LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100492.D
Acq On : 12 Nov 2017 16:20
Operator : SJ/JU
Sample : I6403-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 | 2.204 | 17 | 20 | 32 | rVB | 82919 | 130485 | 3.80% | 0.635% |
| 2 | 5.116 | 512 | 515 | 525 | rBV | 209271 | 210304 | 6.12% | 1.023% |
| 3 | 5.510 | 578 | 582 | 586 | rBV | 1135893 | 1086052 | 31.61% | 5.281% |
| 4 | 6.516 | 749 | 753 | 757 | rBV | 800688 | 734472 | 21.37% | 3.572% |
| 5 | 6.669 | 774 | 779 | 782 | rBV | 1981971 | 1903278 | 55.39% | 9.255% |
| 6 | 6.898 | 815 | 818 | 822 | rBV | 923176 | 786617 | 22.89% | 3.825% |
| 7 | 7.057 | 841 | 845 | 849 | rVB | 2729331 | 2570234 | 74.80% | 12.499% |
| 8 | 7.463 | 908 | 914 | 917 | rBV | 2106867 | 2066462 | 60.14% | 10.049% |
| 9 | 8.180 | 1032 | 1036 | 1040 | rBV | 1120670 | 975506 | 28.39% | 4.744% |
| 10 | 9.257 | 1214 | 1219 | 1222 | rBV | 3655042 | 3436267 | 100.00% | 16.710% |
| 11 | 9.645 | 1282 | 1285 | 1294 | rVB | 128180 | 104060 | 3.03% | 0.506% |
| 12 | 9.939 | 1329 | 1335 | 1339 | rBV | 953590 | 937230 | 27.27% | 4.558% |
| 13 | 10.645 | 1452 | 1455 | 1460 | rBV | 47932 | 40826 | 1.19% | 0.199% |
| 14 | 10.721 | 1464 | 1468 | 1480 | rBV | 1181803 | 1065218 | 31.00% | 5.180% |
| 15 | 11.421 | 1583 | 1587 | 1591 | rBV | 849917 | 744802 | 21.67% | 3.622% |
| 16 | 12.821 | 1822 | 1825 | 1828 | rBV | 119983 | 87414 | 2.54% | 0.425% |
| 17 | 13.010 | 1852 | 1857 | 1860 | rBV | 2611592 | 2415664 | 70.30% | 11.747% |
| 18 | 13.527 | 1942 | 1945 | 1948 | rBV | 82868 | 63883 | 1.86% | 0.311% |
| 19 | 14.062 | 2032 | 2036 | 2045 | rVB | 745458 | 713955 | 20.78% | 3.472% |
| 20 | 15.545 | 2283 | 2288 | 2296 | rBV | 359398 | 491537 | 14.30% | 2.390% |

Sum of corrected areas: 20564266

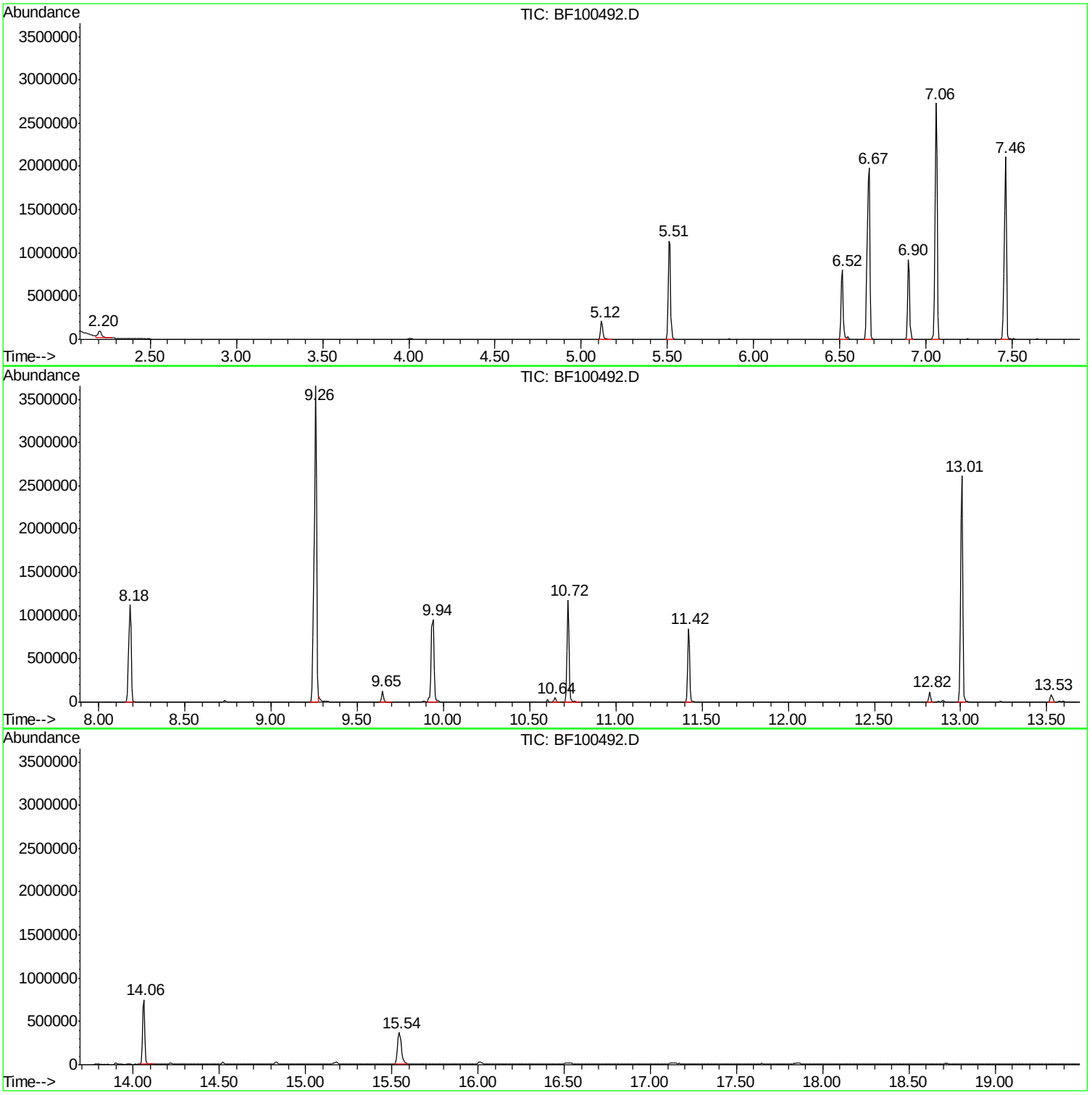
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100492.D
Acq On : 12 Nov 2017 16:20
Operator : SJ/JU
Sample : I6403-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100492.D
Acq On : 12 Nov 2017 16:20
Operator : SJ/JU
Sample : I6403-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

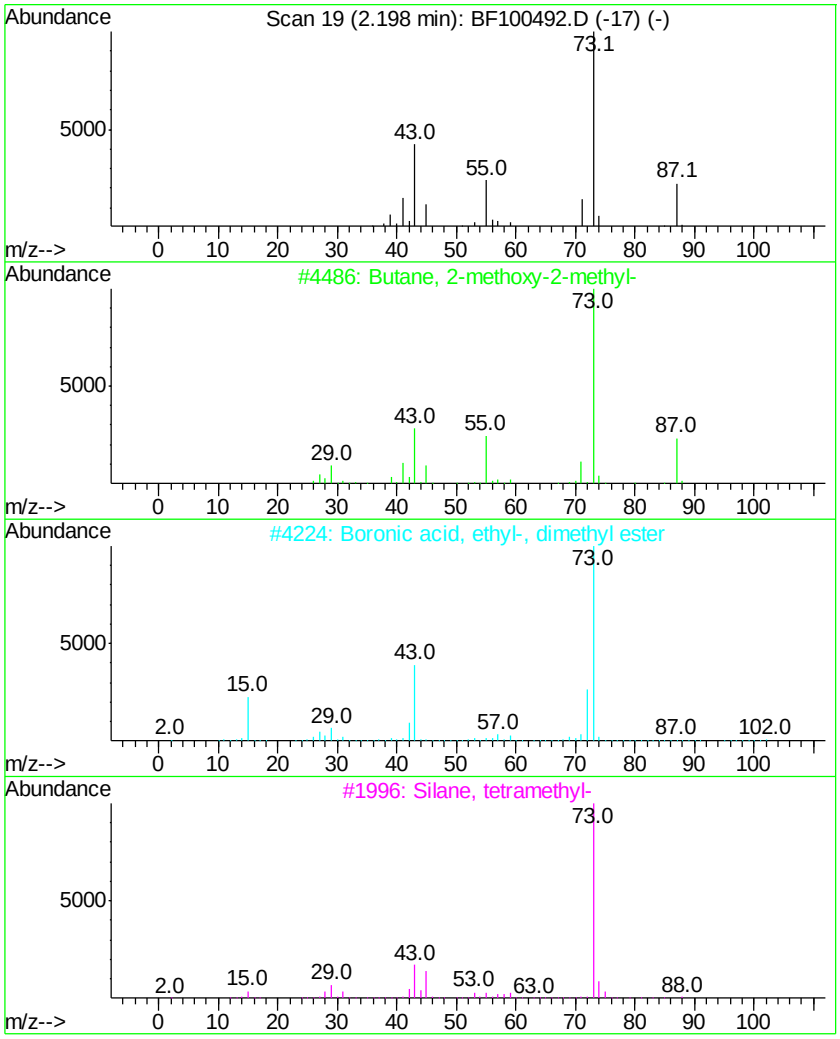
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

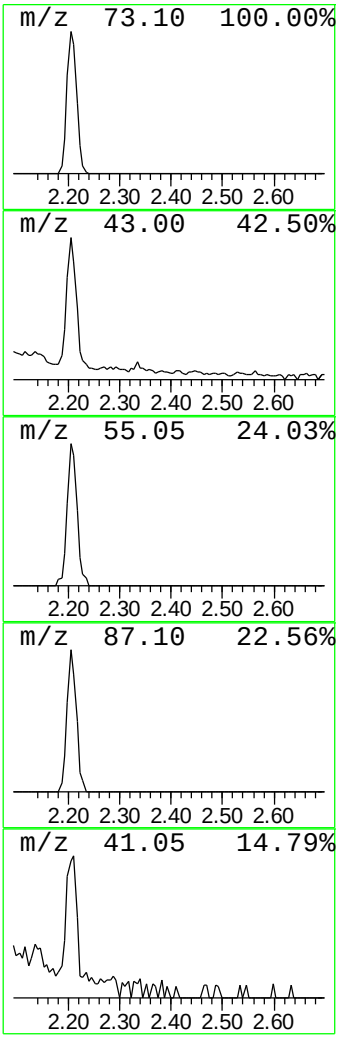
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.20 | 3.32 ng | 130485 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | Boronic acid, ethyl-, dimethyl e... | 102 | C4H11BO2 | 007318-82-3 | 17 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100492.D
Acq On : 12 Nov 2017 16:20
Operator : SJ/JU
Sample : I6403-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

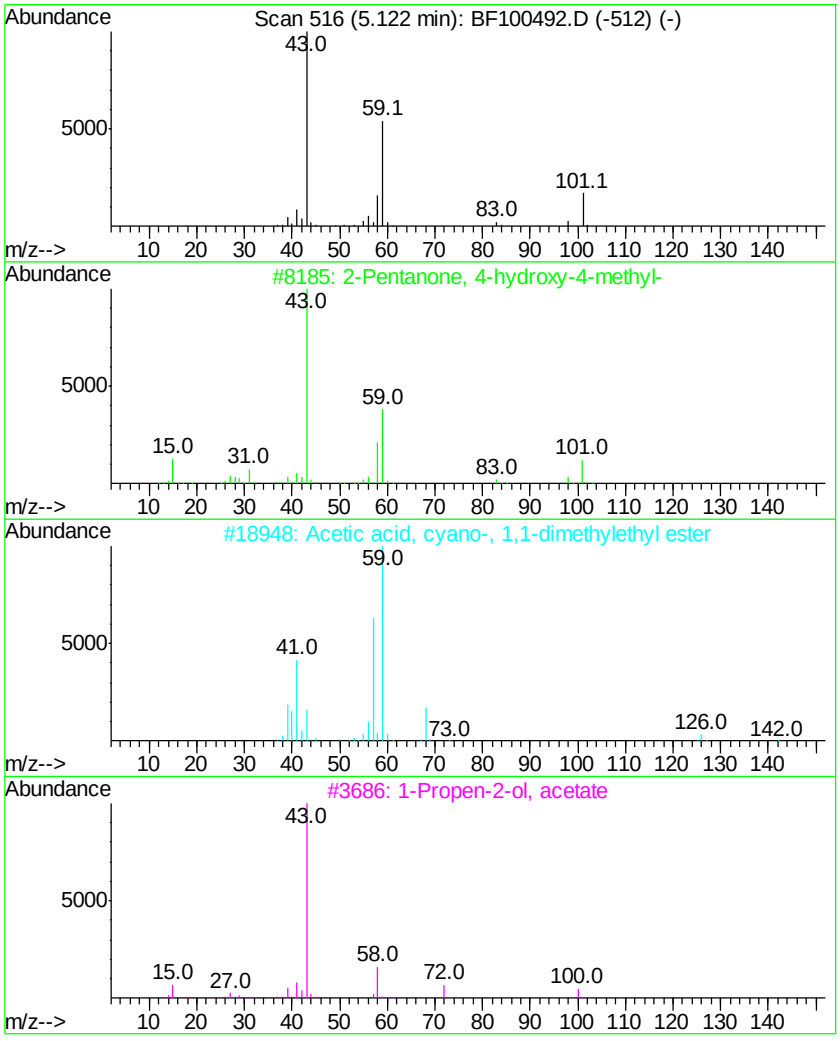
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

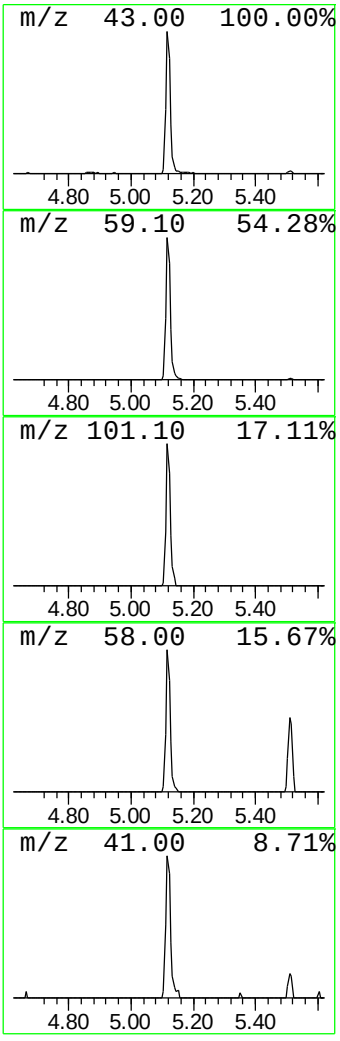
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 5.35 ng | 210304 | 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 | 59 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Hexanamide | 115 | C6H13NO | 000628-02-4 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100492.D
Acq On : 12 Nov 2017 16:20
Operator : SJ/JU
Sample : I6403-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

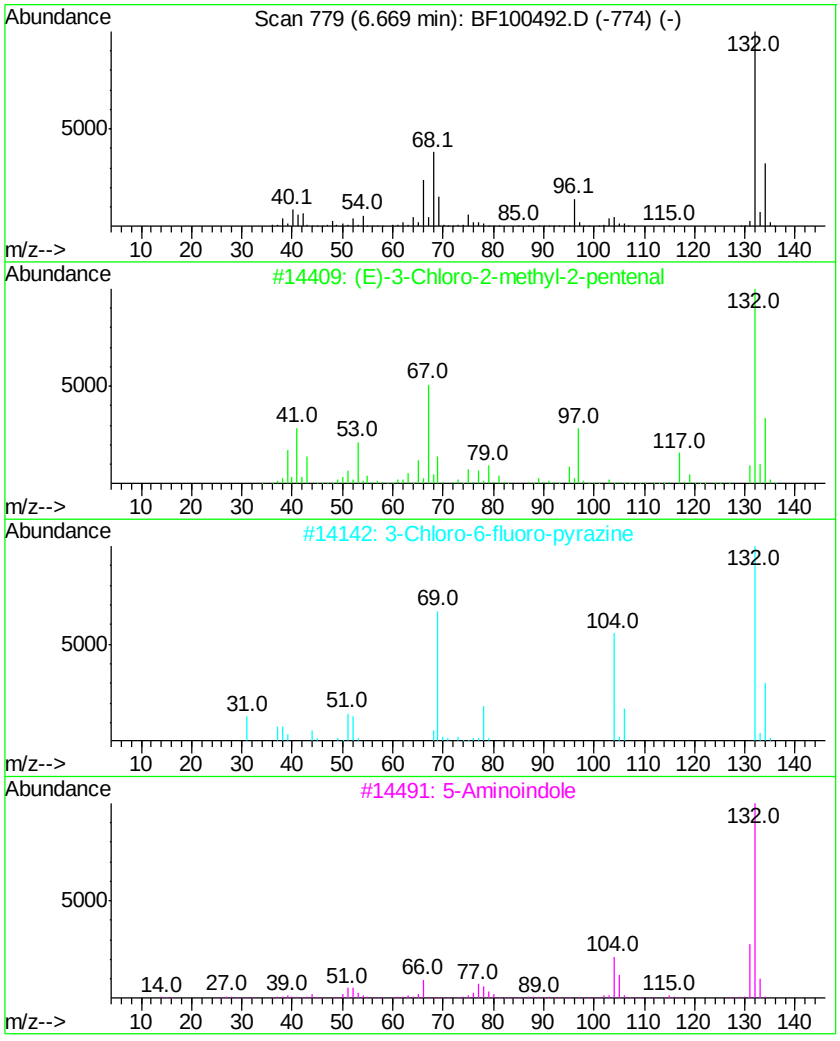
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

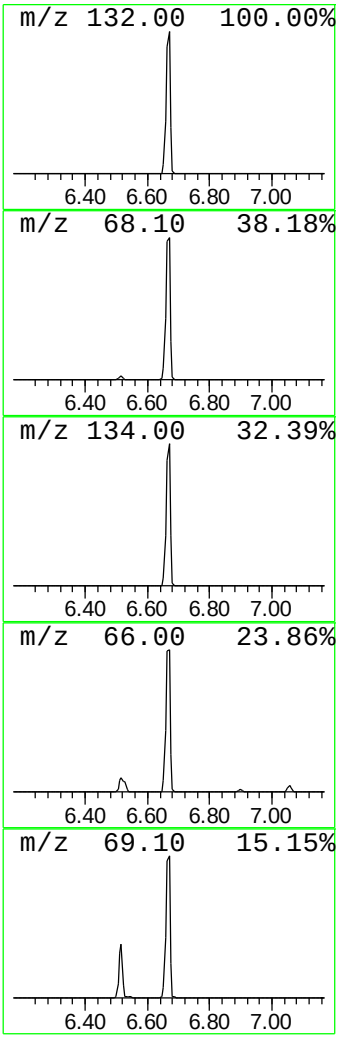
**********

Peak Number 3 unknown6.67 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 48.39 ng | 1903280 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

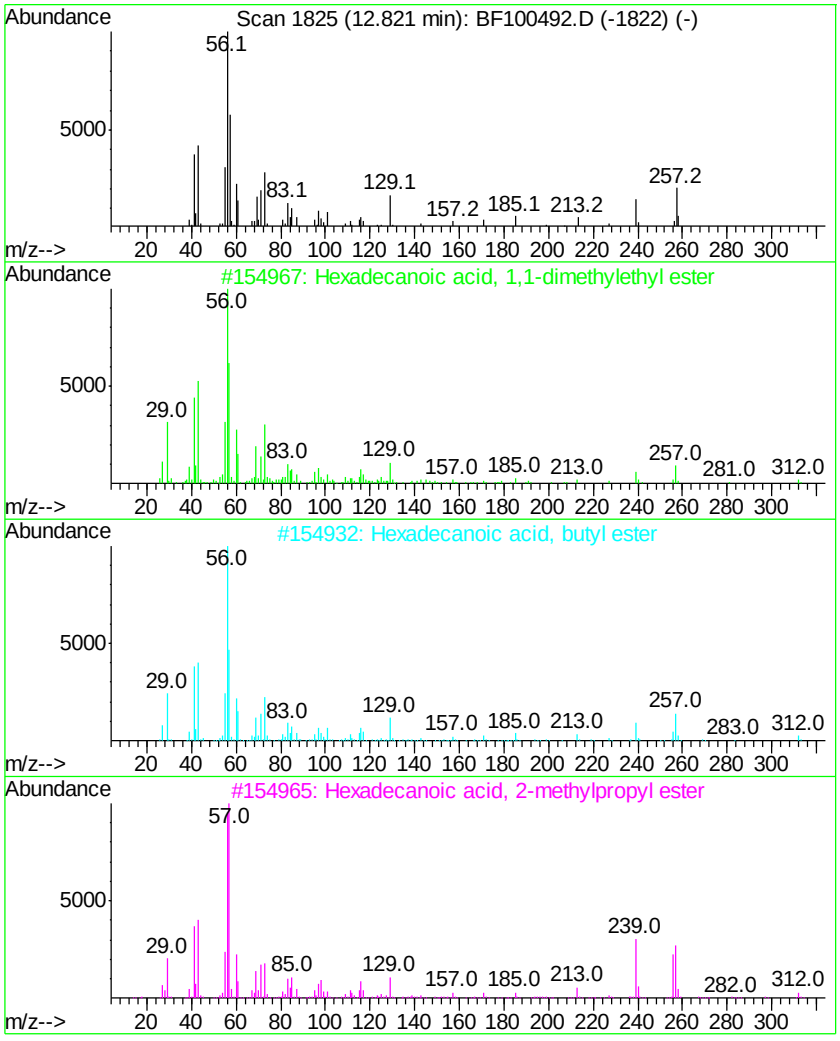
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

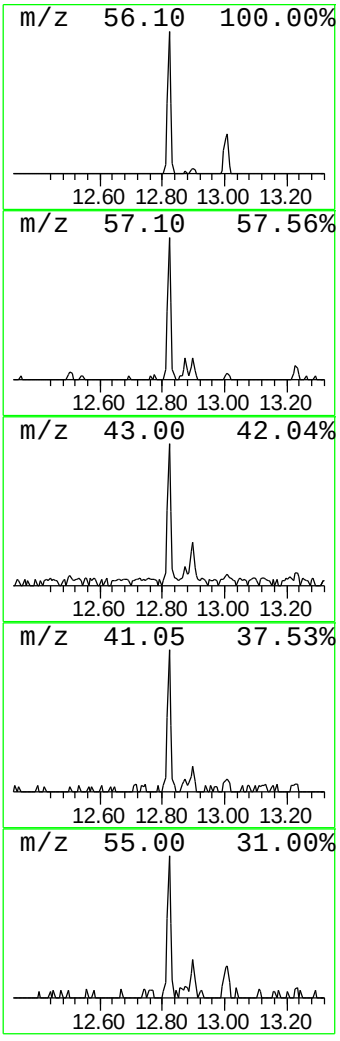
**********

Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.82 | 2.45 ng | 87414 | Chrysene-d12 | 14.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 83 |
| 2 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 83 |
| 3 | Hexadecanoic acid, 2-methylpropy... | 312 | C20H40O2 | 000110-34-9 | 50 |
| 4 | 1-Hexanol, 3,5,5-trimethyl- | 144 | C9H20O | 003452-97-9 | 37 |
| 5 | Cyclohexanol, 4-amino-, trans- | 115 | C6H13NO | 027489-62-9 | 30 |



# Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF111217\
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ALS Vial : 61 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 110817-TIDO-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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... | 2.20 | 3.3 | ng | 130485 | 1 | 6.90 | 786617 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 5.3 | ng | 210304 | 1 | 6.90 | 786617 | 20.0 |
| unknown6.67 | 6.67 | 48.4 | ng | 1903280 | 1 | 6.90 | 786617 | 20.0 |
| Hexadecanoic acid... | 12.82 | 2.5 | ng | 87414 | 5 | 14.06 | 713955 | 20.0 |