LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033507.D
Acq On : 17 Dec 2021 15:52
Operator : CG/JU
Sample : M5064-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SASP2-121-1-(17-32)

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_M\Methods\8270-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033507.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.037 | 301 | 306 | 315 | rBV | 286467 | 424678 | 16.59% | 2.786% |
| 2 | 5.502 | 378 | 385 | 400 | rBV | 1082553 | 1590761 | 62.14% | 10.434% |
| 3 | 6.119 | 484 | 490 | 499 | rBV | 31569 | 48883 | 1.91% | 0.321% |
| 4 | 7.107 | 651 | 658 | 677 | rBV | 1072805 | 1814761 | 70.89% | 11.903% |
| 5 | 7.937 | 792 | 799 | 806 | rBV | 229607 | 365902 | 14.29% | 2.400% |
| 6 | 9.107 | 989 | 998 | 1012 | rBV | 692751 | 1196384 | 46.74% | 7.847% |
| 7 | 10.537 | 1236 | 1241 | 1252 | rBV2 | 24095 | 52653 | 2.06% | 0.345% |
| 8 | 10.748 | 1268 | 1277 | 1284 | rBV | 287567 | 498377 | 19.47% | 3.269% |
| 9 | 13.207 | 1688 | 1695 | 1704 | rBV | 1686964 | 2453701 | 95.85% | 16.094% |
| 10 | 14.583 | 1922 | 1929 | 1942 | rVB | 437021 | 648336 | 25.33% | 4.253% |
| 11 | 16.071 | 2176 | 2182 | 2196 | rBV | 1244741 | 1779369 | 69.51% | 11.671% |
| 12 | 17.330 | 2390 | 2396 | 2403 | rBV | 493159 | 699071 | 27.31% | 4.585% |
| 13 | 18.218 | 2543 | 2547 | 2558 | rBV | 79520 | 115648 | 4.52% | 0.759% |
| 14 | 19.495 | 2760 | 2764 | 2769 | rBV4 | 25791 | 37176 | 1.45% | 0.244% |
| 15 | 19.948 | 2836 | 2841 | 2852 | rBV | 1973819 | 2559857 | 100.00% | 16.791% |
| 16 | 21.206 | 3052 | 3055 | 3062 | rVB | 98370 | 122439 | 4.78% | 0.803% |
| 17 | 21.506 | 3101 | 3106 | 3115 | rBV | 335886 | 462150 | 18.05% | 3.031% |
| 18 | 23.924 | 3511 | 3517 | 3528 | rVB2 | 181142 | 375574 | 14.67% | 2.463% |

Sum of corrected areas: 15245720

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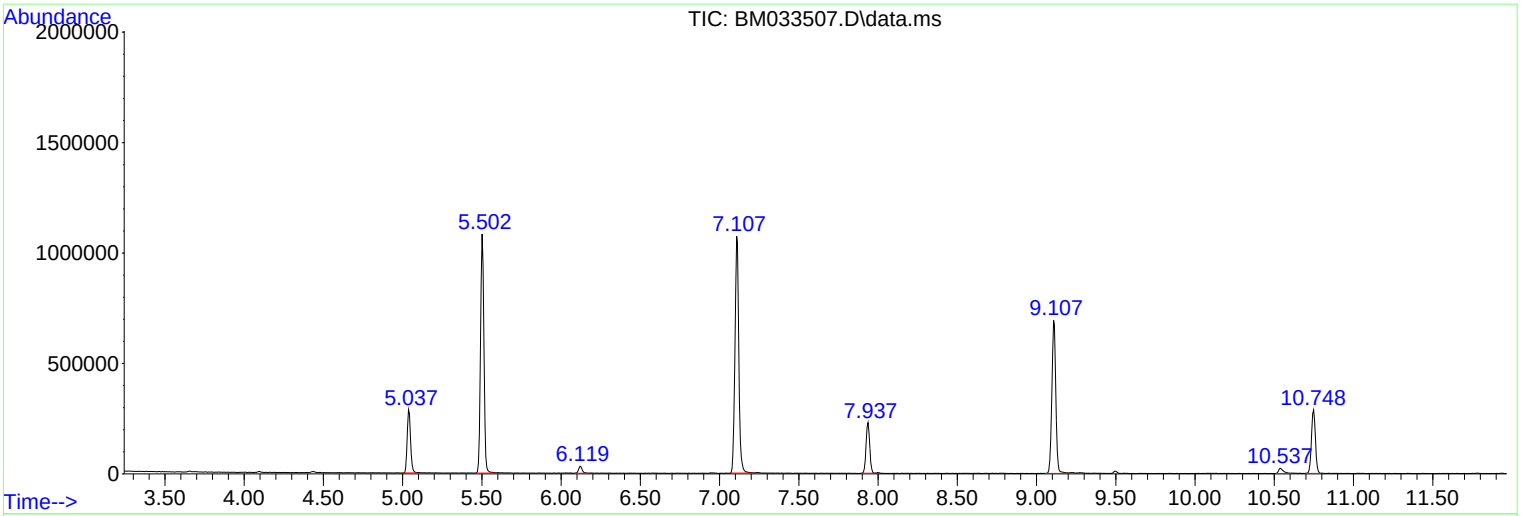
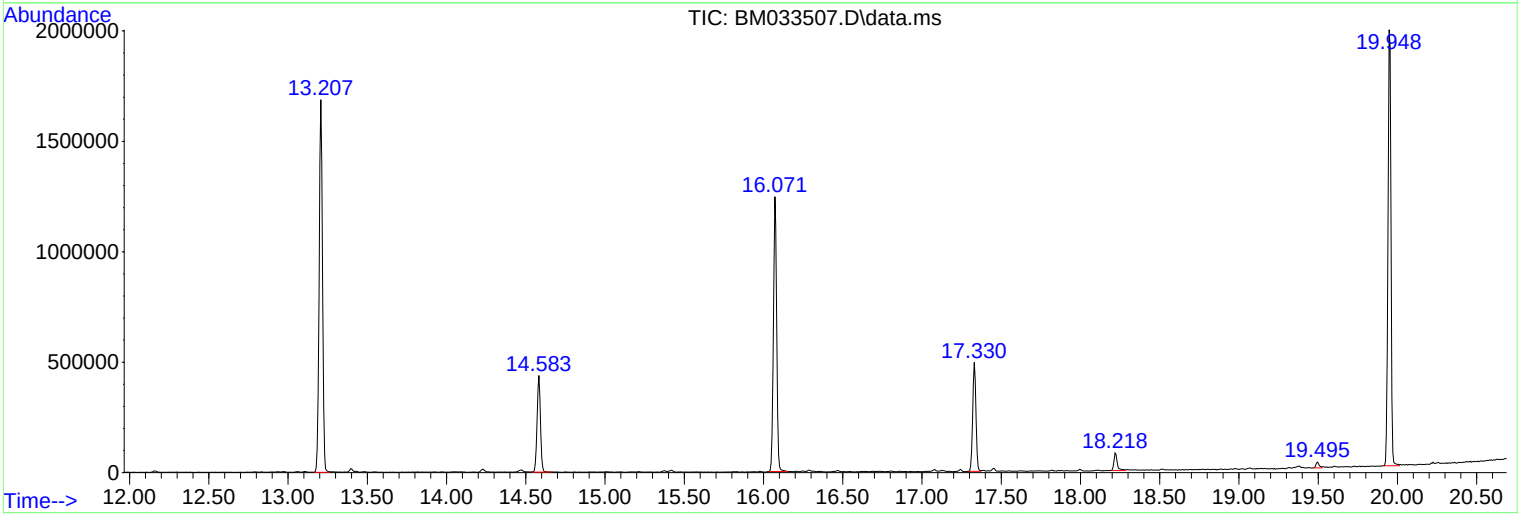
ALS Vial : 12 Sample Multiplier: 1

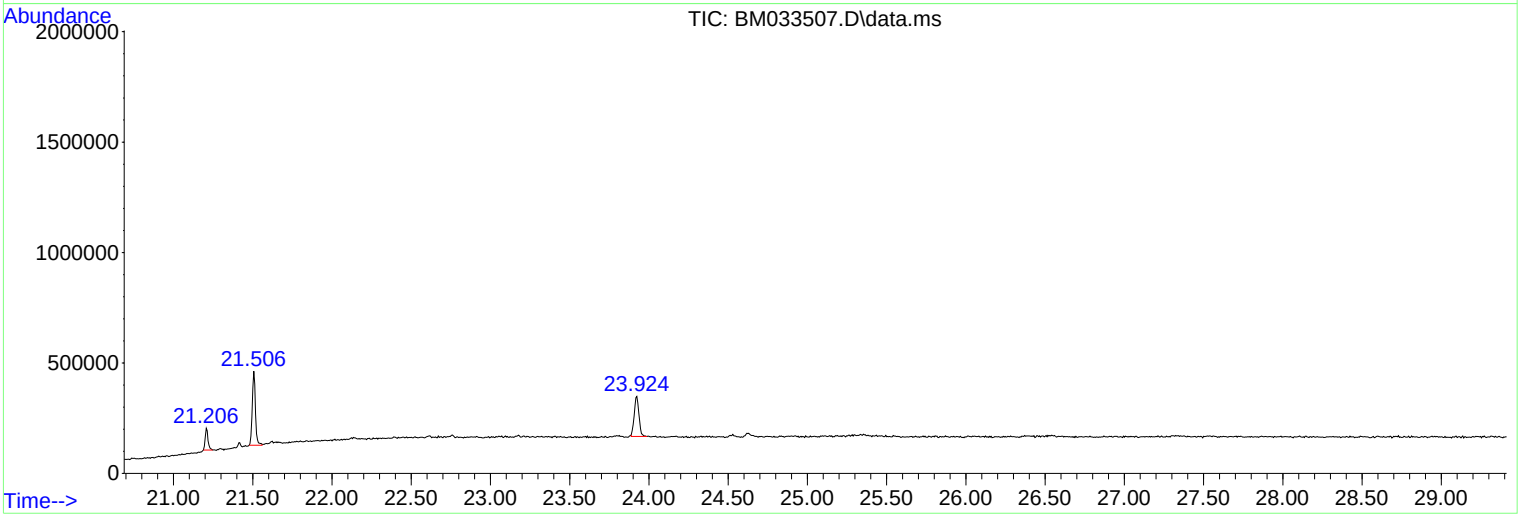
**Instrument :**
BNA_M
**ClientSampleId :**
SASP2-121-1-(17-32)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BM033507.D
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**Instrument :**
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**ClientSampleId :**
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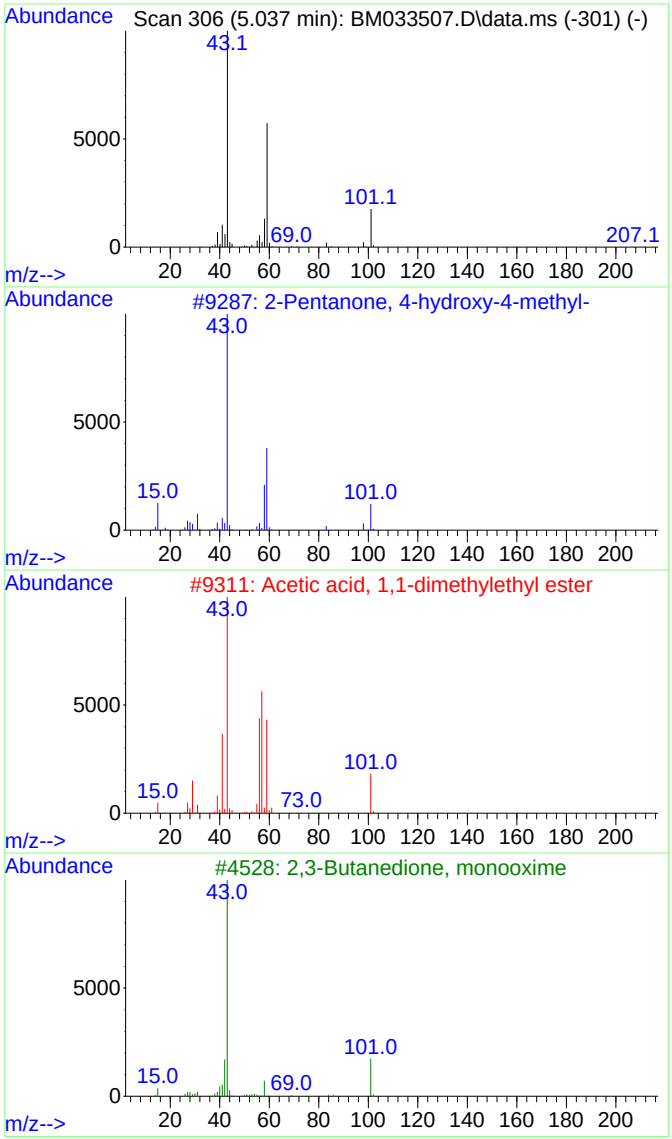
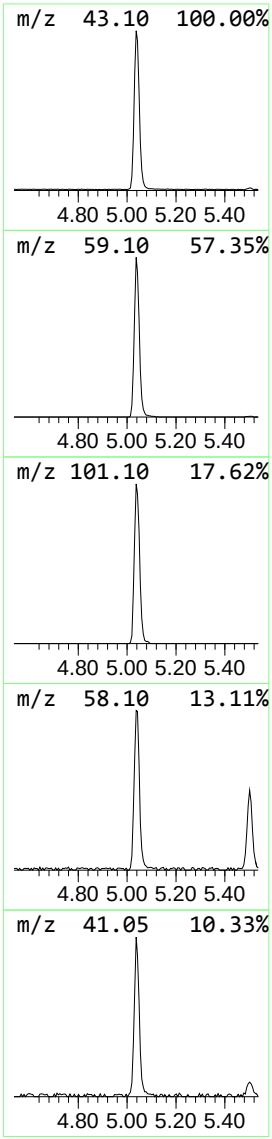
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.037 | 23.21 ng | 424678 | 1,4-Dichlorobenzene-d4 | 7.937 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 5 | Butane | 58 | C4H10 | 000106-97-8 | 9 |



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Operator : CG/JU
Sample : M5064-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SASP2-121-1-(17-32)

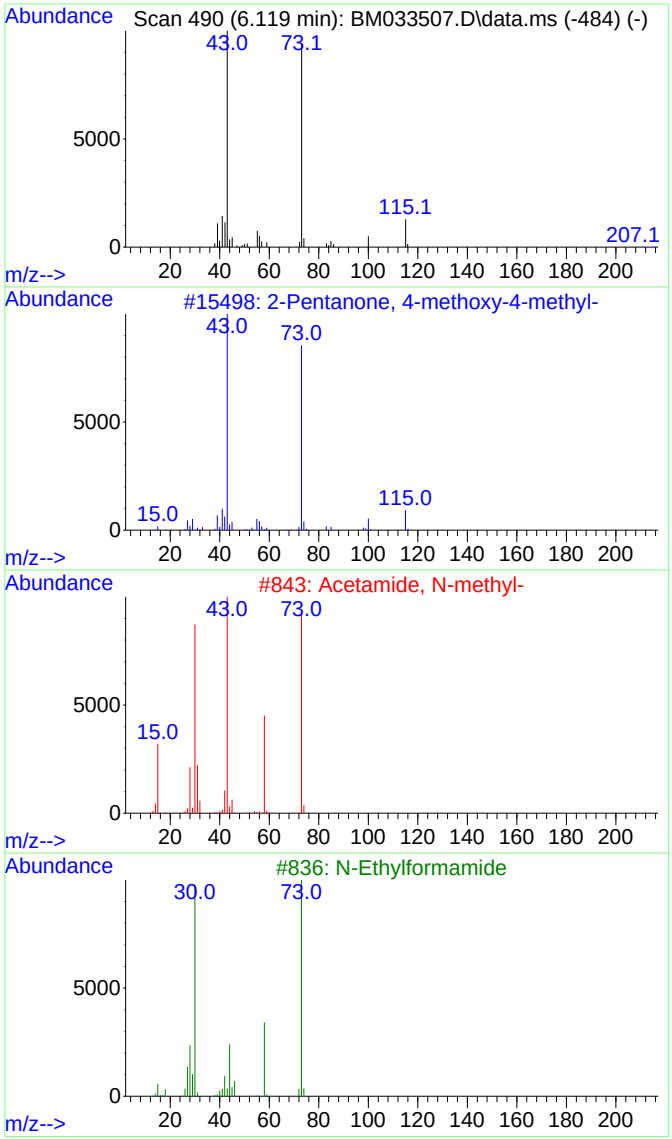
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

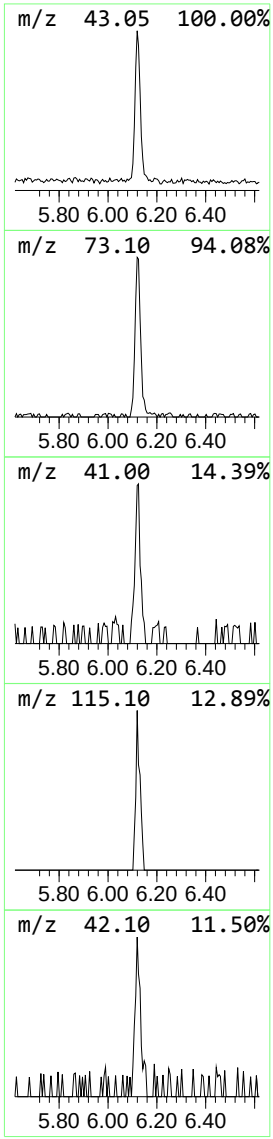
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.119 | 2.67 ng | 48883 | 1,4-Dichlorobenzene-d4 | 7.937 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 78 |
| 2 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 52 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 23 |
| 4 | 1-Methoxyethanimine, N-acetyl- | 115 | C5H9NO2 | 099028-43-0 | 23 |
| 5 | 3,4-Hexanediol, 2,5-dimethyl- | 146 | C8H18O2 | 022607-11-0 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033507.D
Acq On : 17 Dec 2021 15:52
Operator : CG/JU
Sample : M5064-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SASP2-121-1-(17-32)

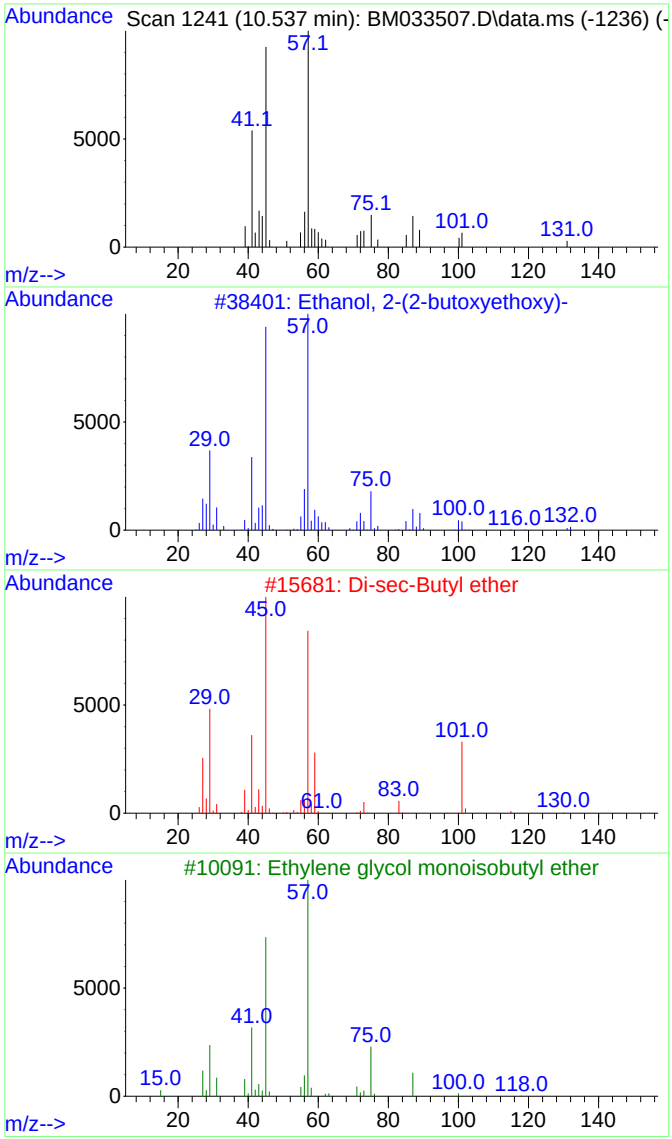
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

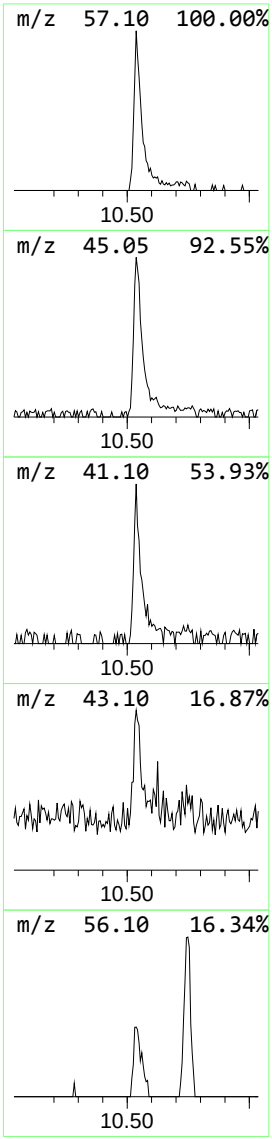
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.537 | 2.11 ng | 52653 | Naphthalene-d8 | 10.748 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Di-sec-Butyl ether | 130 | C8H18O | 006863-58-7 | 59 |
| 3 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 50 |
| 4 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 50 |
| 5 | 3,6,9,12-Tetraoxatetradeca-1,13-... | 202 | C10H18O4 | 000765-12-8 | 45 |



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Operator : CG/JU
Sample : M5064-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

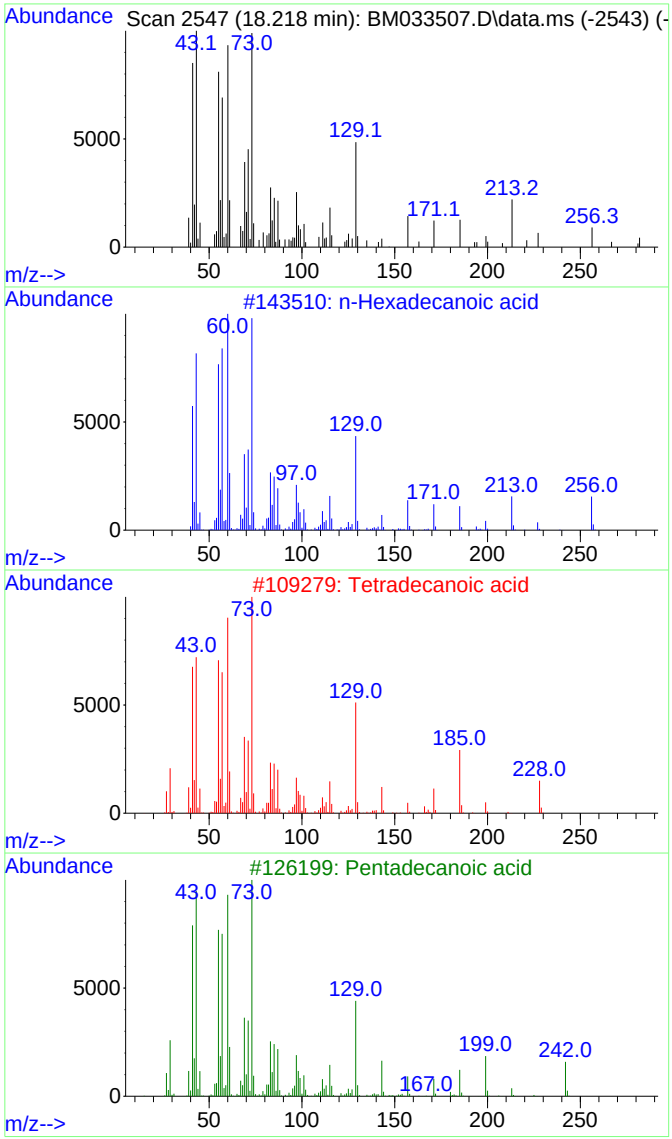
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

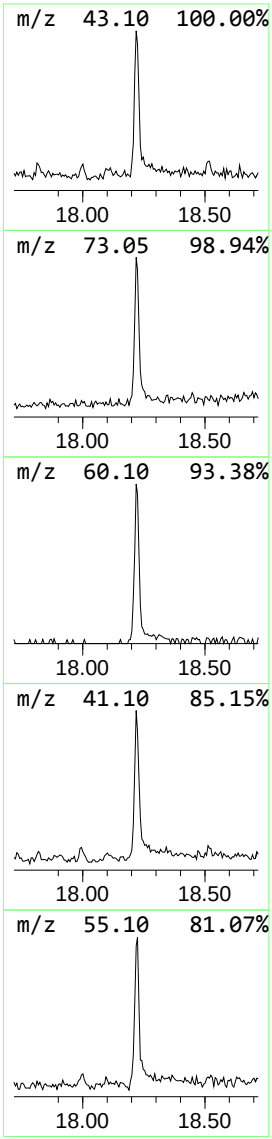
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.218 | 3.31 ng | 115648 | Phenanthrene-d10 | 17.330 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 74 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 72 |
| 5 | Oxalic acid, dodecyl propyl ester | 300 | C17H32O4 | 1000309-26-5 | 18 |



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Sample : M5064-04
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ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_M
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SASP2-121-1-(17-32)

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TIC Library : C:\Database\NIST20.L
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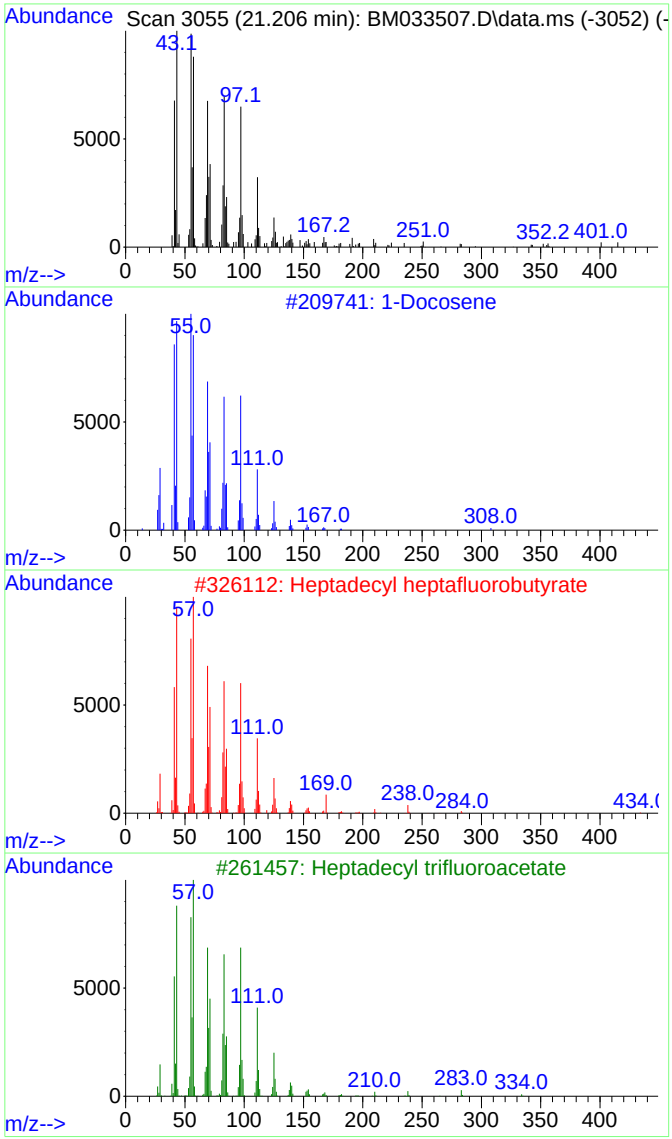
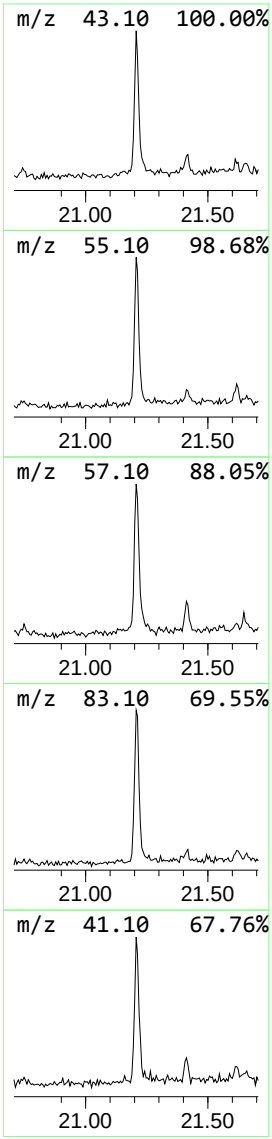
**********

Peak Number 5 1-Docosene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.206 | 5.30 ng | 122439 | Chrysene-d12 | 21.506 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 95 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 3 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1010351-87-0 | 94 |
| 4 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 94 |
| 5 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |



Tentatively Identified Compound (LSC) summary

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| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 5.037 | 23.2 | ng | 424678 | 1 | 7.937 | 365902 | 20.0 |
| 2-Pentanone, 4-... | 6.119 | 2.7 | ng | 48883 | 1 | 7.937 | 365902 | 20.0 |
| Ethanol, 2-(2-b... | 10.537 | 2.1 | ng | 52653 | 2 | 10.748 | 498377 | 20.0 |
| n-Hexadecanoic ... | 18.218 | 3.3 | ng | 115648 | 4 | 17.330 | 699071 | 20.0 |
| 1-Docosene | 21.206 | 5.3 | ng | 122439 | 5 | 21.506 | 462150 | 20.0 |