LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

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:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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 | 2.169 | 7 | 14 | 22 | rVB | 493707 | 686382 | 12.97% | 1.624% |
| 2 | 5.122 | 513 | 516 | 526 | rVB | 141715 | 188457 | 3.56% | 0.446% |
| 3 | 5.510 | 576 | 582 | 585 | rBV | 4859058 | 5137328 | 97.05% | 12.153% |
| 4 | 6.516 | 747 | 753 | 770 | rBV2 | 4361858 | 5293719 | 100.00% | 12.523% |
| 5 | 6.657 | 772 | 777 | 780 | rBV | 4759624 | 4929018 | 93.11% | 11.660% |
| 6 | 6.887 | 812 | 816 | 819 | rBV | 1598587 | 1287492 | 24.32% | 3.046% |
| 7 | 7.045 | 838 | 843 | 846 | rBV | 3977092 | 3680930 | 69.53% | 8.708% |
| 8 | 7.451 | 906 | 912 | 915 | rBV | 3208162 | 3292791 | 62.20% | 7.789% |
| 9 | 8.169 | 1030 | 1034 | 1037 | rBV | 1946714 | 1581606 | 29.88% | 3.741% |
| 10 | 9.245 | 1212 | 1217 | 1220 | rBV | 4429660 | 4255724 | 80.39% | 10.067% |
| 11 | 9.316 | 1227 | 1229 | 1232 | rVB | 124554 | 93035 | 1.76% | 0.220% |
| 12 | 9.633 | 1279 | 1283 | 1286 | rBV | 408140 | 349482 | 6.60% | 0.827% |
| 13 | 9.845 | 1314 | 1319 | 1322 | rBV | 277889 | 214690 | 4.06% | 0.508% |
| 14 | 9.928 | 1329 | 1333 | 1336 | rBV | 1457562 | 1429714 | 27.01% | 3.382% |
| 15 | 10.075 | 1355 | 1358 | 1361 | rBV2 | 47472 | 54638 | 1.03% | 0.129% |
| 16 | 10.169 | 1371 | 1374 | 1378 | rBV2 | 60085 | 55008 | 1.04% | 0.130% |
| 17 | 10.345 | 1401 | 1404 | 1407 | rVB | 287815 | 224413 | 4.24% | 0.531% |
| 18 | 10.569 | 1437 | 1442 | 1444 | rBV | 77828 | 99728 | 1.88% | 0.236% |
| 19 | 10.716 | 1463 | 1467 | 1470 | rBV | 2181214 | 2073008 | 39.16% | 4.904% |
| 20 | 10.822 | 1482 | 1485 | 1490 | rBV2 | 209474 | 266207 | 5.03% | 0.630% |
| 21 | 10.922 | 1498 | 1502 | 1505 | rVV2 | 67011 | 76388 | 1.44% | 0.181% |
| 22 | 10.951 | 1505 | 1507 | 1510 | rVV2 | 56722 | 62658 | 1.18% | 0.148% |
| 23 | 11.022 | 1514 | 1519 | 1520 | rBV2 | 43666 | 61948 | 1.17% | 0.147% |
| 24 | 11.069 | 1524 | 1527 | 1530 | rVB2 | 86847 | 95740 | 1.81% | 0.226% |
| 25 | 11.104 | 1530 | 1533 | 1536 | rBV | 87418 | 72407 | 1.37% | 0.171% |
| 26 | 11.145 | 1538 | 1540 | 1545 | rVB | 66644 | 55279 | 1.04% | 0.131% |
| 27 | 11.269 | 1558 | 1561 | 1563 | rBV | 132267 | 101074 | 1.91% | 0.239% |
| 28 | 11.416 | 1582 | 1586 | 1589 | rBV | 1157674 | 1149311 | 21.71% | 2.719% |
| 29 | 11.927 | 1670 | 1673 | 1683 | rBV2 | 122065 | 151530 | 2.86% | 0.358% |
| 30 | 12.627 | 1789 | 1792 | 1797 | rBV | 62147 | 57813 | 1.09% | 0.137% |
| 31 | 12.998 | 1851 | 1855 | 1858 | rBV | 3064122 | 2790032 | 52.70% | 6.600% |
| 32 | 13.468 | 1932 | 1935 | 1938 | rVB | 121503 | 100103 | 1.89% | 0.237% |
| 33 | 13.880 | 2002 | 2005 | 2012 | rBV | 361432 | 400225 | 7.56% | 0.947% |
| 34 | 14.057 | 2031 | 2035 | 2038 | rBV | 1109977 | 1045393 | 19.75% | 2.473% |

LSC Area Percent Report

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Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

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:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 15.545 | 2283 | 2288 | 2297 | rVB | 595944 | 859479 | 16.24% | 2.033% |

Sum of corrected areas: 42272750

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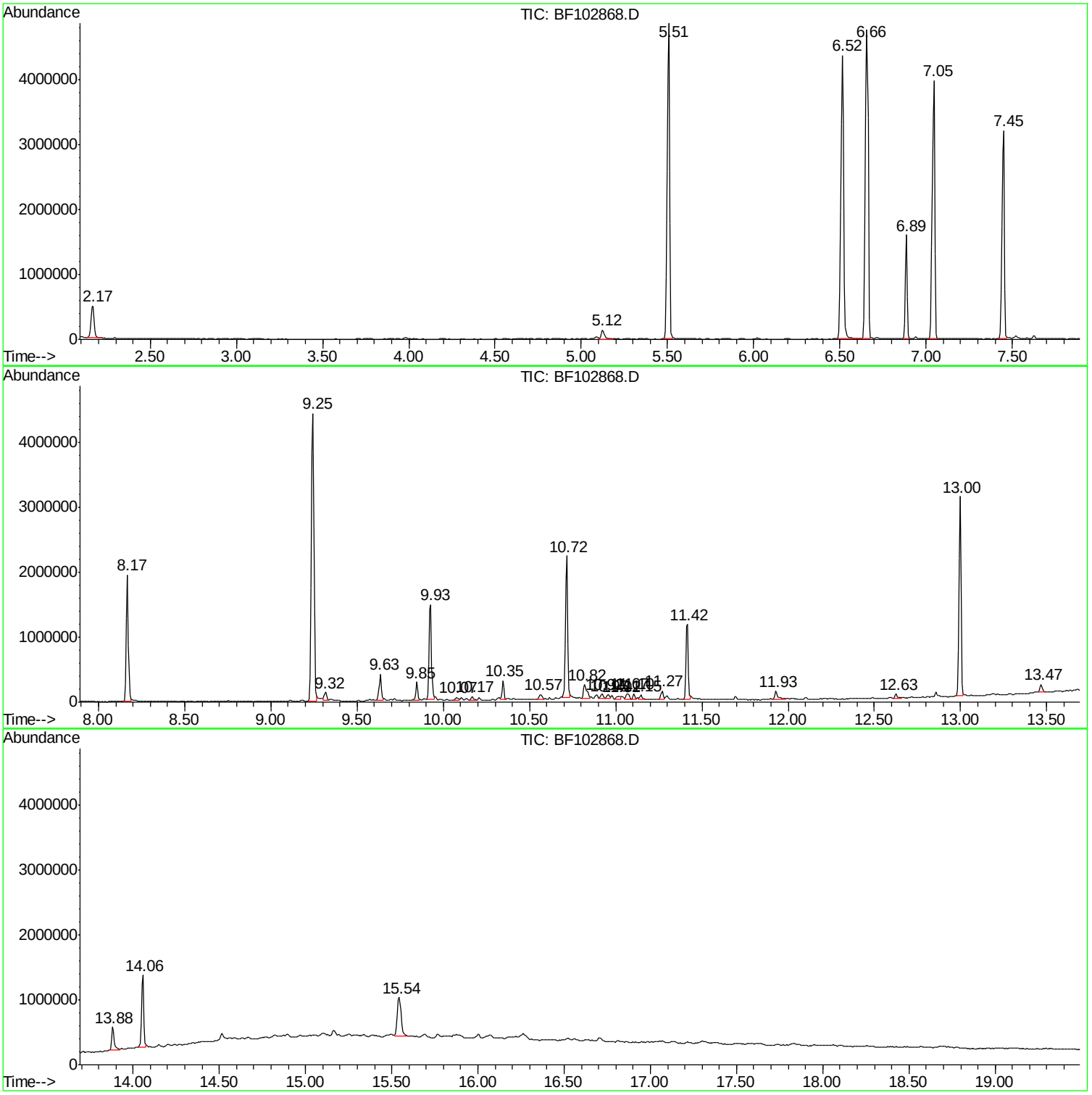
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

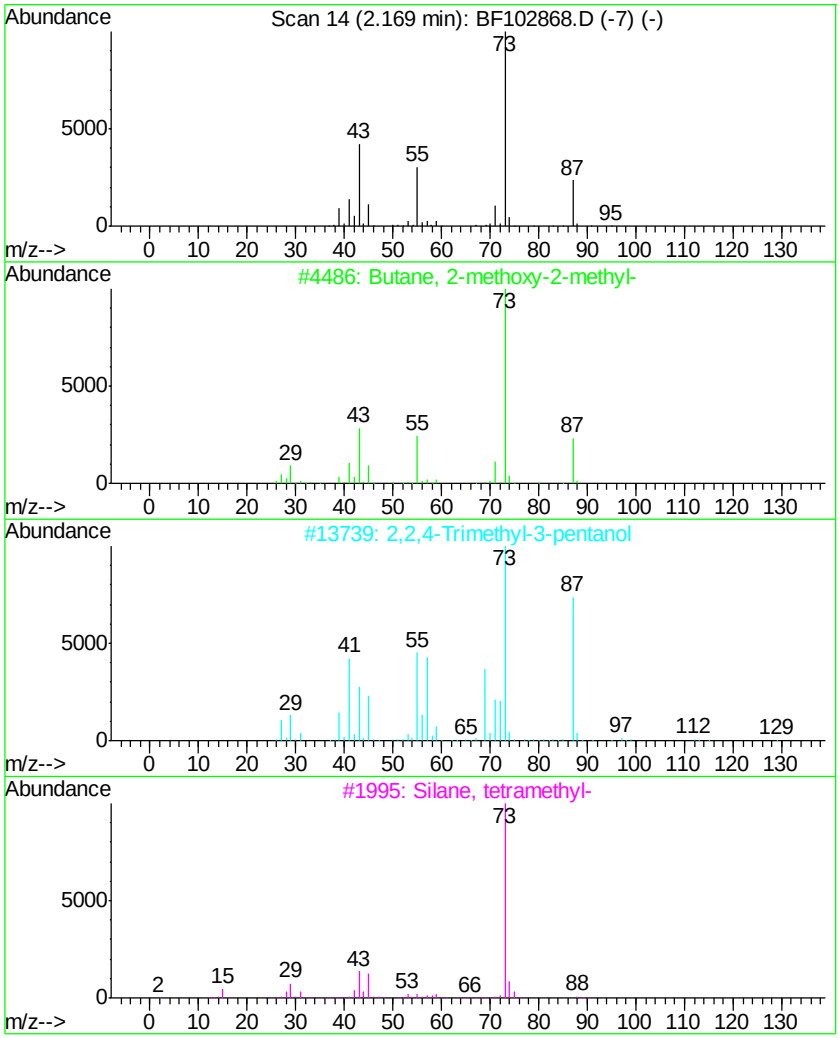
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

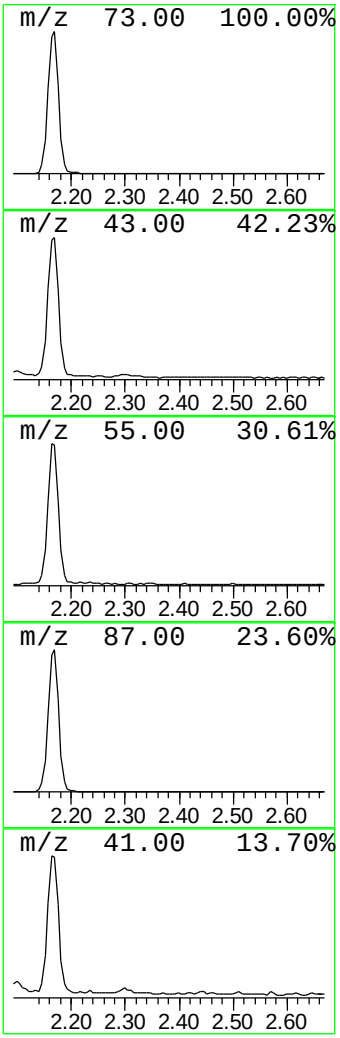
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.17 | 10.66 ng | 686382 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 38 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

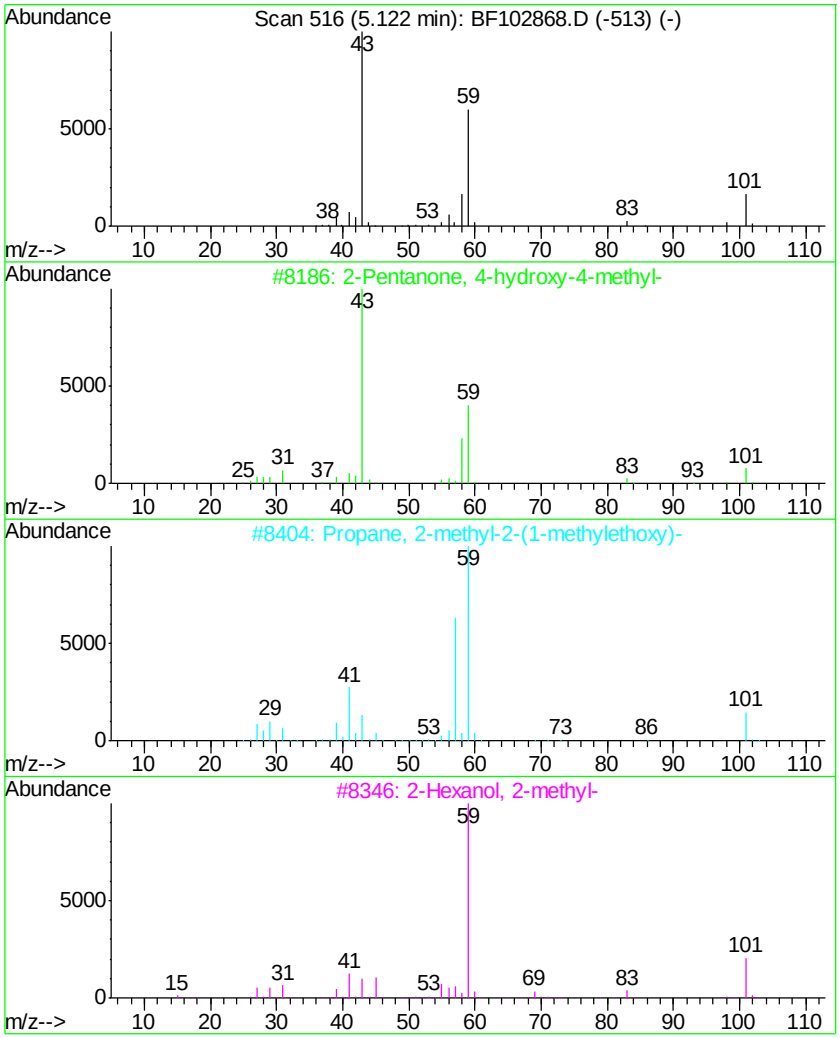
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

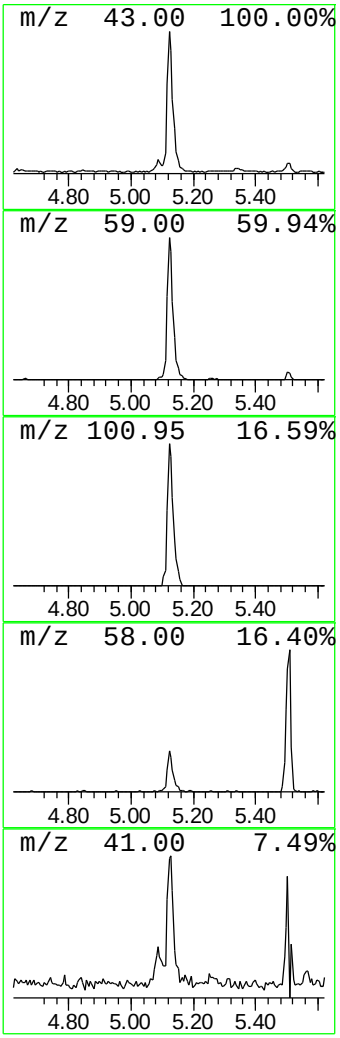
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 2.93 ng | 188457 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 27 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

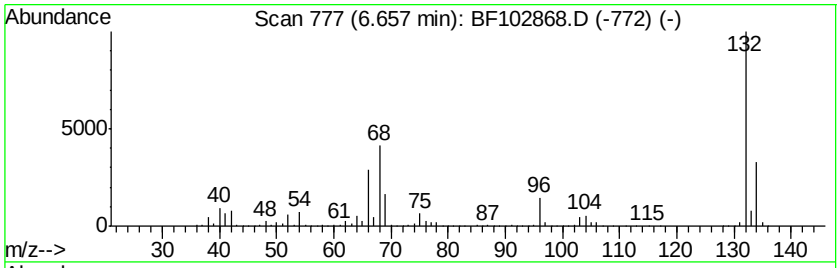
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

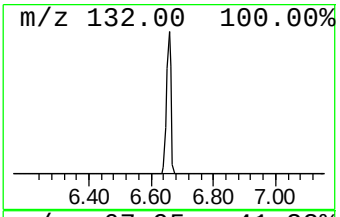
**********

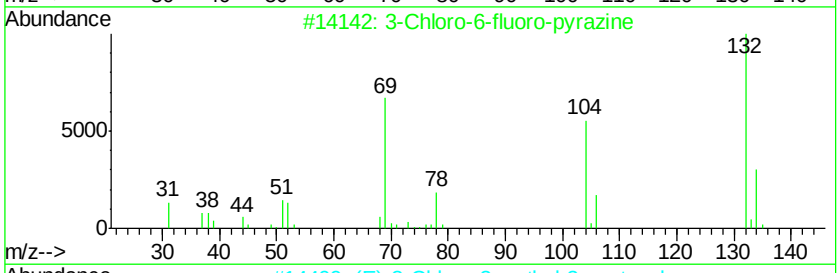
Peak Number 3 unknown6.66 Concentration Rank 1

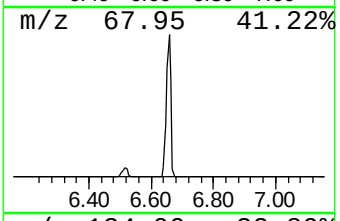
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 76.57 ng | 4929020 | 1,4-Dichlorobenzene-d4 | 6.89 |

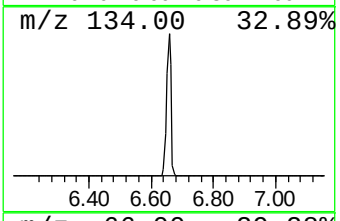
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |

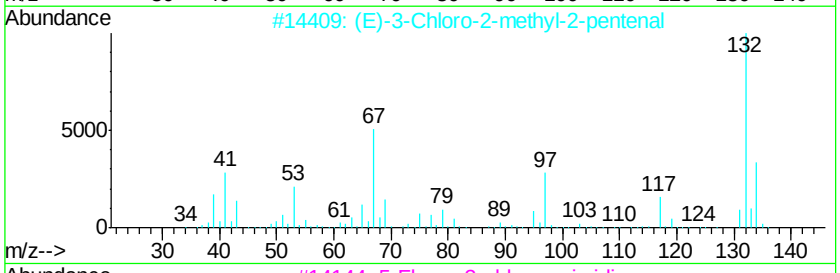


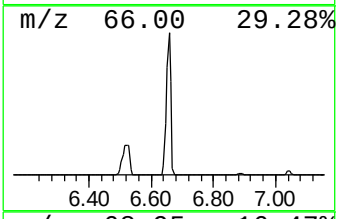



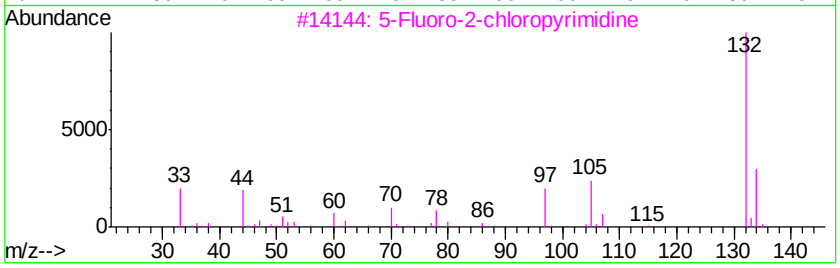



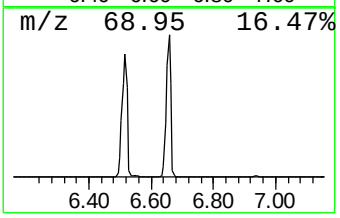



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ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

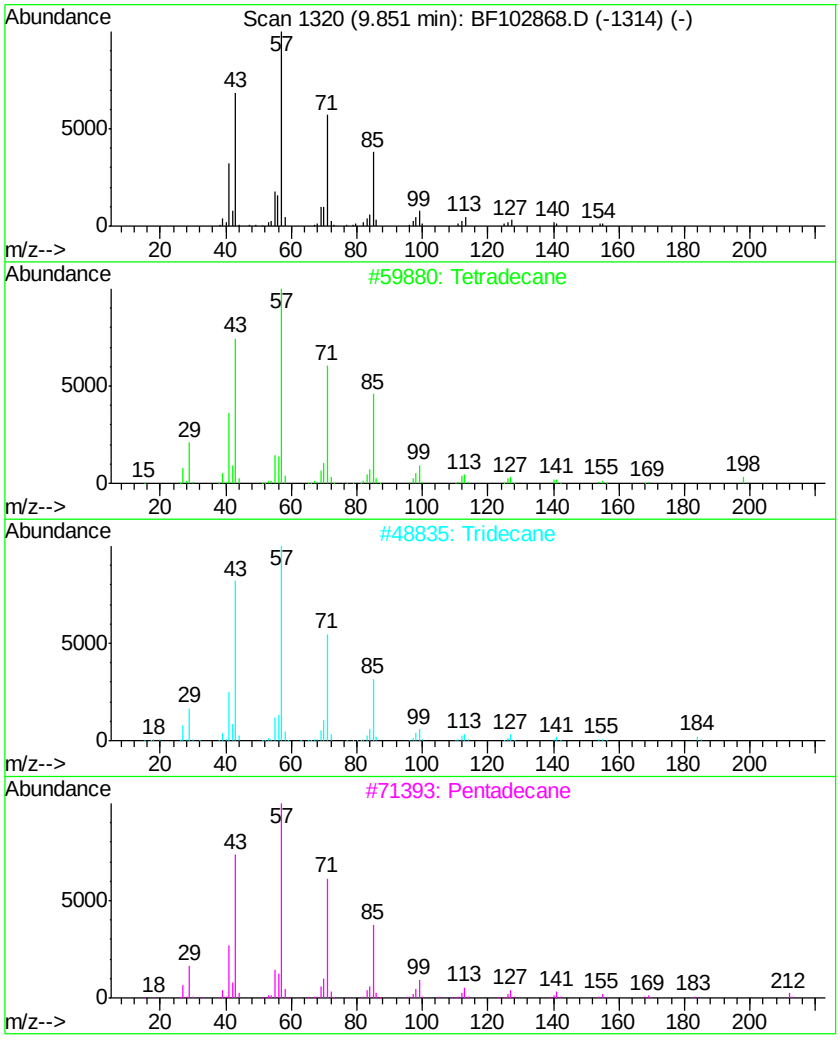
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

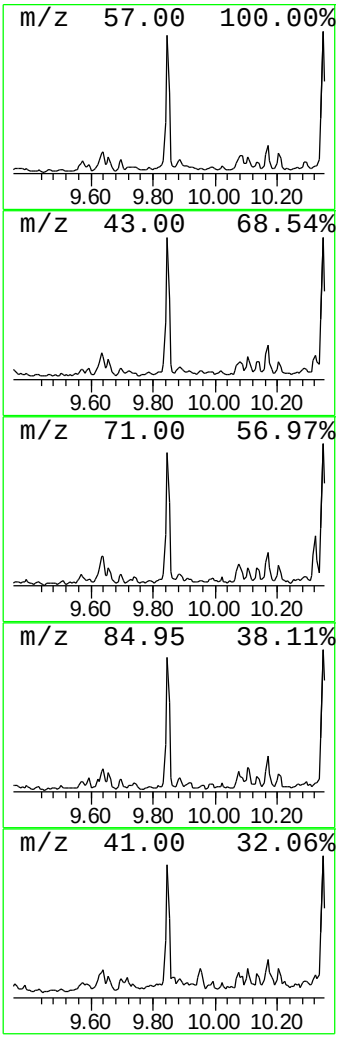
**********

Peak Number 5 Tetradecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.85 | 3.00 ng | 214690 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 90 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |



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Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

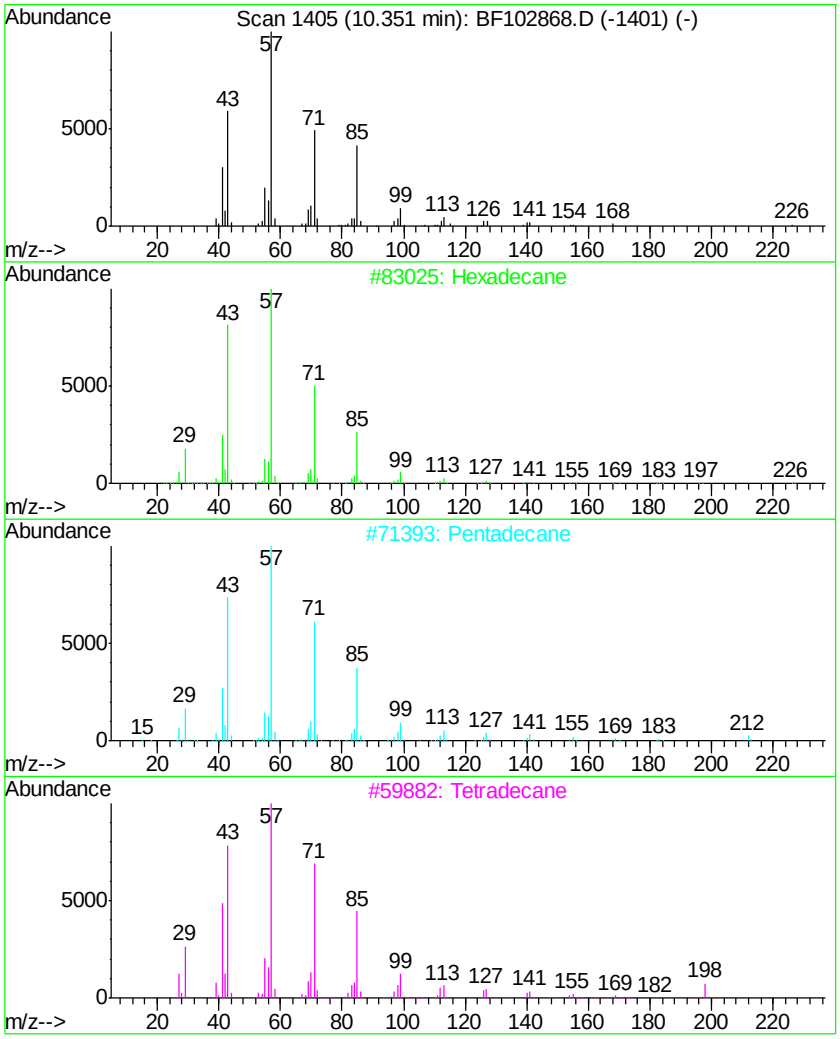
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

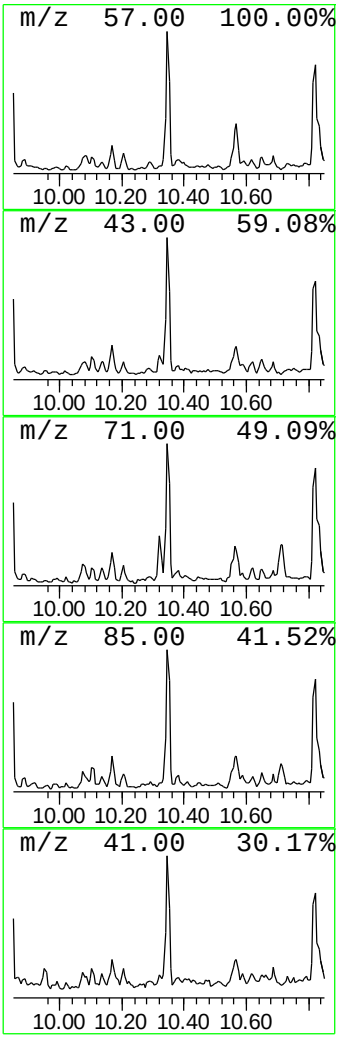
**********

Peak Number 6 Hexadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.35 | 3.14 ng | 224413 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 4 | Sulfurous acid, 2-propyl tetrade... | 320 | C17H36O3S | 1000309-12-5 | 80 |
| 5 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 80 |



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Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

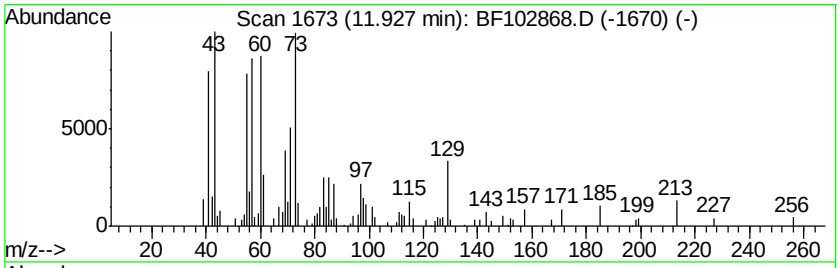
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

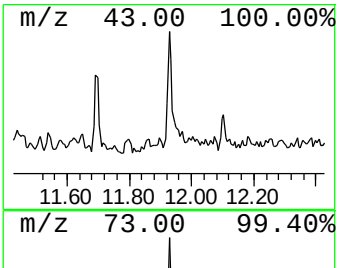
**********

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.93 | 2.64 ng | 151530 | Phenanthrene-d10 | 11.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 74 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 25 |
| 5 | .beta.-D-Mannofuranoside, 1-O-(1... | 332 | C17H32O6 | 1000155-29-9 | 25 |



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Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

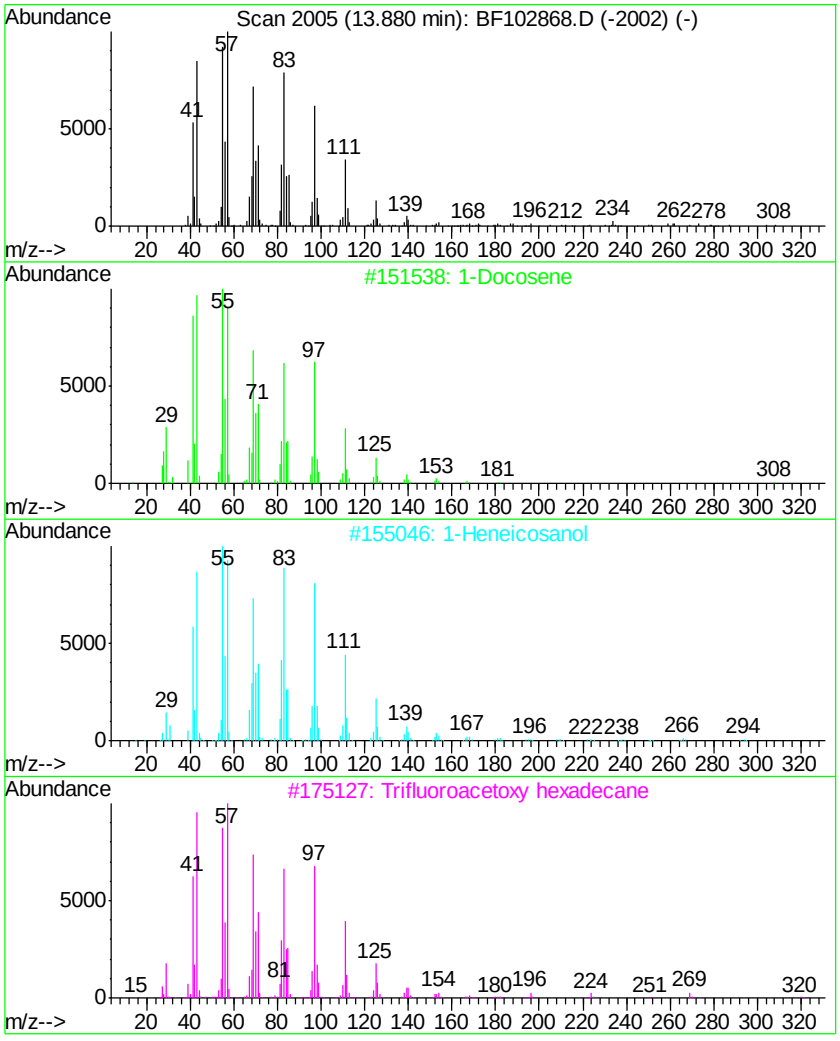
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

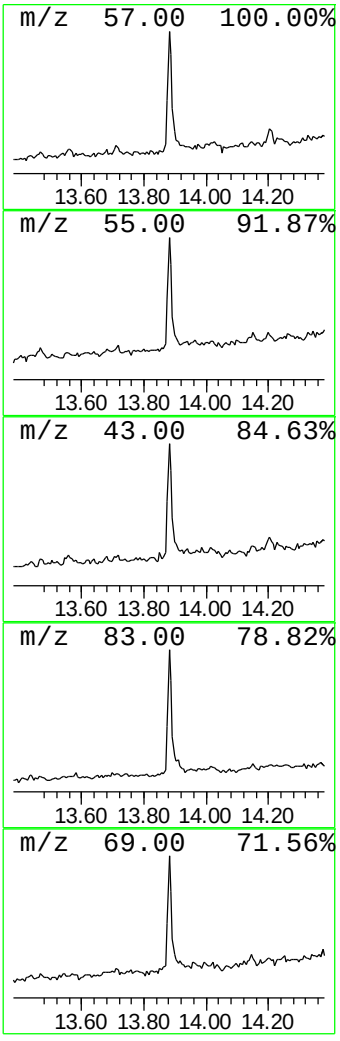
**********

Peak Number 9 1-Docosene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.88 | 7.66 ng | 400225 | Chrysene-d12 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 98 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 3 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 4 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 5 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102868.D
Acq On : 8 Feb 2018 20:43
Operator : SJ/JU
Sample : J1471-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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 |
| Butane, 2-methoxy... | 2.17 | 10.7 | ng | 686382 | 1 | 6.89 | 1287490 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 2.9 | ng | 188457 | 1 | 6.89 | 1287490 | 20.0 |
| unknown6.66 | 6.66 | 76.6 | ng | 4929020 | 1 | 6.89 | 1287490 | 20.0 |
| Tetradecane | 9.85 | 3.0 | ng | 214690 | 3 | 9.93 | 1429710 | 20.0 |
| Hexadecane | 10.35 | 3.1 | ng | 224413 | 3 | 9.93 | 1429710 | 20.0 |
| n-Hexadecanoic acid | 11.93 | 2.6 | ng | 151530 | 4 | 11.42 | 1149310 | 20.0 |
| 1-Docosene | 13.88 | 7.7 | ng | 400225 | 5 | 14.06 | 1045390 | 20.0 |