LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103208.D
Acq On : 26 Feb 2018 10:34
Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

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-BF022218.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 | 2.175 | 7 | 15 | 22 | rVB | 88107 | 133340 | 3.57% | 0.403% |
| 2 | 5.110 | 511 | 514 | 527 | rVB | 142384 | 191357 | 5.12% | 0.579% |
| 3 | 5.498 | 575 | 580 | 583 | rBV | 3530989 | 3604337 | 96.44% | 10.905% |
| 4 | 6.504 | 746 | 751 | 754 | rBV | 3106336 | 3409629 | 91.23% | 10.316% |
| 5 | 6.639 | 770 | 774 | 777 | rBV | 3659818 | 3517622 | 94.12% | 10.642% |
| 6 | 6.869 | 809 | 813 | 821 | rBV | 1066172 | 898380 | 24.04% | 2.718% |
| 7 | 7.022 | 835 | 839 | 843 | rBV | 2848335 | 2792268 | 74.71% | 8.448% |
| 8 | 7.434 | 904 | 909 | 912 | rBV | 2367794 | 2336925 | 62.53% | 7.070% |
| 9 | 8.151 | 1027 | 1031 | 1049 | rBV | 1280770 | 1220369 | 32.65% | 3.692% |
| 10 | 9.227 | 1209 | 1214 | 1217 | rBV | 3634462 | 3737544 | 100.00% | 11.308% |
| 11 | 9.910 | 1325 | 1330 | 1345 | rBV | 1234770 | 1290211 | 34.52% | 3.904% |
| 12 | 10.698 | 1460 | 1464 | 1480 | rBV | 2098600 | 2251710 | 60.25% | 6.812% |
| 13 | 11.398 | 1579 | 1583 | 1597 | rBV | 1343574 | 1277679 | 34.18% | 3.866% |
| 14 | 12.792 | 1816 | 1820 | 1823 | rBV | 363085 | 319559 | 8.55% | 0.967% |
| 15 | 12.868 | 1830 | 1833 | 1839 | rVB | 50145 | 43787 | 1.17% | 0.132% |
| 16 | 12.986 | 1848 | 1853 | 1856 | rBV | 3388205 | 3533385 | 94.54% | 10.690% |
| 17 | 13.492 | 1936 | 1939 | 1944 | rBV | 276692 | 250834 | 6.71% | 0.759% |
| 18 | 14.045 | 2028 | 2033 | 2042 | rBV | 1030645 | 1152725 | 30.84% | 3.488% |
| 19 | 14.186 | 2053 | 2057 | 2060 | rBV | 46540 | 40687 | 1.09% | 0.123% |
| 20 | 14.804 | 2159 | 2162 | 2167 | rVB | 47199 | 43677 | 1.17% | 0.132% |
| 21 | 15.145 | 2216 | 2220 | 2224 | rBV2 | 37748 | 41876 | 1.12% | 0.127% |
| 22 | 15.533 | 2280 | 2286 | 2298 | rBV | 644870 | 964730 | 25.81% | 2.919% |

Sum of corrected areas: 33052631

LSC Report - Integrated Chromatogram

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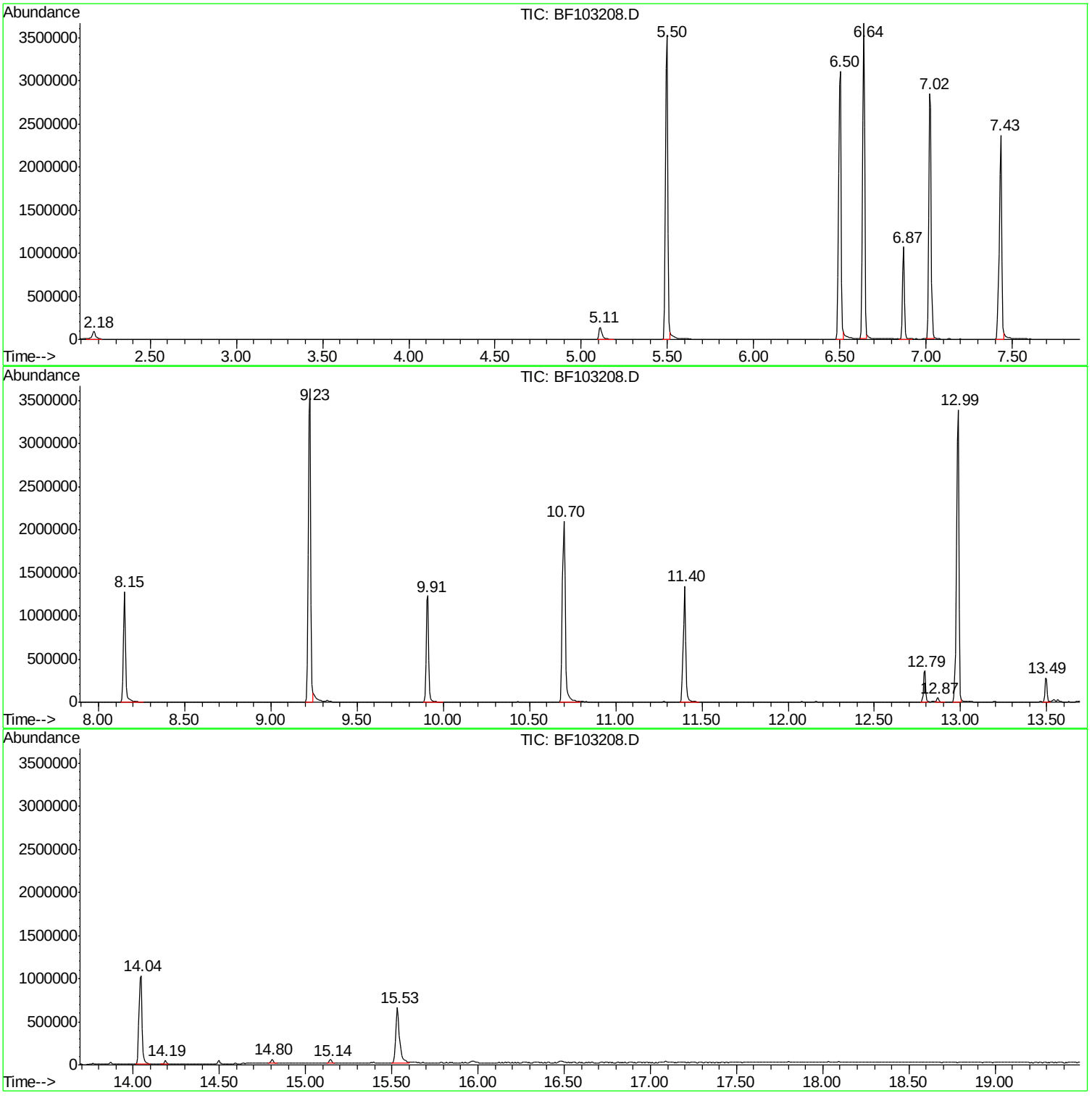
Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103208.D
Acq On : 26 Feb 2018 10:34
Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

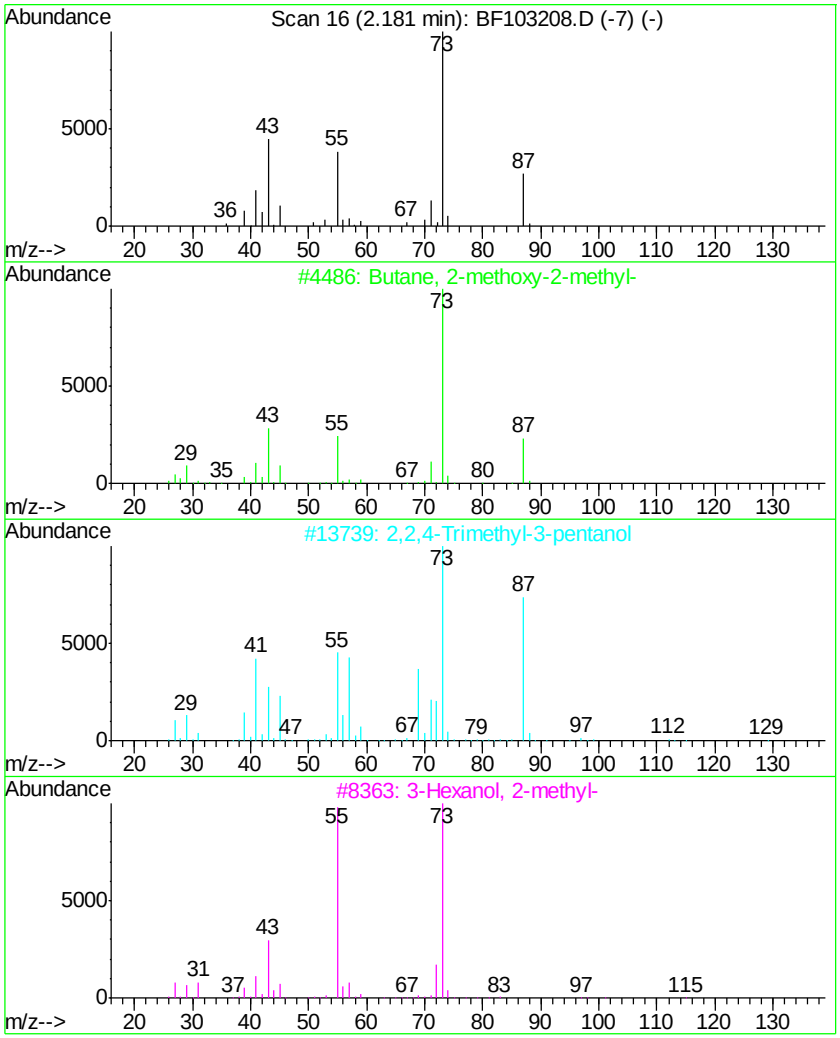
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

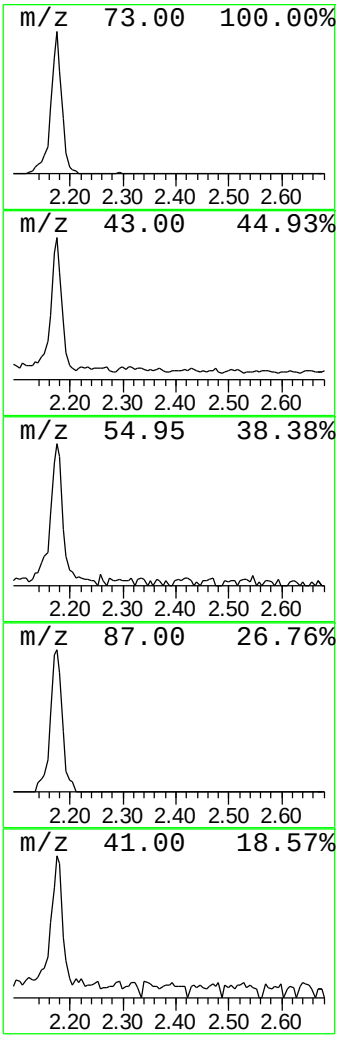
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.18 | 2.97 ng | 133340 | 1,4-Dichlorobenzene-d4 | 6.87 |

| 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 | 39 |
| 3 | 3-Hexanol, 2-methyl- | 116 | C7H16O | 000617-29-8 | 25 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 5 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 25 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103208.D
Acq On : 26 Feb 2018 10:34
Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

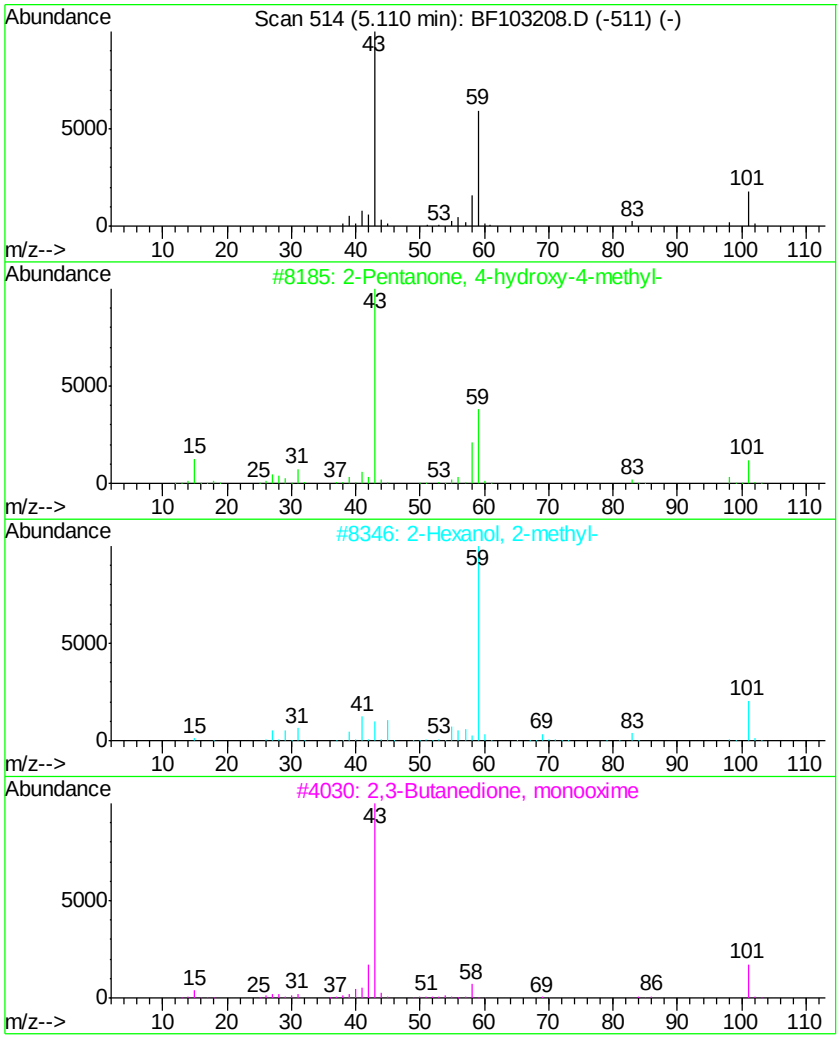
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

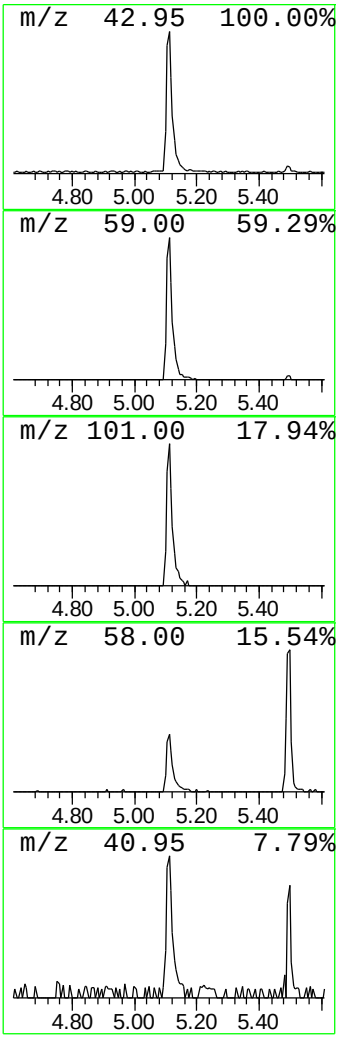
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 4.26 ng | 191357 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 27 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 23 |
| 5 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103208.D
Acq On : 26 Feb 2018 10:34
Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

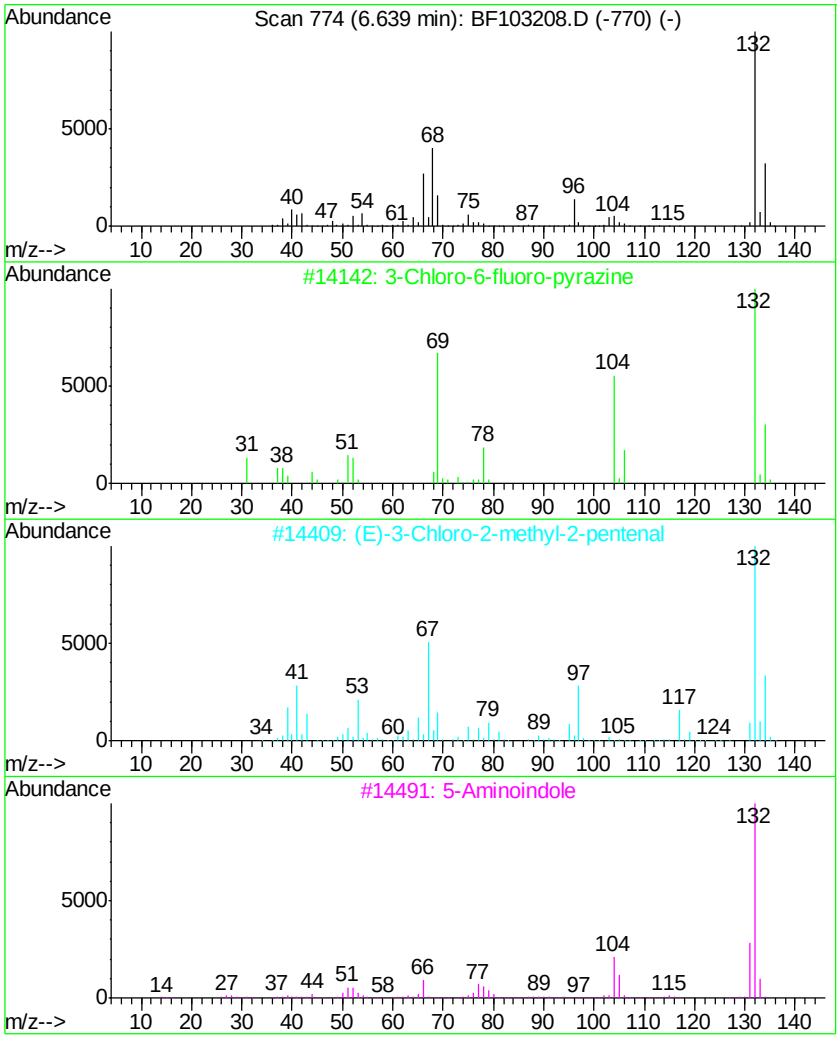
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

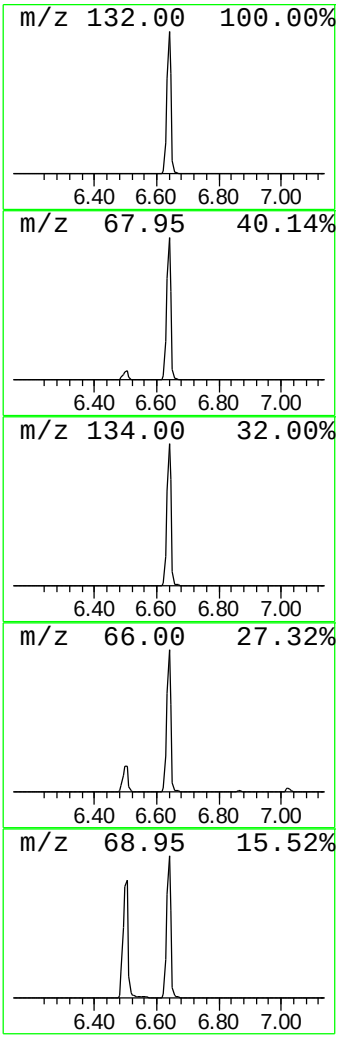
**********

Peak Number 3 unknown6.64 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.64 | 78.31 ng | 3517620 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



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Operator : SJ/JU
Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

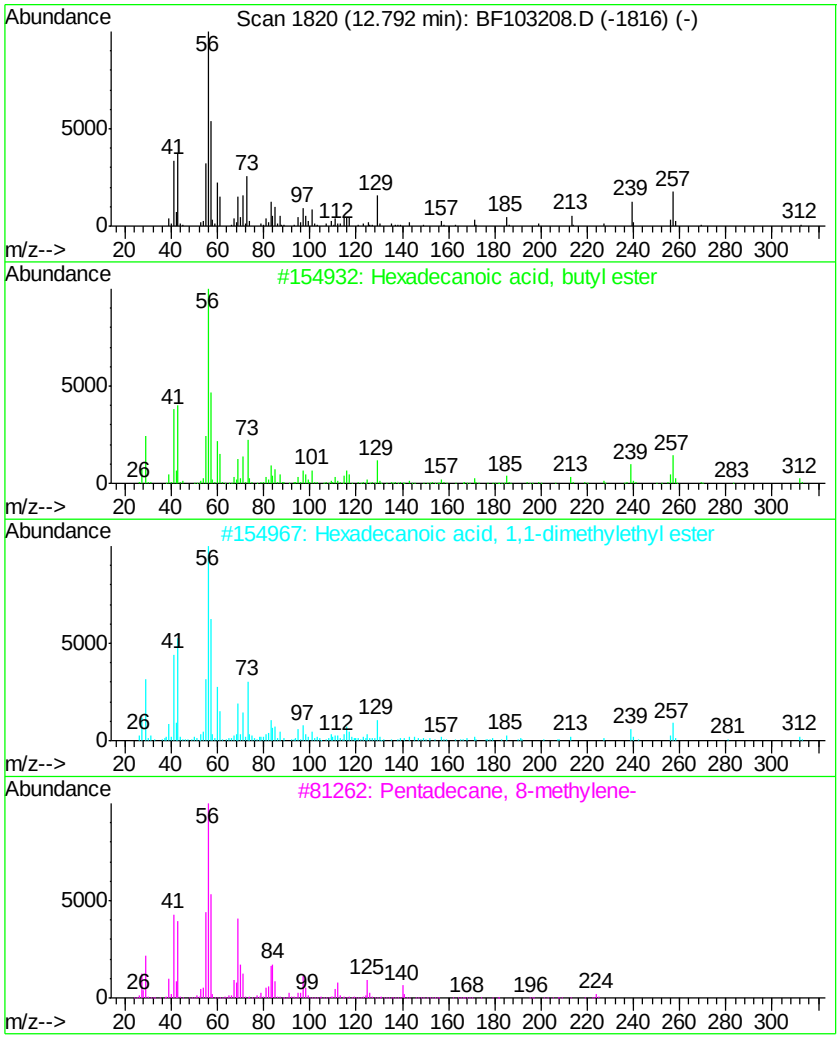
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

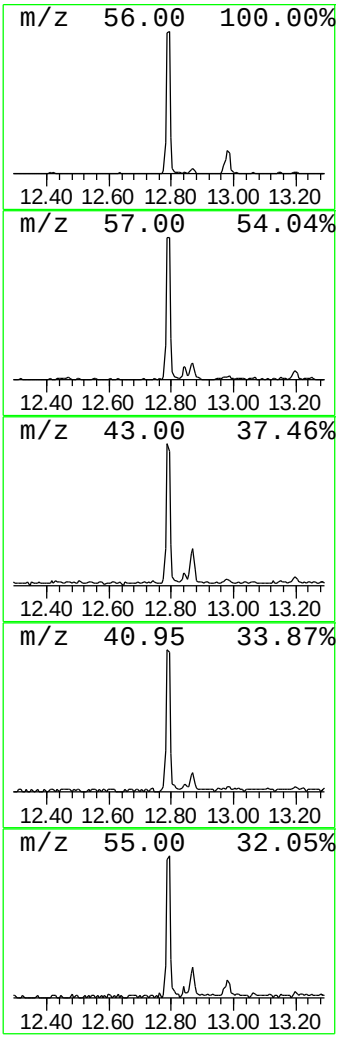
**********

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.79 | 5.54 ng | 319559 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 91 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 91 |
| 3 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 43 |
| 4 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 38 |
| 5 | Cyclopentanecarboxylic acid, 2-a... | 129 | C6H11NO2 | 040482-05-1 | 38 |



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Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PB106778BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

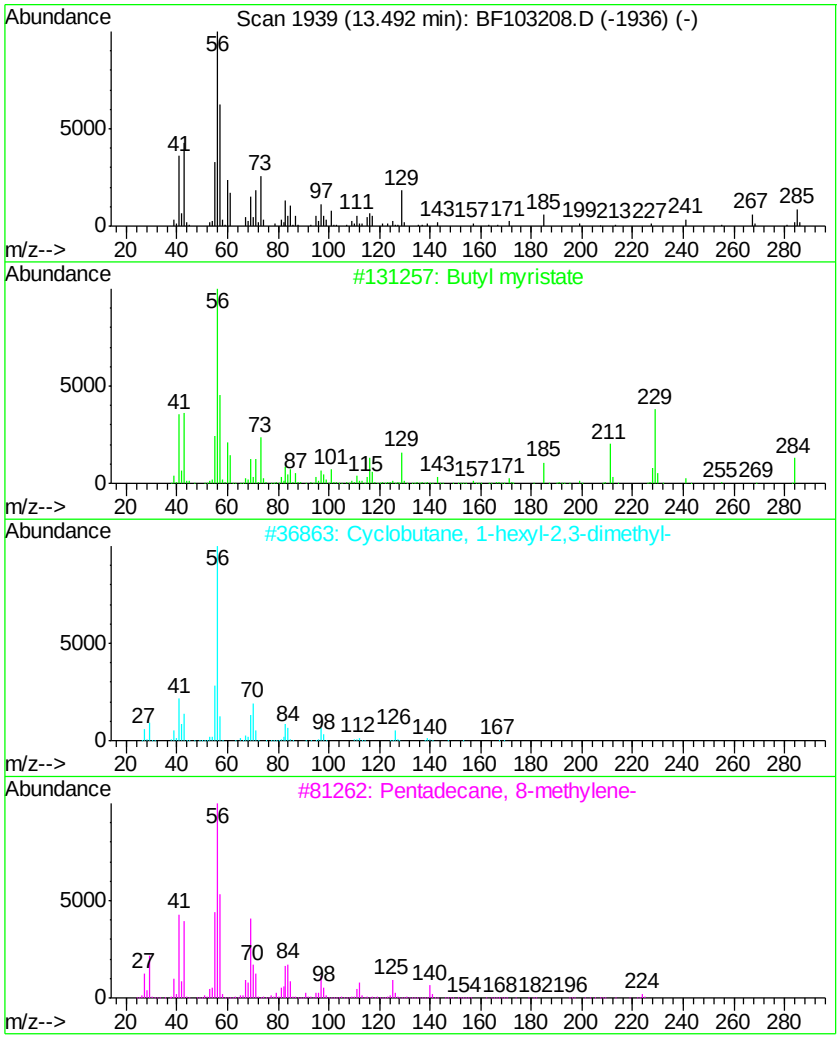
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

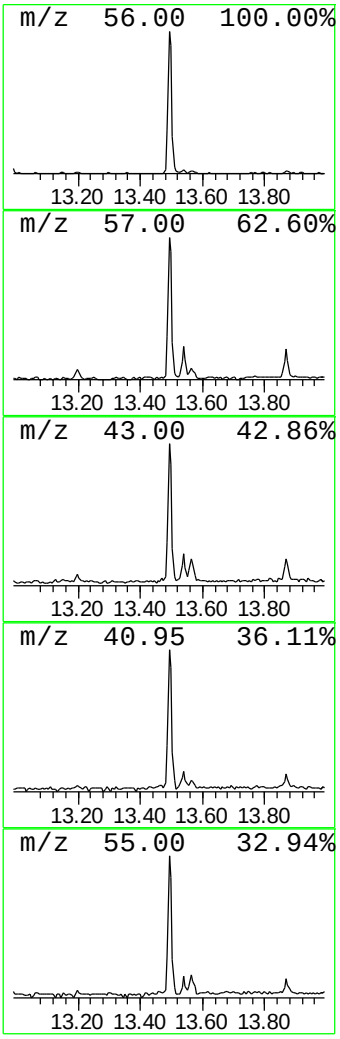
**********

Peak Number 6 Butyl myristate Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.49 | 4.35 ng | 250834 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 90 |
| 2 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 38 |
| 3 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 37 |
| 4 | Cyclohexane, (1,1-dimethylethyl)- | 140 | C10H20 | 003178-22-1 | 35 |
| 5 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 35 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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Sample : PB106778BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
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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... | 2.18 | 3.0 | ng | 133340 | 1 | 6.87 | 898380 | 20.0 |
| 2-Pentanone, 4-hy... | 5.11 | 4.3 | ng | 191357 | 1 | 6.87 | 898380 | 20.0 |
| unknown6.64 | 6.64 | 78.3 | ng | 3517620 | 1 | 6.87 | 898380 | 20.0 |
| Hexadecanoic acid... | 12.79 | 5.5 | ng | 319559 | 5 | 14.04 | 1152730 | 20.0 |
| Butyl myristate | 13.49 | 4.3 | ng | 250834 | 5 | 14.04 | 1152730 | 20.0 |