LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117625.D
Acq On : 30 Oct 2019 15:32
Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

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_F\METHODS\8270-BF101819.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 | 5.357 | 552 | 556 | 579 | rBV | 505574 | 752277 | 85.34% | 10.919% |
| 2 | 6.387 | 727 | 731 | 747 | rBV | 641928 | 852118 | 96.66% | 12.368% |
| 3 | 6.504 | 747 | 751 | 769 | rVB | 910526 | 881543 | 100.00% | 12.795% |
| 4 | 6.728 | 785 | 789 | 800 | rVB | 219380 | 205044 | 23.26% | 2.976% |
| 5 | 6.881 | 812 | 815 | 830 | rBV | 633554 | 579726 | 65.76% | 8.414% |
| 6 | 7.293 | 882 | 885 | 904 | rBV | 366033 | 471988 | 53.54% | 6.850% |
| 7 | 8.010 | 1004 | 1007 | 1024 | rBV | 201044 | 251260 | 28.50% | 3.647% |
| 8 | 9.081 | 1186 | 1189 | 1203 | rBV | 711431 | 691749 | 78.47% | 10.040% |
| 9 | 9.481 | 1254 | 1257 | 1269 | rBV | 54543 | 62372 | 7.08% | 0.905% |
| 10 | 9.757 | 1301 | 1304 | 1320 | rBB | 253018 | 270968 | 30.74% | 3.933% |
| 11 | 10.557 | 1436 | 1440 | 1454 | rBV | 336973 | 384108 | 43.57% | 5.575% |
| 12 | 11.251 | 1554 | 1558 | 1567 | rBV | 203772 | 229041 | 25.98% | 3.324% |
| 13 | 11.775 | 1645 | 1647 | 1654 | rBV | 24505 | 29570 | 3.35% | 0.429% |
| 14 | 12.469 | 1763 | 1765 | 1769 | rBV | 12632 | 14189 | 1.61% | 0.206% |
| 15 | 12.698 | 1801 | 1804 | 1807 | rVB | 10698 | 9317 | 1.06% | 0.135% |
| 16 | 12.827 | 1822 | 1826 | 1834 | rVB | 554554 | 495992 | 56.26% | 7.199% |
| 17 | 13.392 | 1918 | 1922 | 1926 | rBV5 | 6915 | 10336 | 1.17% | 0.150% |
| 18 | 13.739 | 1976 | 1981 | 1988 | rBV3 | 55346 | 110878 | 12.58% | 1.609% |
| 19 | 13.898 | 2004 | 2008 | 2015 | rBV | 199953 | 224371 | 25.45% | 3.257% |
| 20 | 14.345 | 2081 | 2084 | 2086 | rBV | 15855 | 15689 | 1.78% | 0.228% |
| 21 | 14.639 | 2131 | 2134 | 2138 | rBV3 | 18819 | 21803 | 2.47% | 0.316% |
| 22 | 14.710 | 2143 | 2146 | 2151 | rVB | 58418 | 61041 | 6.92% | 0.886% |
| 23 | 14.957 | 2186 | 2188 | 2193 | rVB | 26986 | 25903 | 2.94% | 0.376% |
| 24 | 15.339 | 2245 | 2253 | 2262 | rVB | 132088 | 203883 | 23.13% | 2.959% |
| 25 | 15.715 | 2314 | 2317 | 2321 | rVB4 | 19810 | 25216 | 2.86% | 0.366% |
| 26 | 16.345 | 2422 | 2424 | 2429 | rVB6 | 7466 | 9538 | 1.08% | 0.138% |

Sum of corrected areas: 6889920

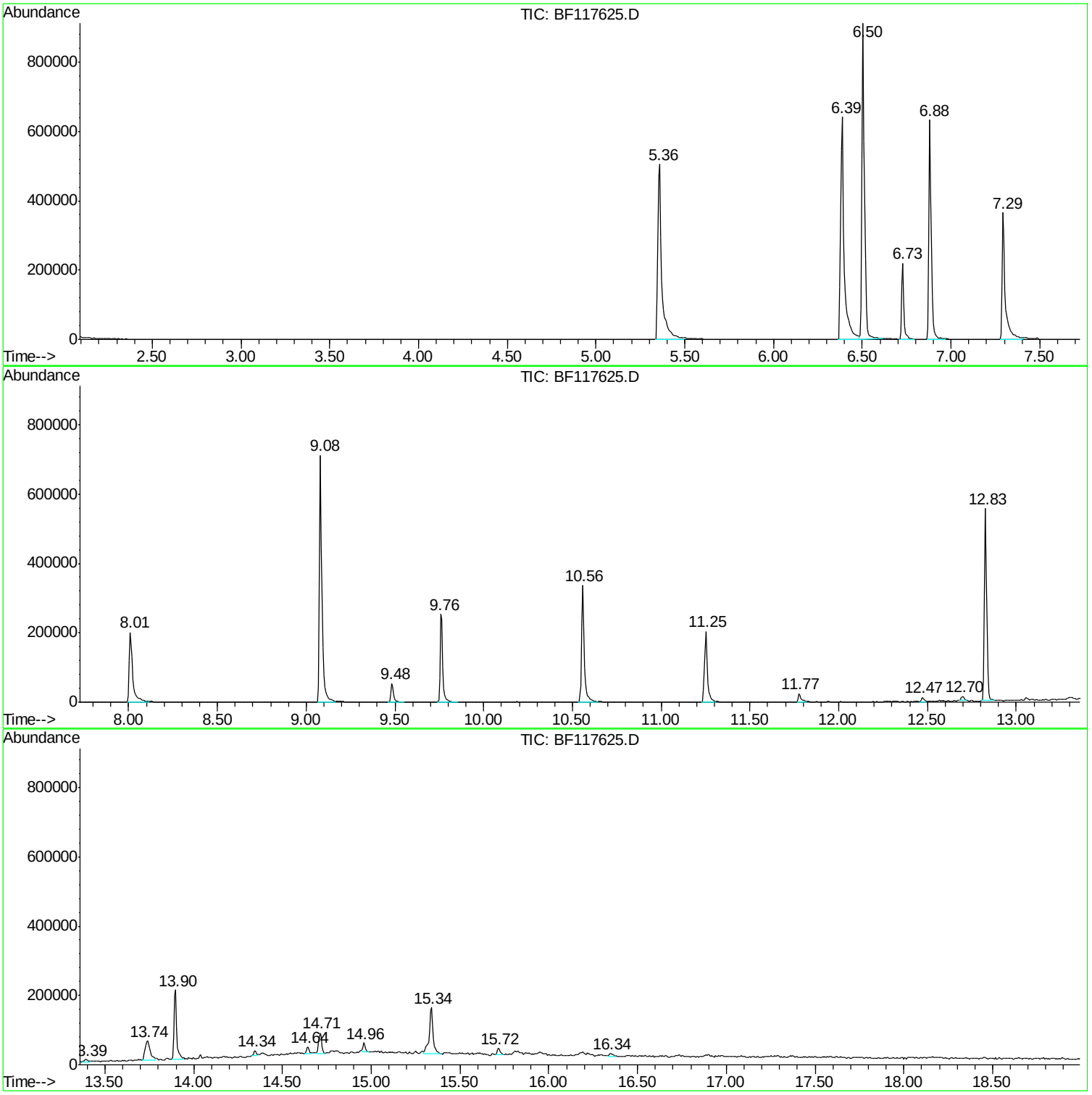
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117625.D
Acq On : 30 Oct 2019 15:32
Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117625.D
Acq On : 30 Oct 2019 15:32
Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

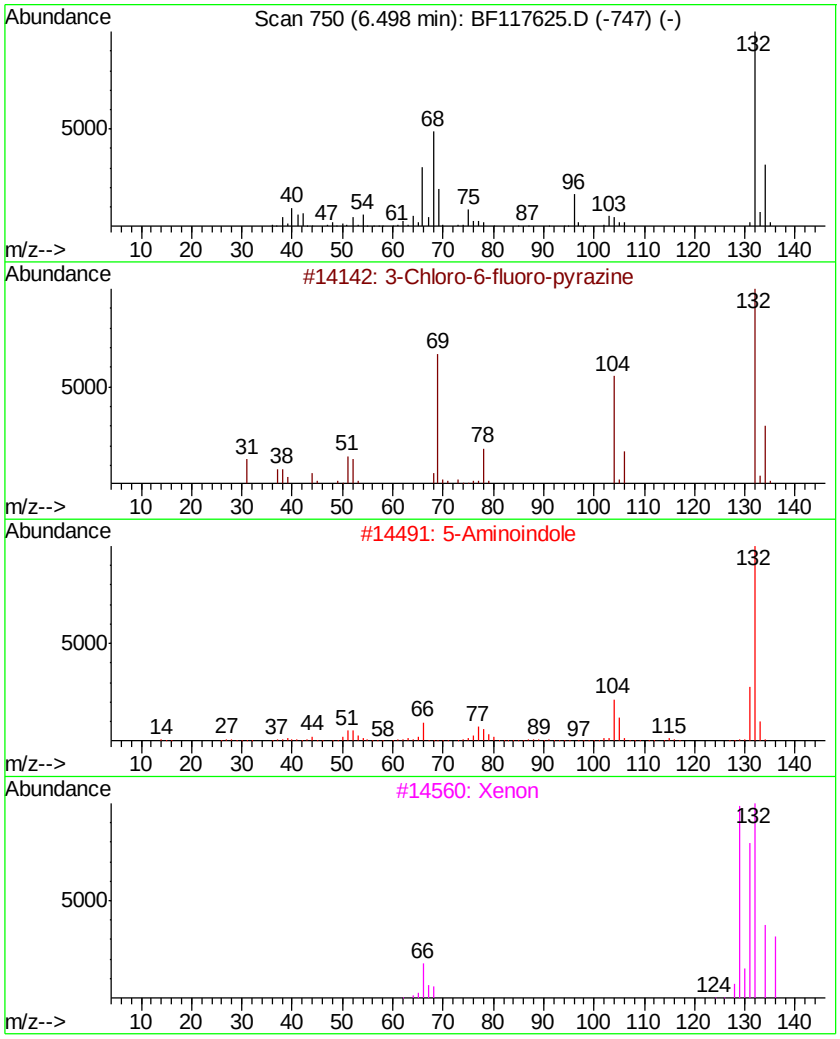
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

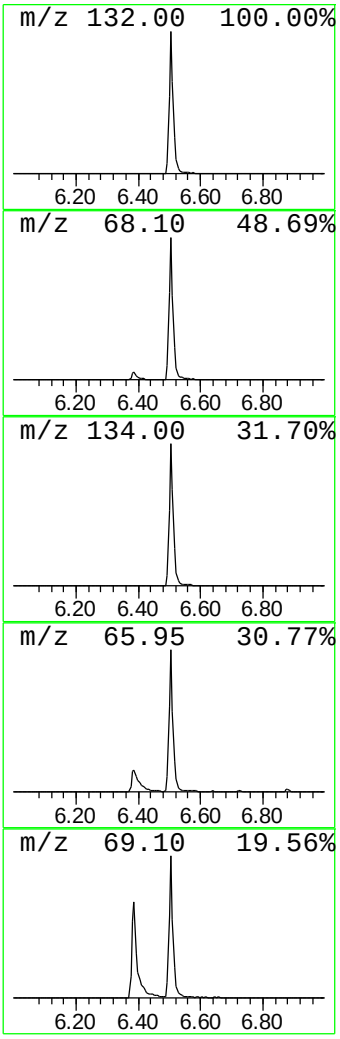
**********

Peak Number 1 unknown6.50 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.50 | 85.99 ng | 881543 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 10 |
| 3 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



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Data File : BF117625.D
Acq On : 30 Oct 2019 15:32
Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

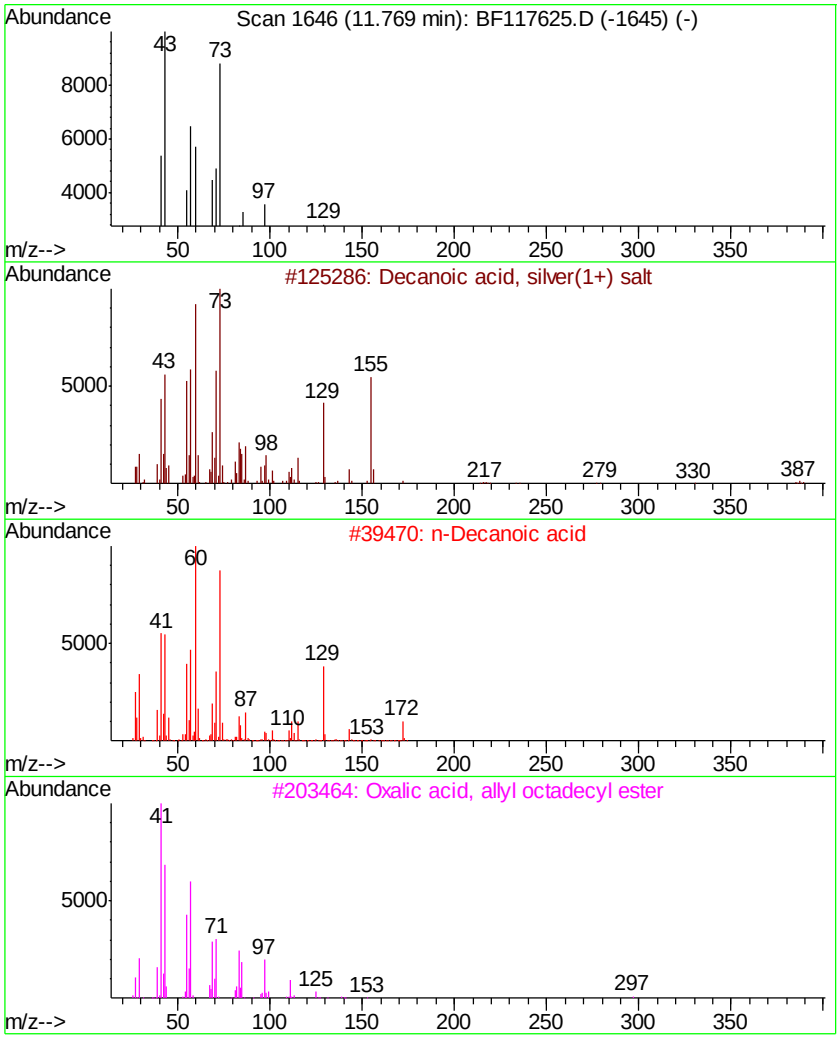
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

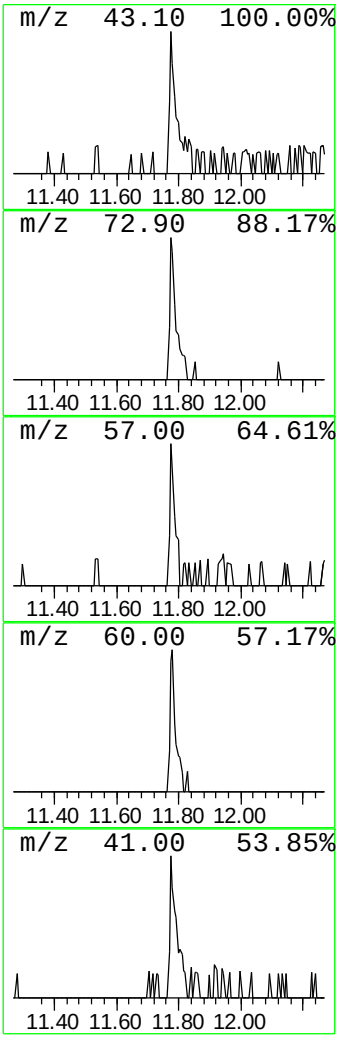
**********

Peak Number 3 Decanoic acid, silver(1+) salt Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.77 | 2.58 ng | 29570 | Phenanthrene-d10 | 11.25 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 59 |
| 2 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 50 |
| 3 | Oxalic acid, allyl octadecyl ester | 382 | C23H42O4 | 1000309-24-5 | 27 |
| 4 | Oxalic acid, cyclobutyl tridecyl... | 326 | C19H34O4 | 1000309-70-4 | 22 |
| 5 | Oxalic acid, allyl tridecyl ester | 312 | C18H32O4 | 1000309-24-1 | 22 |



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Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

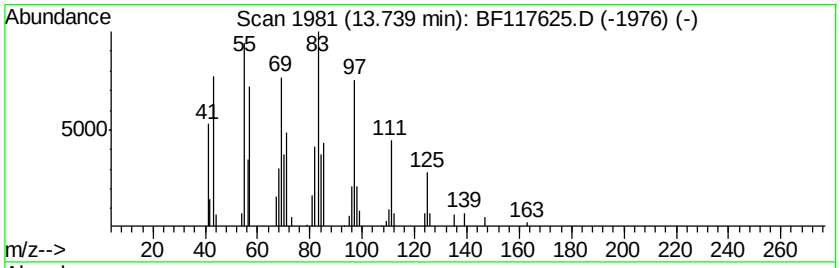
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

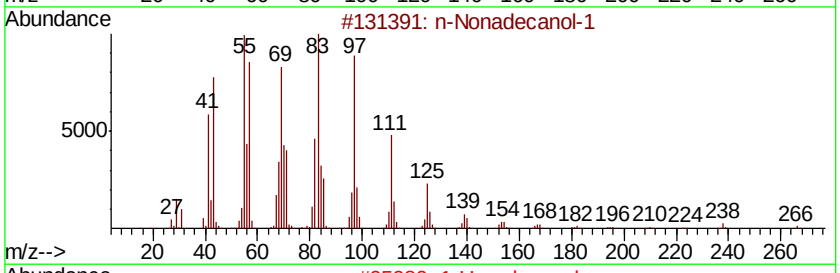
**********

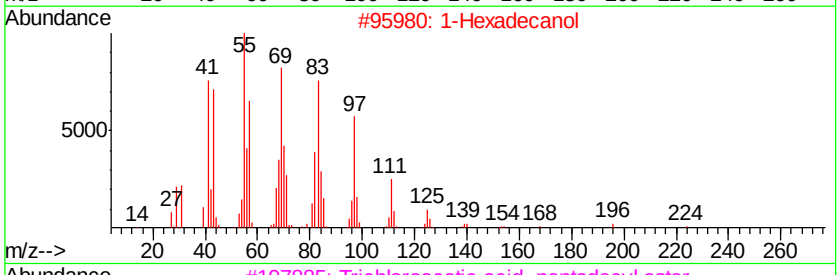
Peak Number 4 n-Nonadecanol-1 Concentration Rank 3

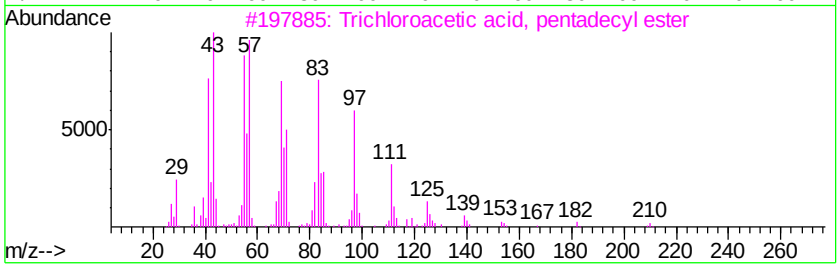
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.74 | 9.88 ng | 110878 | Chrysene-d12 | 13.90 |

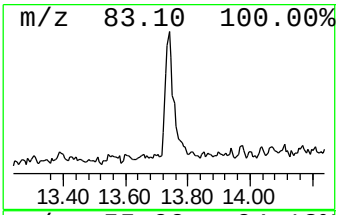
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 90 |
| 2 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 86 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 83 |
| 4 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 83 |
| 5 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 80 |

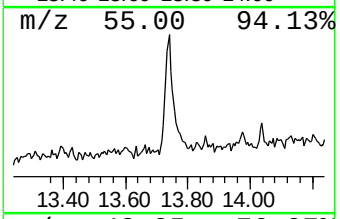


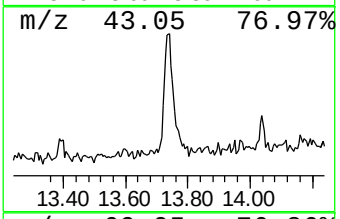



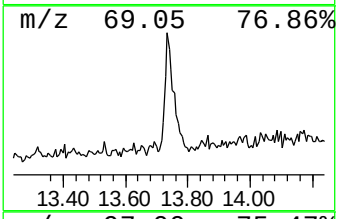



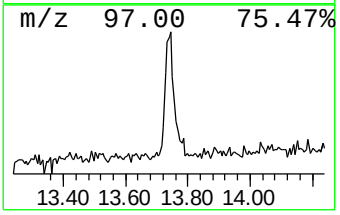



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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

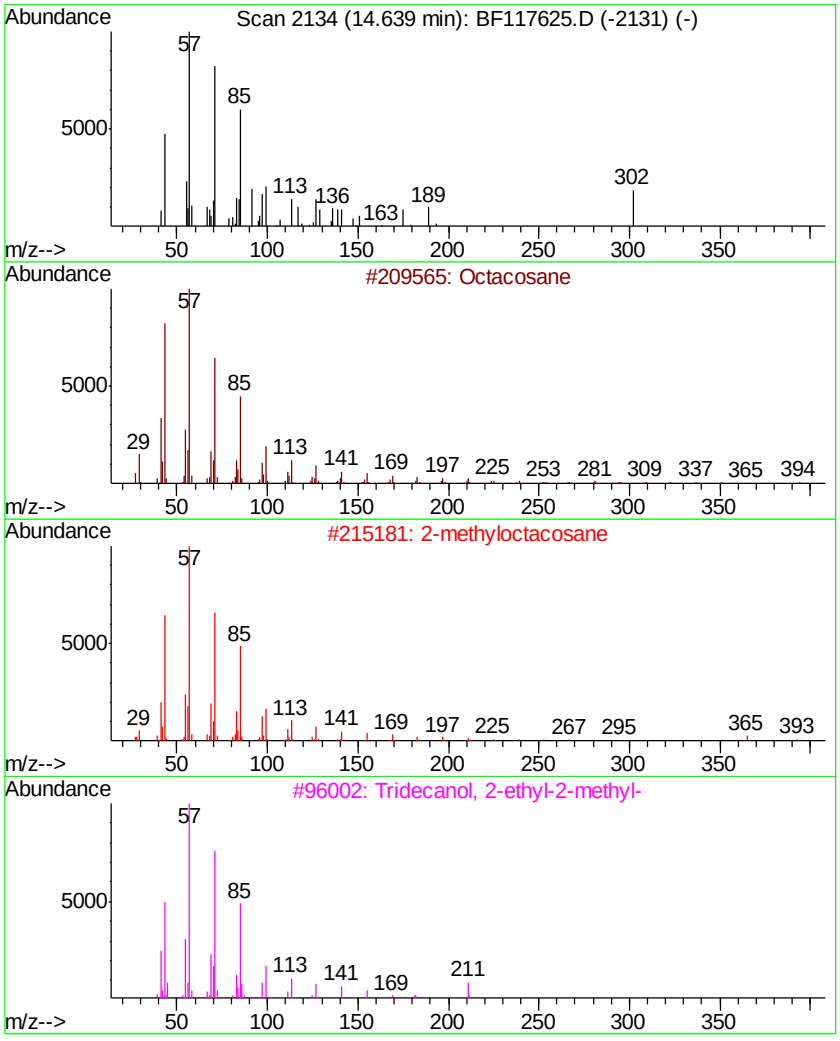
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

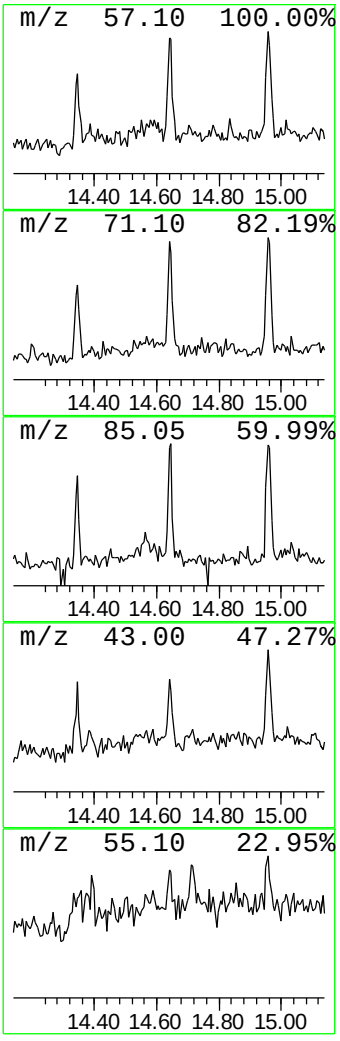
**********

Peak Number 5 Octacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.64 | 2.14 ng | 21803 | Perylene-d12 | 15.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 72 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 72 |
| 3 | Tridecanol, 2-ethyl-2-methyl- | 242 | C16H34O | 1000115-66-1 | 64 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 64 |
| 5 | Pentacosane | 352 | C25H52 | 000629-99-2 | 64 |



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**Instrument :** BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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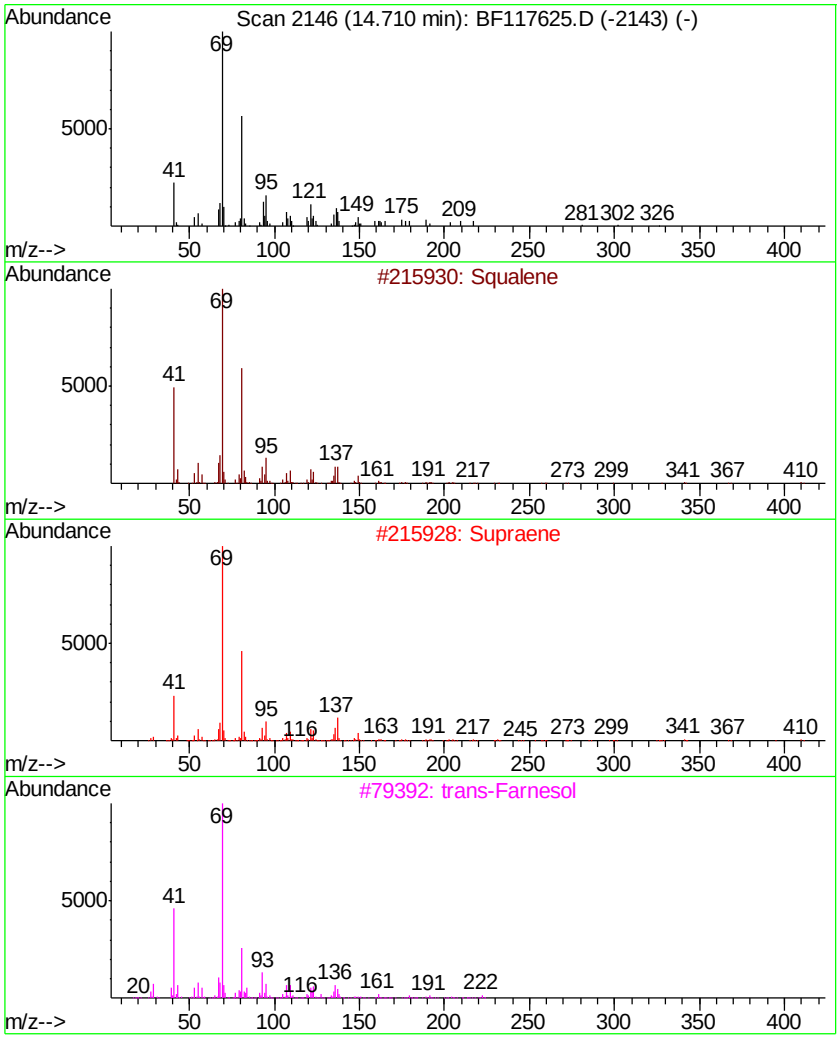
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

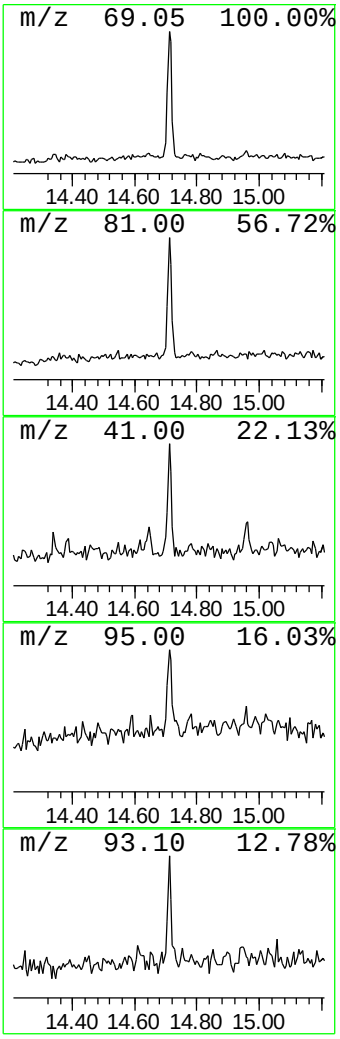
**********

Peak Number 6 Squalene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.71 | 5.99 ng | 61041 | Perylene-d12 | 15.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 86 |
| 3 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 64 |
| 4 | 2,6-Octadiene, 2,6-dimethyl- | 138 | C10H18 | 002792-39-4 | 52 |
| 5 | Butane, 1,3-dibromo-3-methyl- | 228 | C5H10Br2 | 024443-15-0 | 50 |



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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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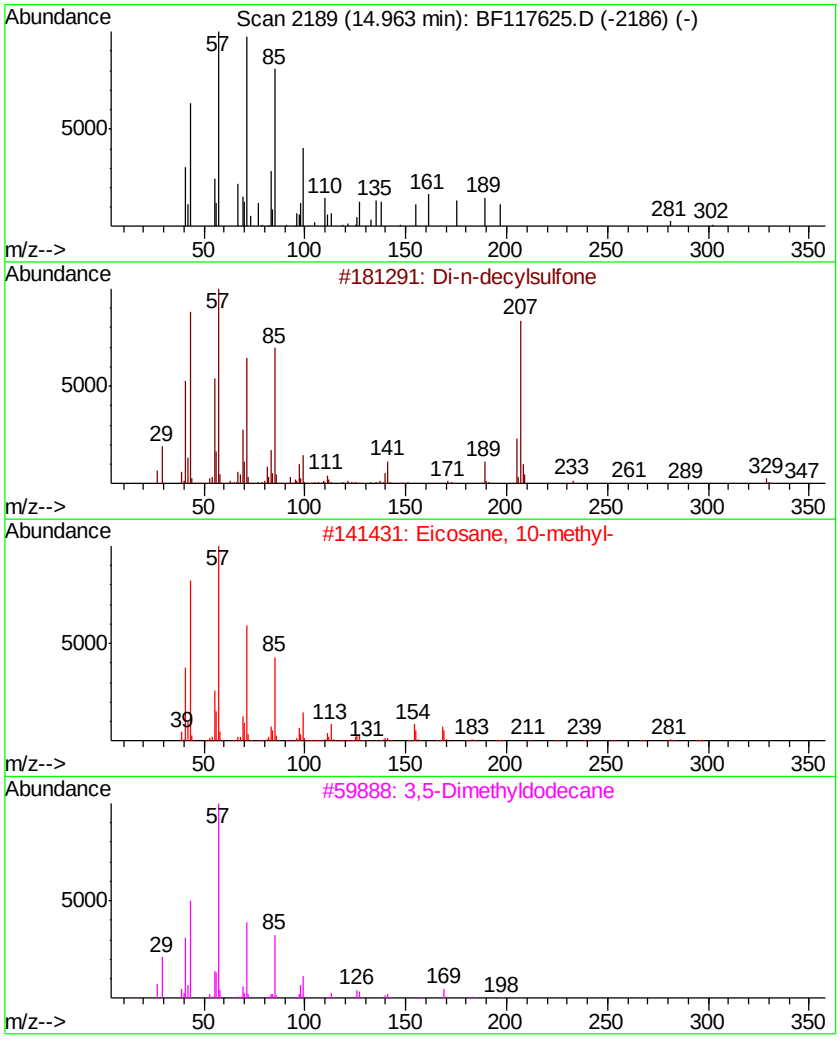
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

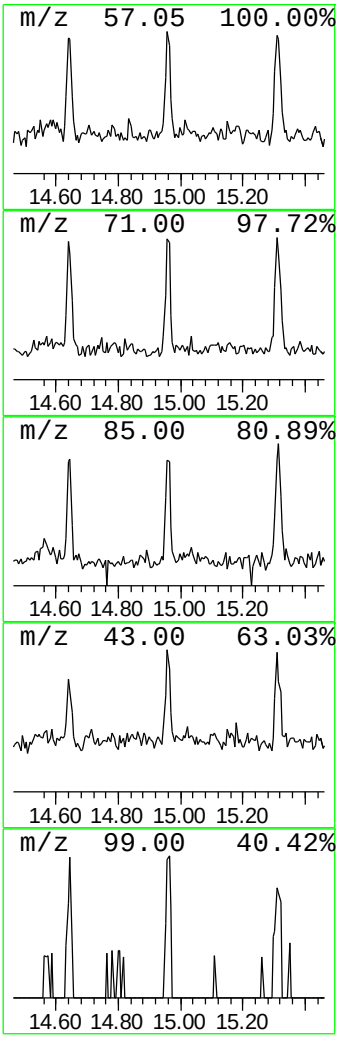
**********

Peak Number 7 Di-n-decylsulfone Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.96 | 2.54 ng | 25903 | Perylene-d12 | 15.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Di-n-decylsulfone | 346 | C20H42O2S | 111530-37-1 | 50 |
| 2 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 50 |
| 3 | 3,5-Dimethyldodecane | 198 | C14H30 | 107770-99-0 | 50 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 50 |
| 5 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 50 |



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Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

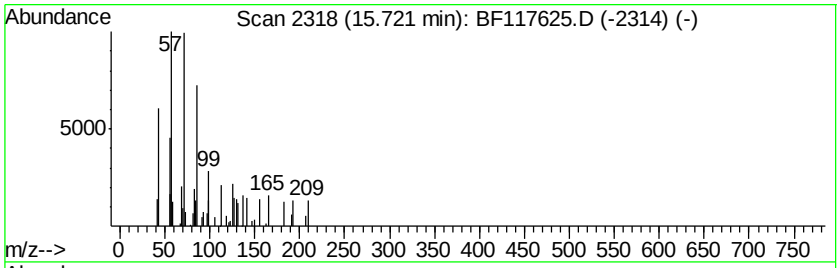
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

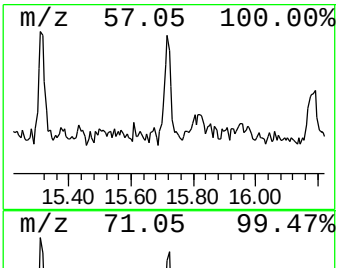
**********

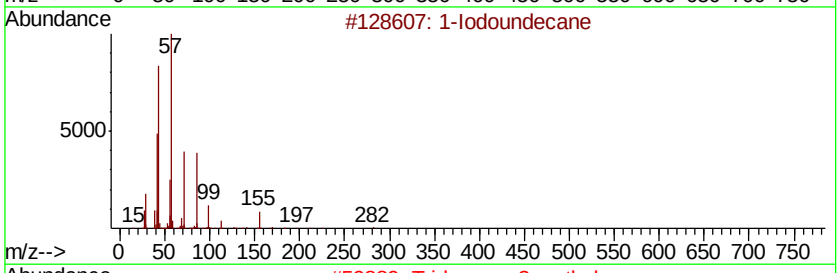
Peak Number 8 1-Iodoundecane Concentration Rank 7

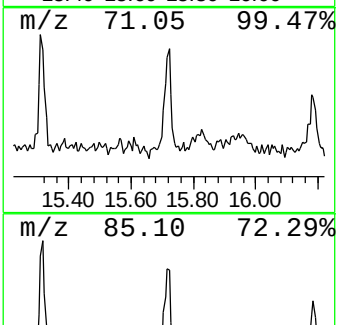
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.72 | 2.47 ng | 25216 | Perylene-d12 | 15.34 |

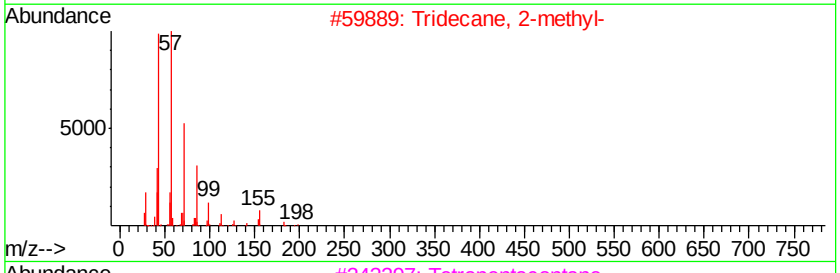
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Iodoundecane | 282 | C11H23I | 004282-44-4 | 50 |
| 2 | Tridecane, 2-methyl- | 198 | C14H30 | 001560-96-9 | 50 |
| 3 | Tetrapentacontane | 759 | C54H110 | 005856-66-6 | 50 |
| 4 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 47 |
| 5 | Tetratriacontane | 479 | C34H70 | 014167-59-0 | 47 |

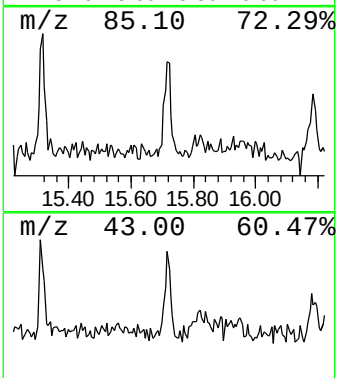


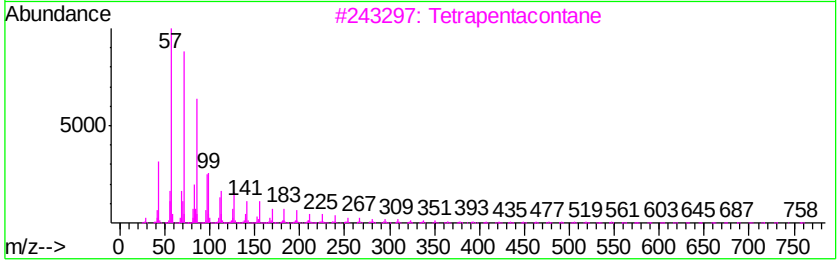



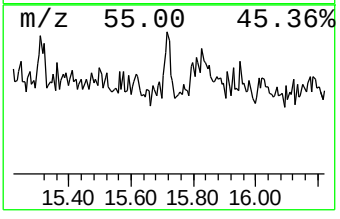









Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117625.D
Acq On : 30 Oct 2019 15:32
Operator : JU
Sample : K5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 161-78-(0-1.1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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 |
| unknown6.50 | 6.50 | 86.0 | ng | 881543 | 1 | 6.73 | 205044 | 20.0 |
| Decanoic acid, si... | 11.77 | 2.6 | ng | 29570 | 4 | 11.25 | 229041 | 20.0 |
| n-Nonadecanol-1 | 13.74 | 9.9 | ng | 110878 | 5 | 13.90 | 224371 | 20.0 |
| Octacosane | 14.64 | 2.1 | ng | 21803 | 6 | 15.34 | 203883 | 20.0 |
| Squalene | 14.71 | 6.0 | ng | 61041 | 6 | 15.34 | 203883 | 20.0 |
| Di-n-decylsulfone | 14.96 | 2.5 | ng | 25903 | 6 | 15.34 | 203883 | 20.0 |
| 1-Iodoundecane | 15.72 | 2.5 | ng | 25216 | 6 | 15.34 | 203883 | 20.0 |