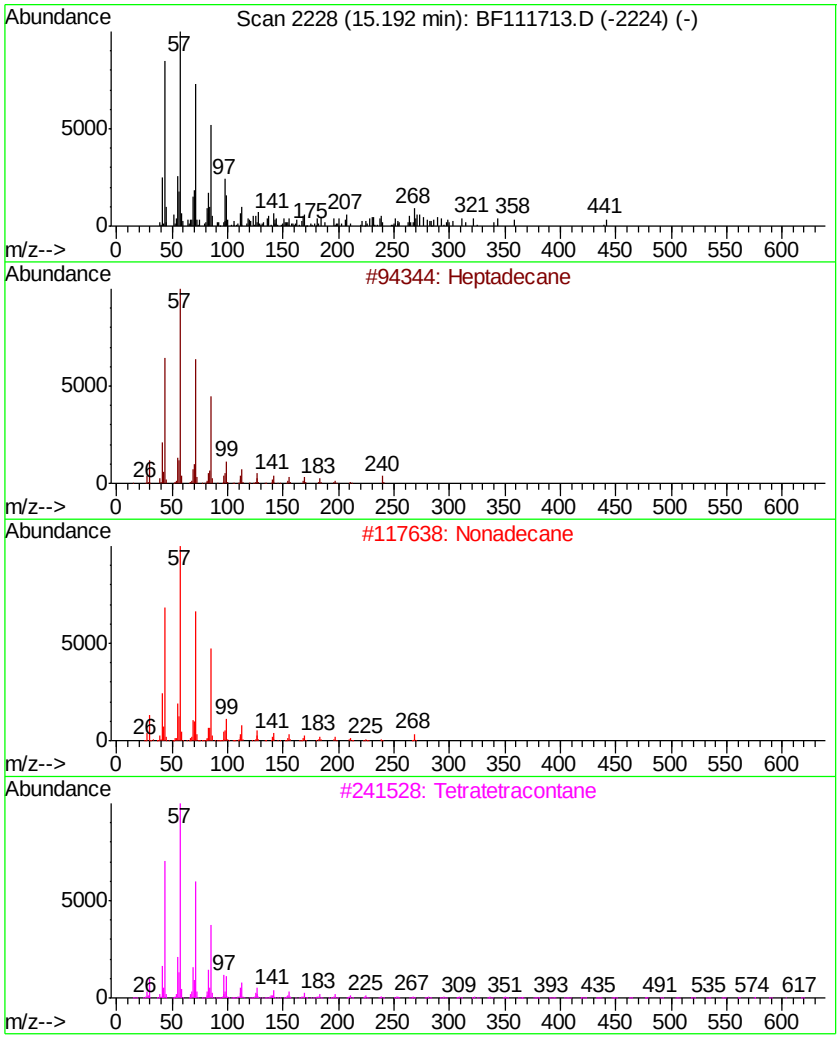
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

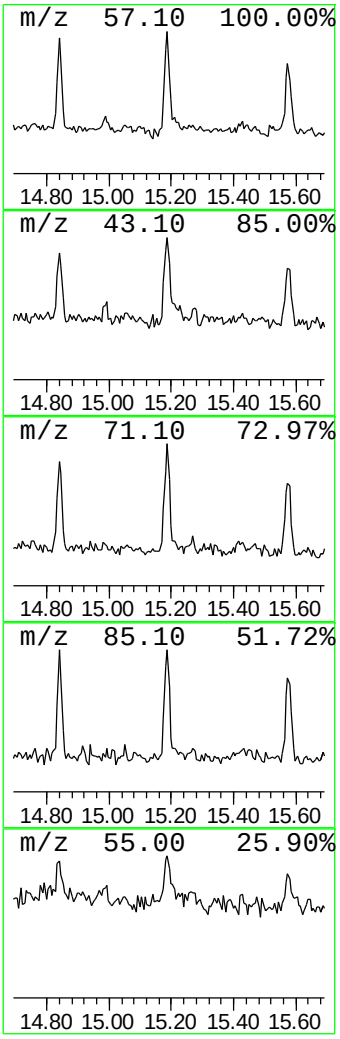
**********

Peak Number 7 Heptadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.19 | 2.03 ng | 107291 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 95 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 80 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 74 |
| 5 | Heptadecane, 3-methyl- | 254 | C18H38 | 006418-44-6 | 74 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122618\
Data File : BF111713.D
Acq On : 26 Dec 2018 13:56
Operator : JU/SJ
Sample : J6498-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SSSI-1218-S-DH-9-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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... | 5.11 | 3.1 | ng | 149137 | 1 | 6.90 | 946100 | 20.0 |
| unknown6.67 | 6.67 | 55.0 | ng | 2599780 | 1 | 6.90 | 946100 | 20.0 |
| Hexathiane | 10.26 | 3.0 | ng | 207359 | 3 | 9.93 | 1377300 | 20.0 |
| 1-Octadecene | 13.90 | 4.6 | ng | 292000 | 5 | 14.06 | 1263240 | 20.0 |
| Eicosane | 14.53 | 2.0 | ng | 128729 | 5 | 14.06 | 1263240 | 20.0 |
| Heptadecane | 15.19 | 2.0 | ng | 107291 | 6 | 15.54 | 1055850 | 20.0 |