LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
Data File : BM042591.D
Acq On : 04 Nov 2023 14:53
Operator : MA/JU
Sample : 05234-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SP-A

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-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042591.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.446 | 378 | 384 | 396 | rBV | 631536 | 935391 | 34.98% | 6.956% |
| 2 | 7.075 | 654 | 661 | 678 | rBV | 590654 | 983476 | 36.78% | 7.313% |
| 3 | 7.910 | 797 | 803 | 812 | rBV | 181332 | 286701 | 10.72% | 2.132% |
| 4 | 9.110 | 1000 | 1007 | 1023 | rBV | 372864 | 622208 | 23.27% | 4.627% |
| 5 | 10.728 | 1272 | 1282 | 1296 | rBV | 211418 | 368912 | 13.80% | 2.743% |
| 6 | 13.186 | 1693 | 1700 | 1712 | rBV | 870157 | 1281203 | 47.91% | 9.528% |
| 7 | 13.410 | 1731 | 1738 | 1747 | rBV | 309088 | 475962 | 17.80% | 3.539% |
| 8 | 14.563 | 1928 | 1934 | 1940 | rBV | 338697 | 490625 | 18.35% | 3.648% |
| 9 | 15.298 | 2055 | 2059 | 2064 | rBV2 | 29543 | 39648 | 1.48% | 0.295% |
| 10 | 15.398 | 2070 | 2076 | 2080 | rBV6 | 16715 | 32520 | 1.22% | 0.242% |
| 11 | 16.057 | 2183 | 2188 | 2197 | rBV | 890085 | 1280183 | 47.88% | 9.520% |
| 12 | 17.315 | 2397 | 2402 | 2408 | rBV | 473816 | 657910 | 24.60% | 4.892% |
| 13 | 18.168 | 2543 | 2547 | 2553 | rBV | 520728 | 701720 | 26.24% | 5.218% |
| 14 | 19.303 | 2737 | 2740 | 2742 | rBV2 | 96053 | 105558 | 3.95% | 0.785% |
| 15 | 19.445 | 2760 | 2764 | 2777 | rBV | 355672 | 534328 | 19.98% | 3.973% |
| 16 | 19.933 | 2842 | 2847 | 2852 | rBV | 2279291 | 2673962 | 100.00% | 19.885% |
| 17 | 21.156 | 3053 | 3055 | 3065 | rVB | 155794 | 245779 | 9.19% | 1.828% |
| 18 | 21.497 | 3109 | 3113 | 3120 | rVB | 693960 | 848737 | 31.74% | 6.312% |
| 19 | 23.915 | 3518 | 3524 | 3532 | rVB | 446981 | 882589 | 33.01% | 6.563% |

Sum of corrected areas: 13447412

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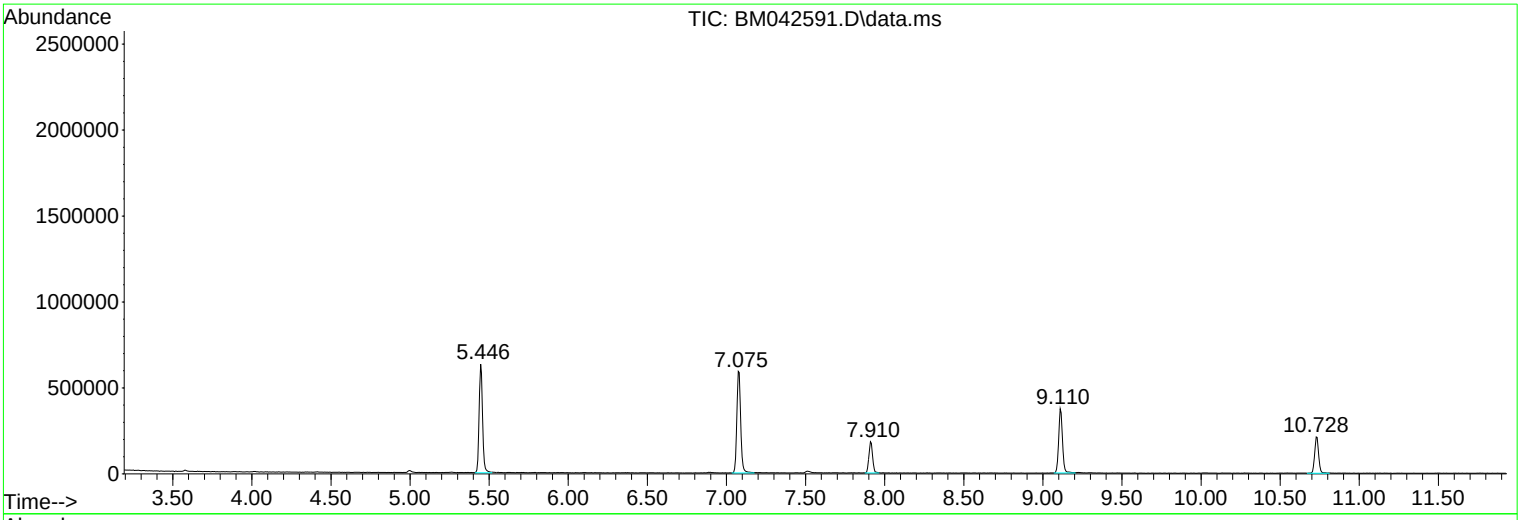
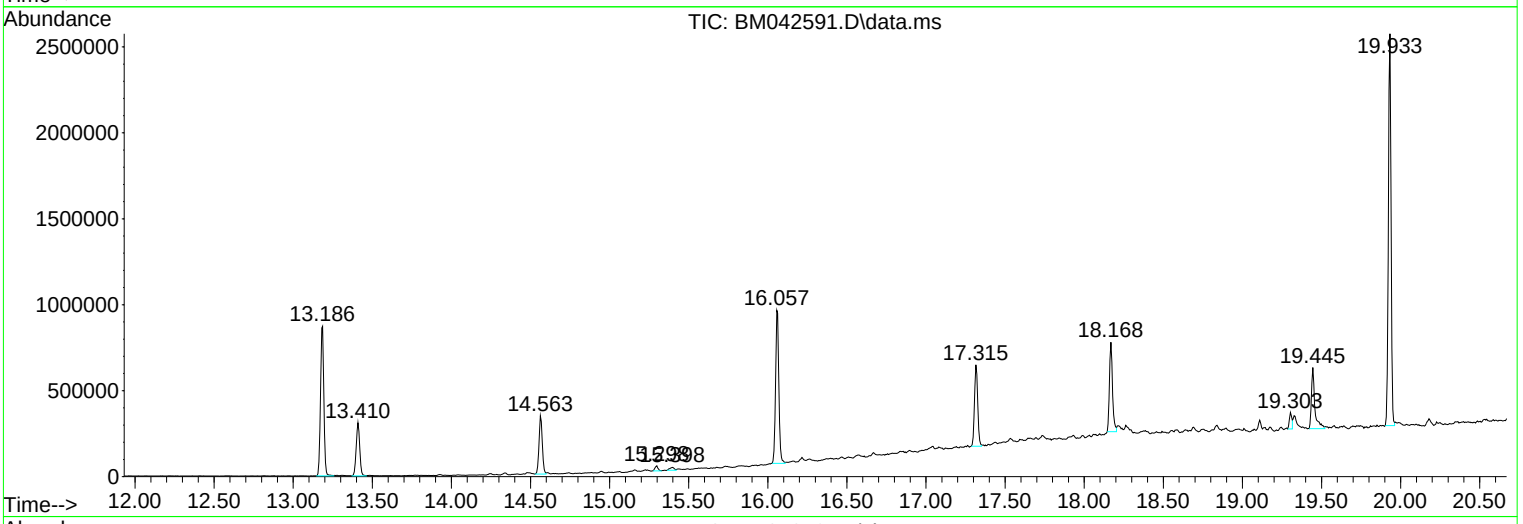
ALS Vial : 8 Sample Multiplier: 1

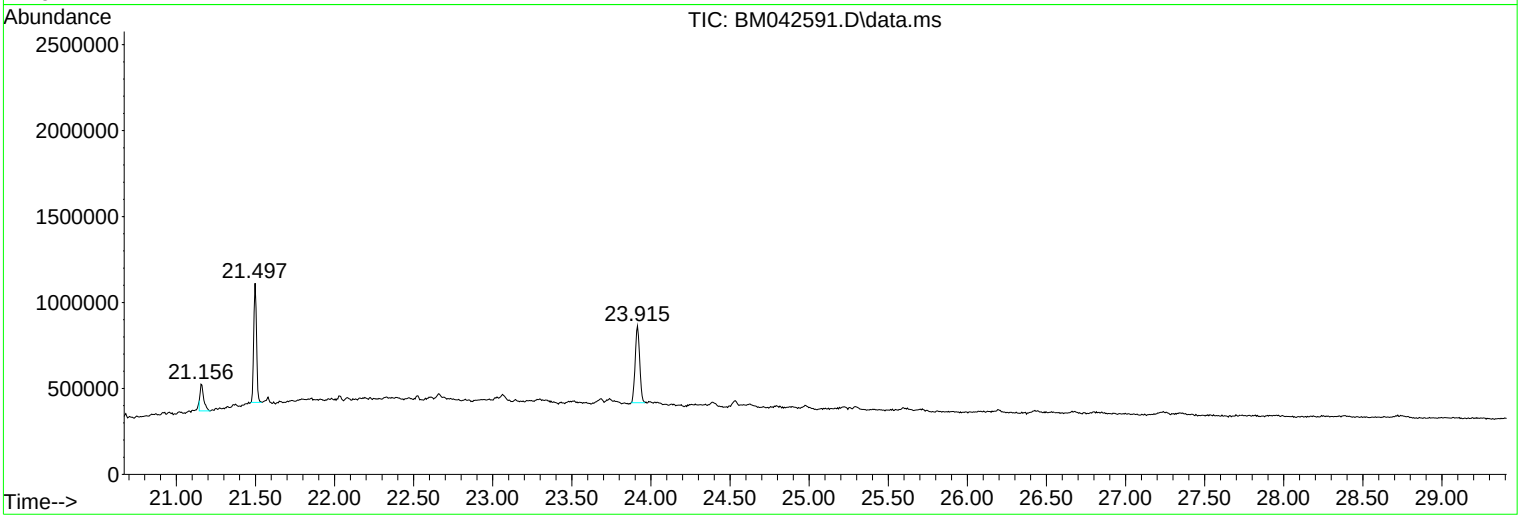
**Instrument :**
BNA_M
**ClientSampleId :**
SP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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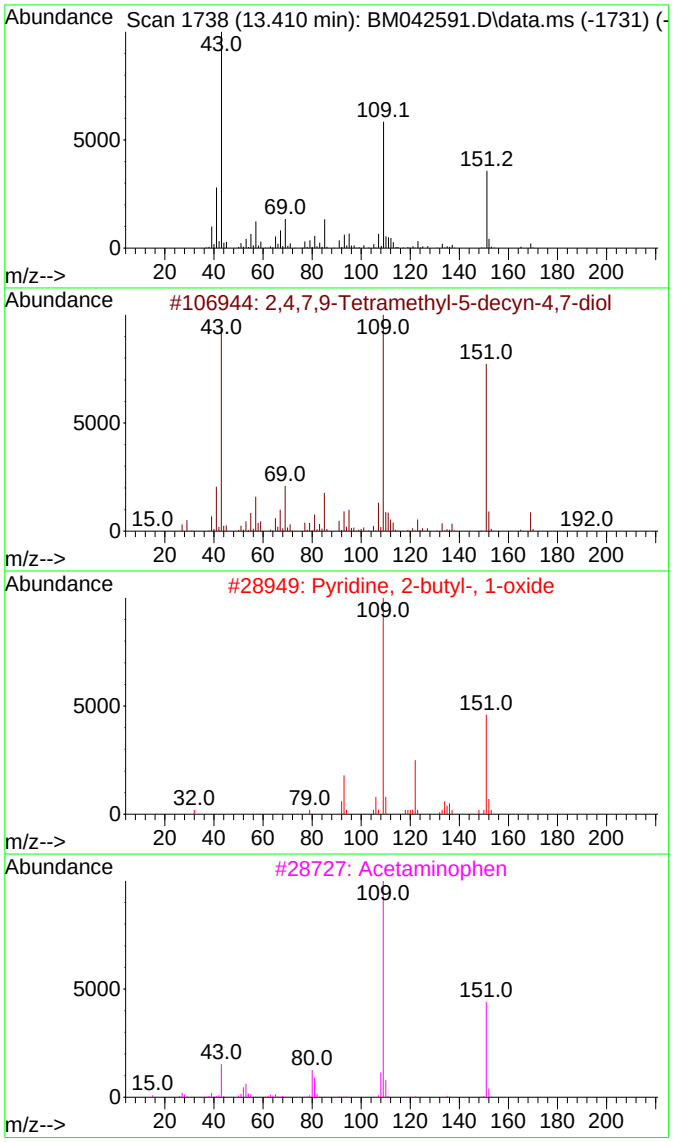
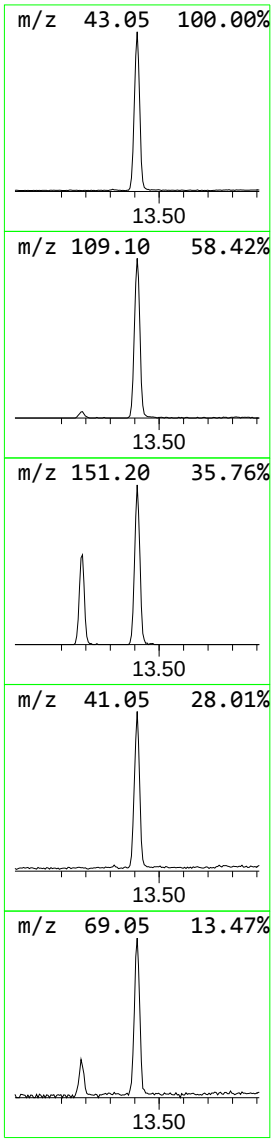
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.410 | 19.40 ng | 475962 | Acenaphthene-d10 | 14.563 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226 | C14H26O2 | 000126-86-3 | 87 |
| 2 | Pyridine, 2-butyl-, 1-oxide | 151 | C9H13NO | 031396-32-4 | 53 |
| 3 | Acetaminophen | 151 | C8H9NO2 | 000103-90-2 | 47 |
| 4 | 3-Pyridinol, 4-methyl-, acetate ... | 151 | C8H9NO2 | 001006-96-8 | 38 |
| 5 | Pyridine, 3-butyl-, 1-oxide | 151 | C9H13NO | 031396-33-5 | 38 |



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ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

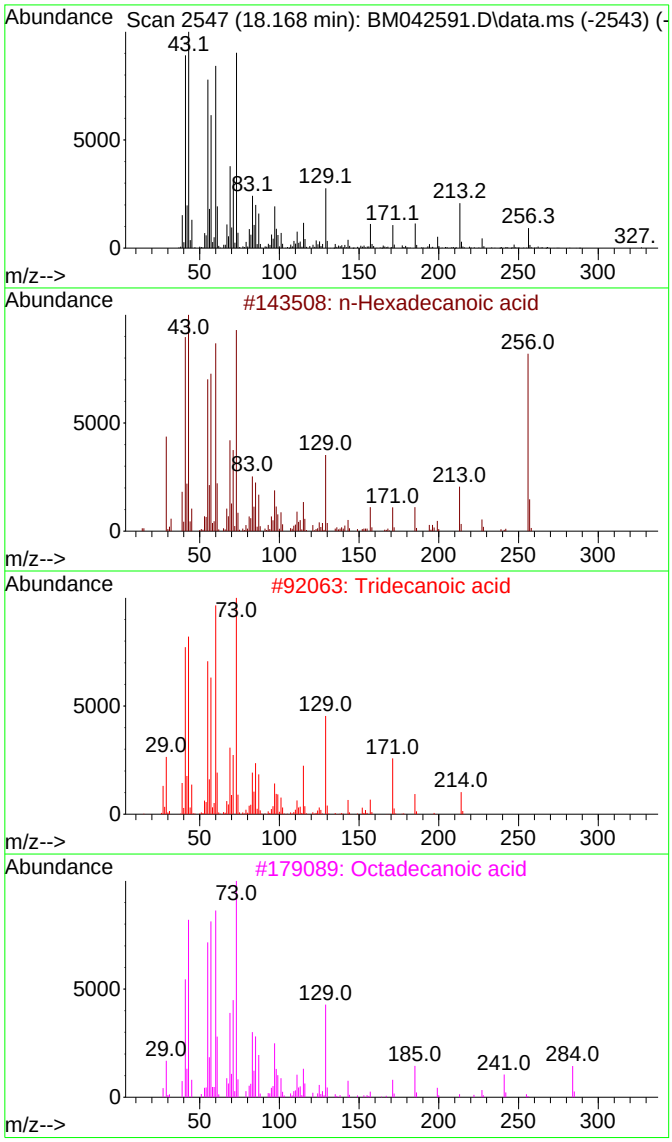
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

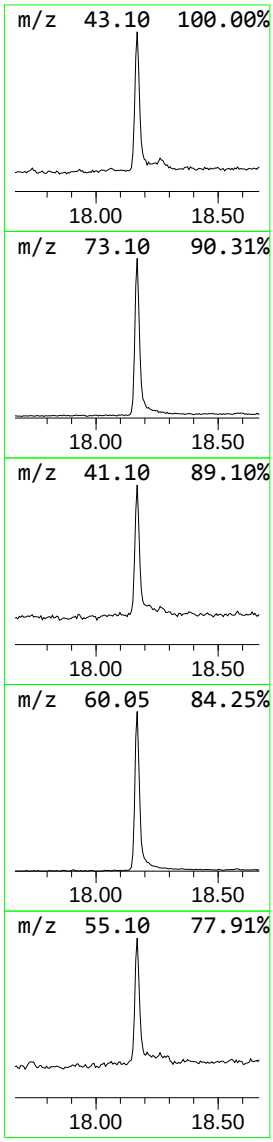
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.168 | 21.33 ng | 701720 | Phenanthrene-d10 | 17.315 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 80 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |



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Data File : BM042591.D
Acq On : 04 Nov 2023 14:53
Operator : MA/JU
Sample : 05234-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
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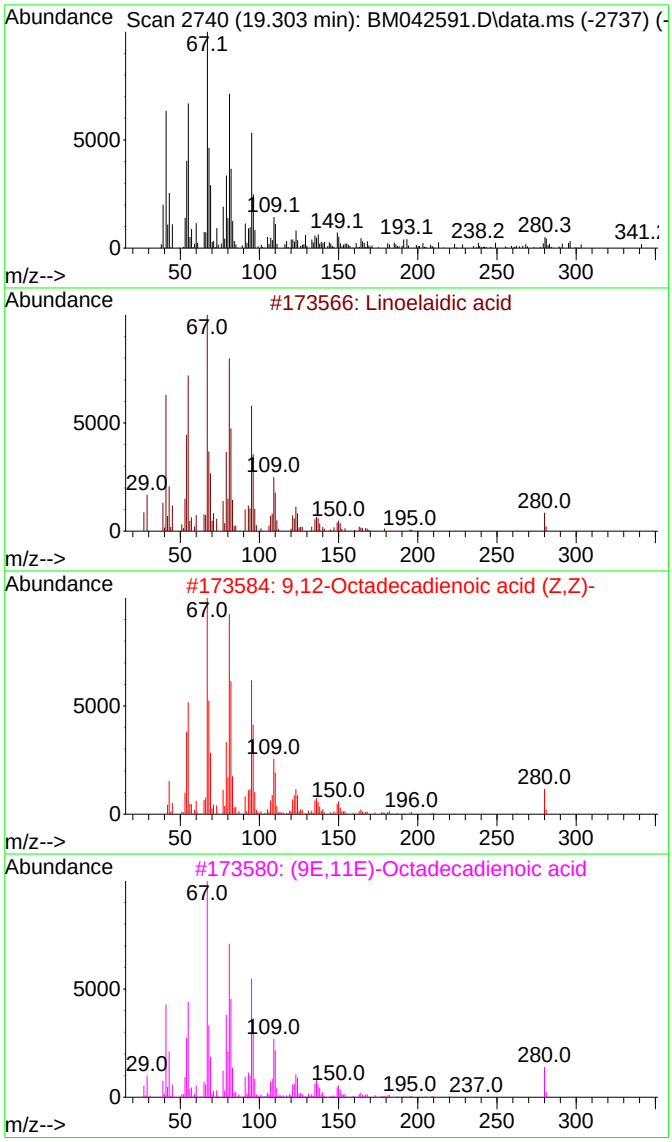
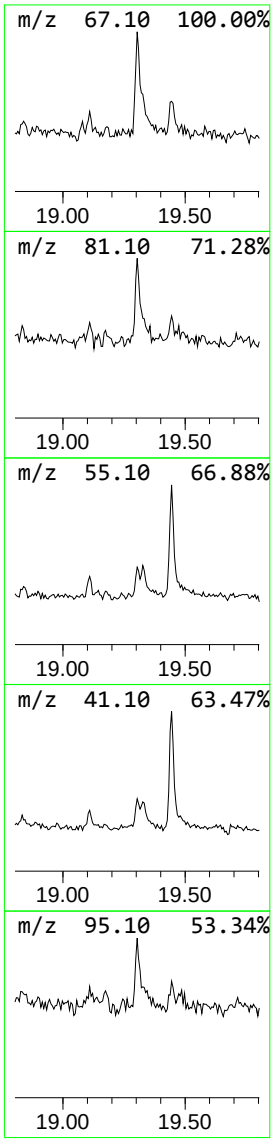
Peak Number 3 Linoelaidic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.304 | 3.21 ng | 105558 | Phenanthrene-d10 | 17.315 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Linoelaidic acid | 280 | C18H32O2 | 000506-21-8 | 97 |
| 2 | 9,12-Octadecadienoic acid (Z,Z)- | 280 | C18H32O2 | 000060-33-3 | 95 |
| 3 | (9E,11E)-Octadecadienoic acid | 280 | C18H32O2 | 000544-71-8 | 93 |
| 4 | 10E,12Z-Octadecadienoic acid | 280 | C18H32O2 | 002420-56-6 | 93 |
| 5 | 1,9-Tetradecadiene | 194 | C14H26 | 112929-06-3 | 90 |



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Sample : 05234-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
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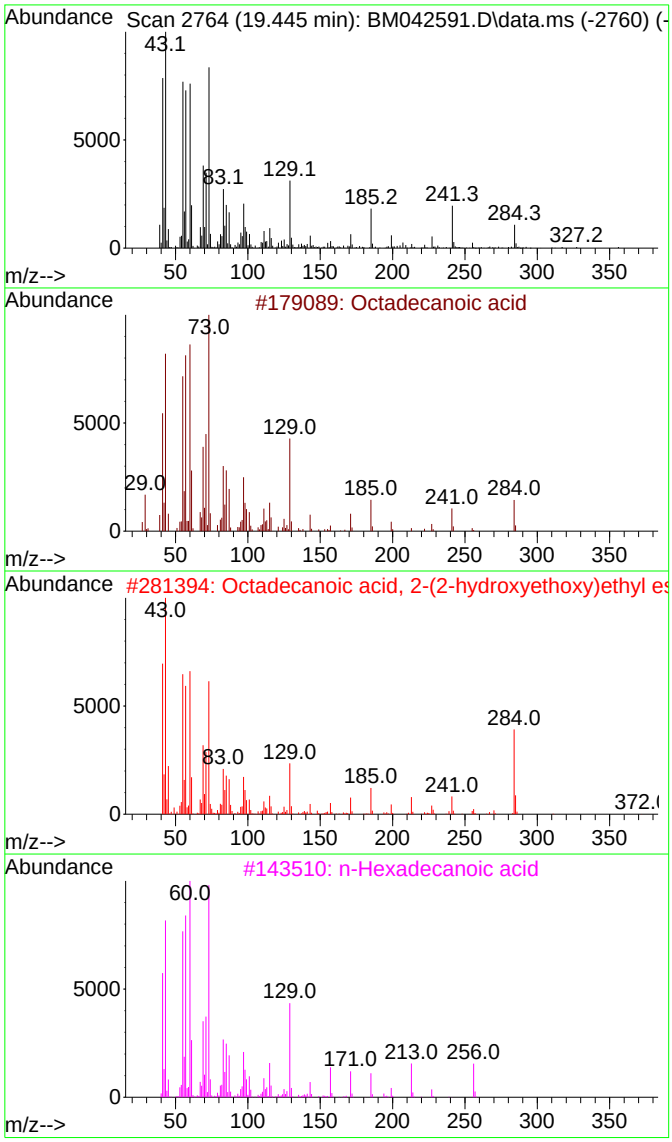
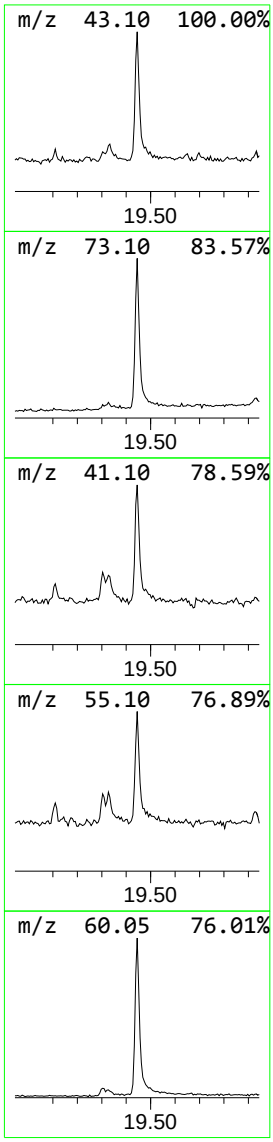
Peak Number 4 Octadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.445 | 12.59 ng | 534328 | Chrysene-d12 | 21.497 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 80 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 74 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 64 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 62 |



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Sample : 05234-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
SP-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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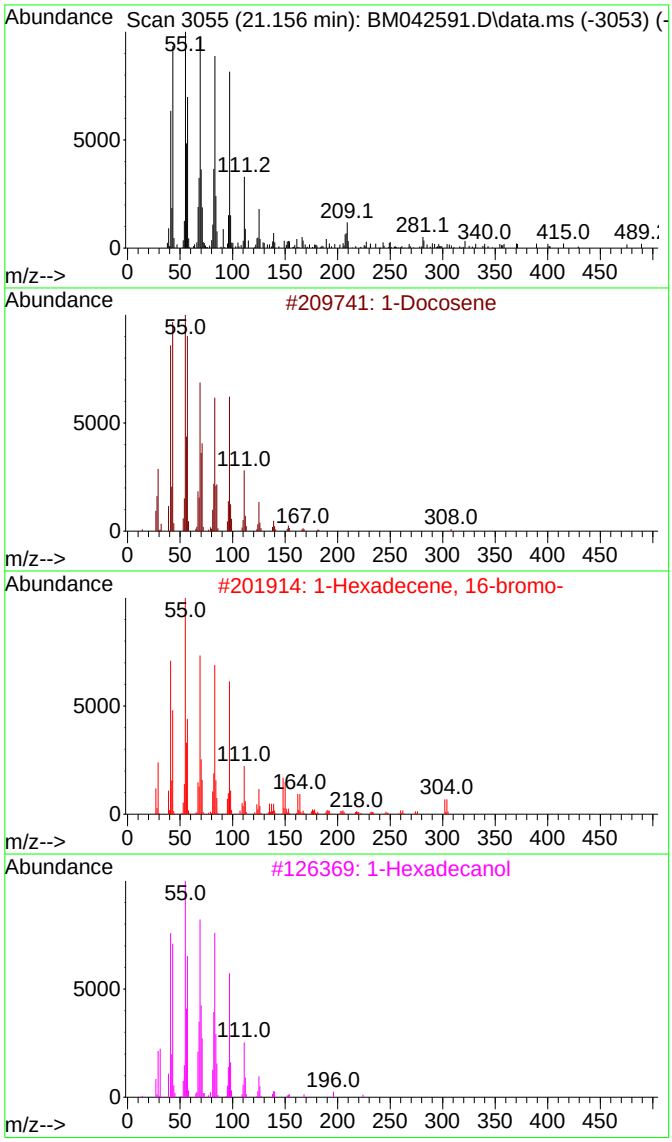
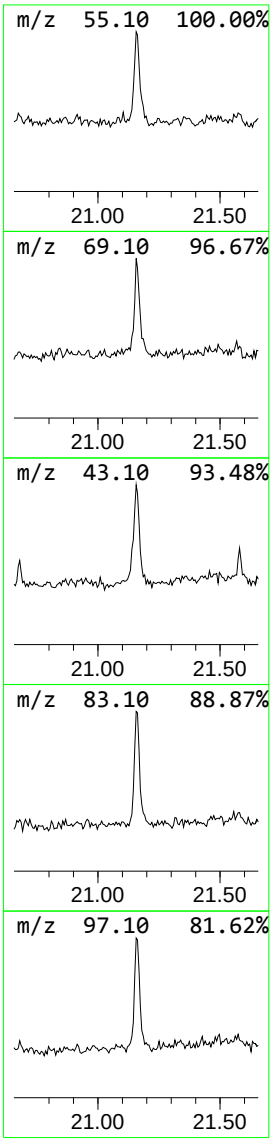
Peak Number 5 1-Docosene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.156 | 5.79 ng | 245779 | Chrysene-d12 | 21.497 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 90 |
| 2 | 1-Hexadecene, 16-bromo- | 302 | C16H31Br | 118625-56-2 | 90 |
| 3 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 83 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 70 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 68 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110423\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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BNA_M
**ClientSampleId :**
SP-A

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2,4,7,9-Tetrame... | 13.410 | 19.4 | ng | 475962 | 3 | 14.563 | 490625 | 20.0 |
| n-Hexadecanoic ... | 18.168 | 21.3 | ng | 701720 | 4 | 17.315 | 657910 | 20.0 |
| Linoelaidic acid | 19.304 | 3.2 | ng | 105558 | 4 | 17.315 | 657910 | 20.0 |
| Octadecanoic acid | 19.445 | 12.6 | ng | 534328 | 5 | 21.497 | 848737 | 20.0 |
| 1-Docosene | 21.156 | 5.8 | ng | 245779 | 5 | 21.497 | 848737 | 20.0 |