LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-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-BF051019.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 | 5.463 | 570 | 574 | 602 | rBV | 5051944 | 5642774 | 94.49% | 10.476% |
| 2 | 6.475 | 741 | 746 | 764 | rBV | 5028057 | 5971909 | 100.00% | 11.087% |
| 3 | 6.604 | 764 | 768 | 772 | rBV | 5659759 | 5609657 | 93.93% | 10.415% |
| 4 | 6.828 | 803 | 806 | 814 | rVB | 1483320 | 1267854 | 21.23% | 2.354% |
| 5 | 6.987 | 829 | 833 | 836 | rBV | 4918889 | 4366563 | 73.12% | 8.107% |
| 6 | 7.392 | 897 | 902 | 915 | rBV | 3672790 | 3762549 | 63.00% | 6.985% |
| 7 | 8.110 | 1020 | 1024 | 1046 | rBV | 1675190 | 1632289 | 27.33% | 3.030% |
| 8 | 9.186 | 1202 | 1207 | 1210 | rBV | 6529846 | 5886622 | 98.57% | 10.929% |
| 9 | 9.581 | 1270 | 1274 | 1285 | rBV | 675933 | 685913 | 11.49% | 1.273% |
| 10 | 9.863 | 1318 | 1322 | 1333 | rBV | 1858213 | 1772841 | 29.69% | 3.291% |
| 11 | 10.657 | 1453 | 1457 | 1473 | rBV | 3969179 | 3924779 | 65.72% | 7.287% |
| 12 | 11.351 | 1571 | 1575 | 1585 | rBV | 2018099 | 1933714 | 32.38% | 3.590% |
| 13 | 11.874 | 1661 | 1664 | 1673 | rBV | 386548 | 427602 | 7.16% | 0.794% |
| 14 | 12.657 | 1794 | 1797 | 1804 | rBV | 56344 | 81311 | 1.36% | 0.151% |
| 15 | 12.933 | 1839 | 1844 | 1848 | rBV | 5524832 | 5853185 | 98.01% | 10.867% |
| 16 | 13.157 | 1878 | 1882 | 1891 | rBV | 56955 | 78105 | 1.31% | 0.145% |
| 17 | 13.498 | 1935 | 1940 | 1943 | rBV2 | 72564 | 79866 | 1.34% | 0.148% |
| 18 | 13.827 | 1992 | 1996 | 2012 | rBV | 426236 | 936570 | 15.68% | 1.739% |
| 19 | 13.992 | 2020 | 2024 | 2032 | rBV | 1572465 | 1504732 | 25.20% | 2.794% |
| 20 | 14.139 | 2045 | 2049 | 2053 | rBV | 125443 | 116083 | 1.94% | 0.216% |
| 21 | 14.445 | 2097 | 2101 | 2104 | rBV | 169796 | 169970 | 2.85% | 0.316% |
| 22 | 14.745 | 2148 | 2152 | 2156 | rBV | 132154 | 132508 | 2.22% | 0.246% |
| 23 | 15.074 | 2204 | 2208 | 2215 | rBV | 192444 | 226375 | 3.79% | 0.420% |
| 24 | 15.457 | 2268 | 2273 | 2282 | rBV | 1061857 | 1425980 | 23.88% | 2.647% |
| 25 | 15.874 | 2340 | 2344 | 2353 | rVB | 123151 | 174889 | 2.93% | 0.325% |
| 26 | 15.992 | 2355 | 2364 | 2371 | rBV | 38530 | 127450 | 2.13% | 0.237% |
| 27 | 16.374 | 2424 | 2429 | 2433 | rBV | 37235 | 70949 | 1.19% | 0.132% |

Sum of corrected areas: 53863039

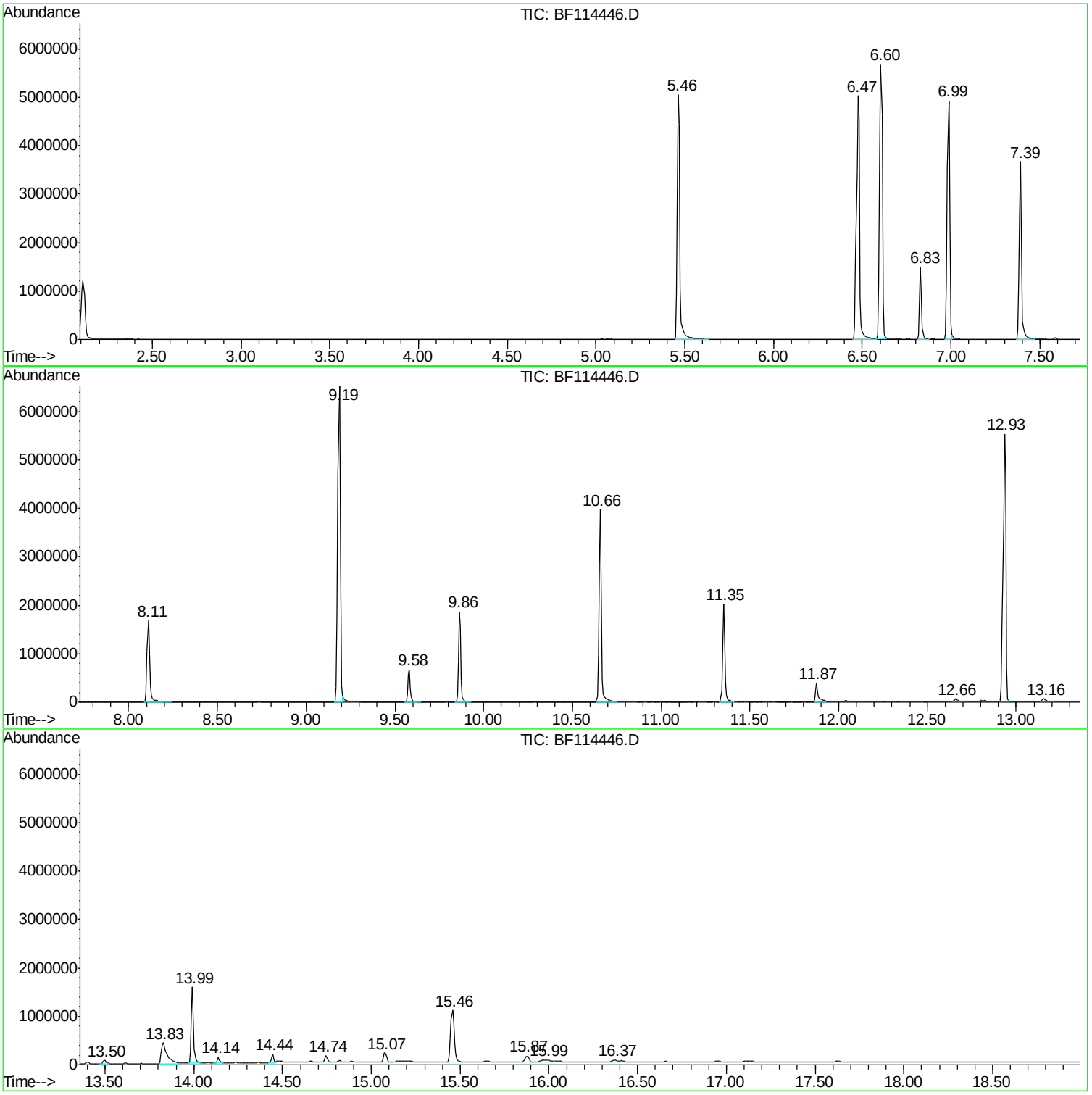
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

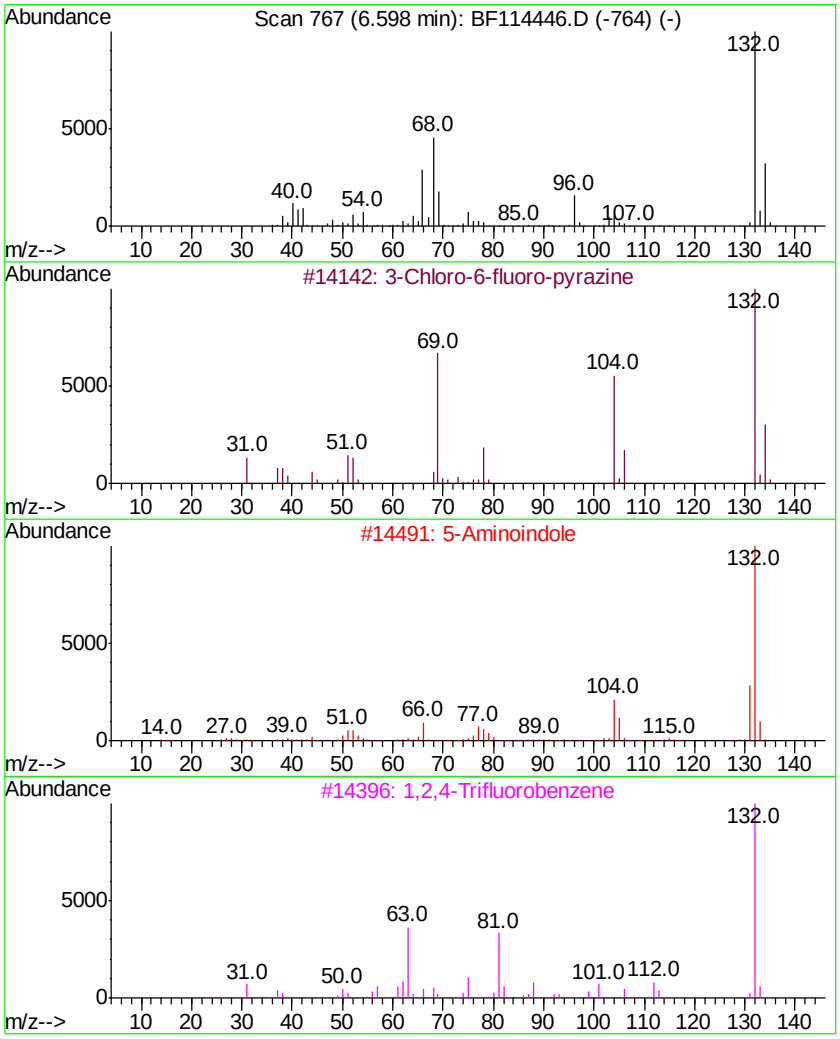
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

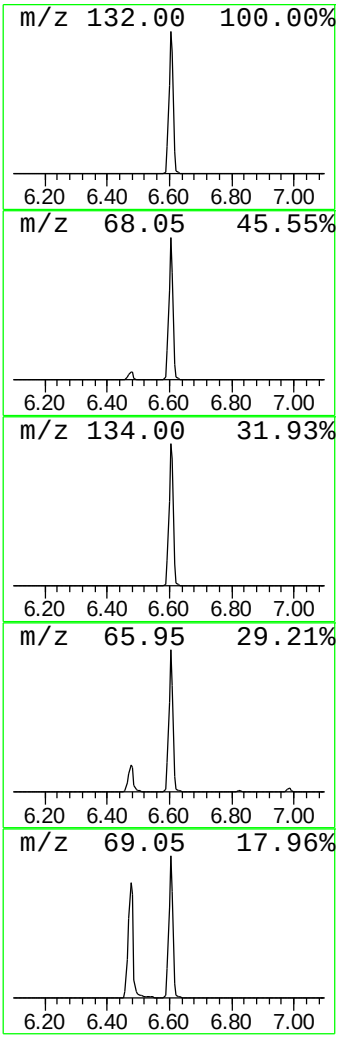
**********

Peak Number 1 unknown6.60 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.60 | 88.49 ng | 5609660 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

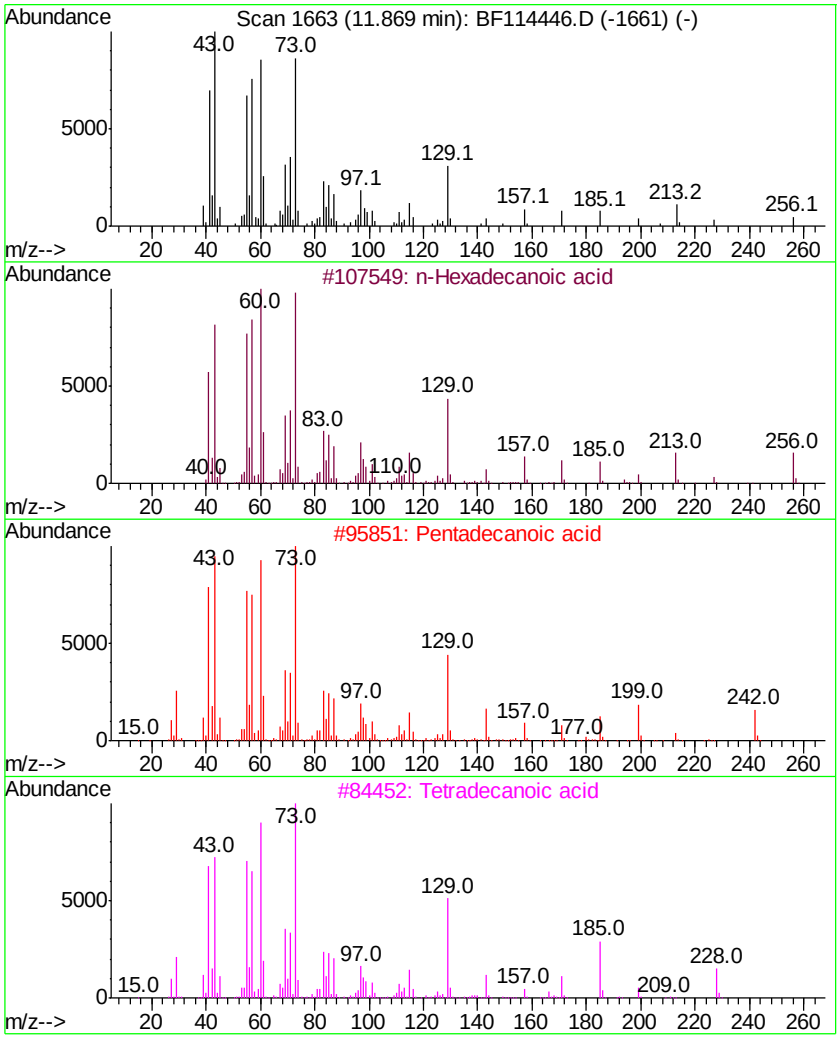
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

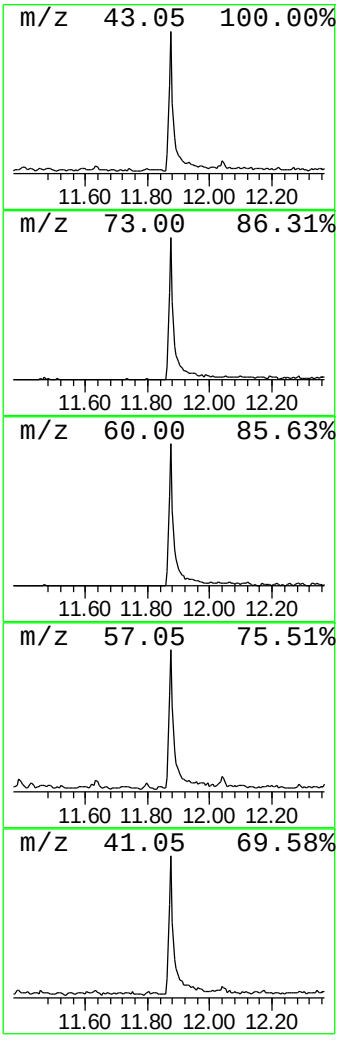
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.87 | 4.42 ng | 427602 | Phenanthrene-d10 | 11.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 83 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

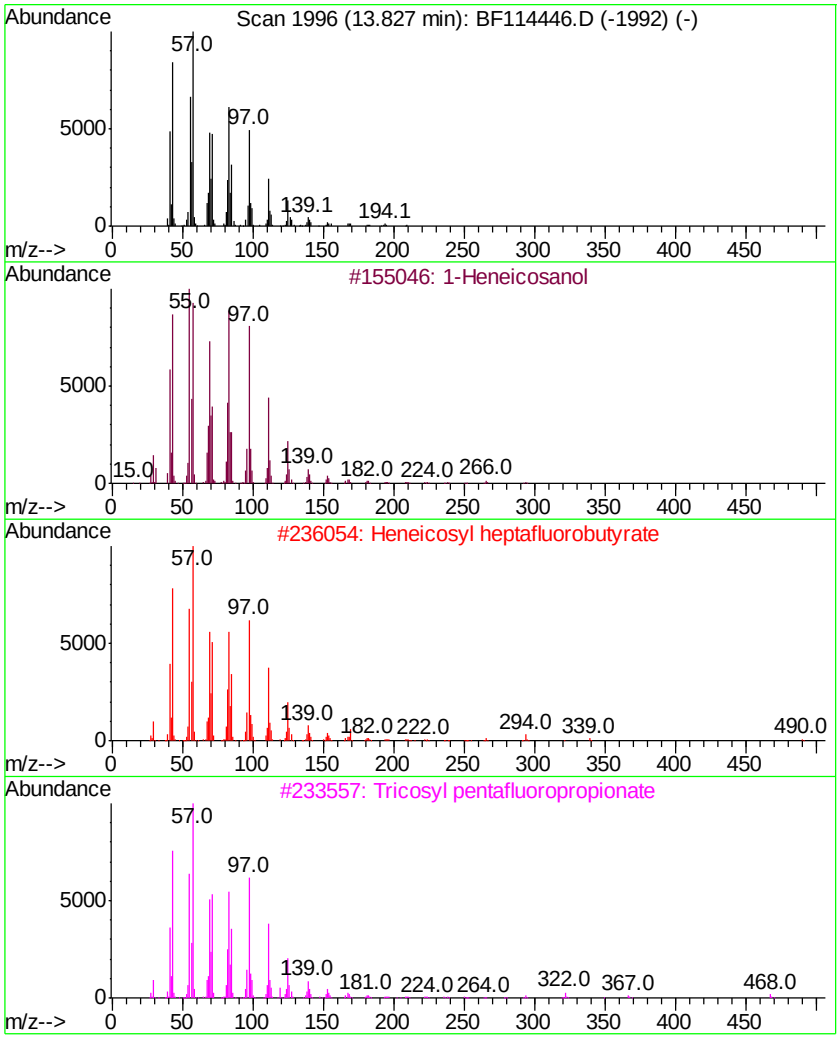
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

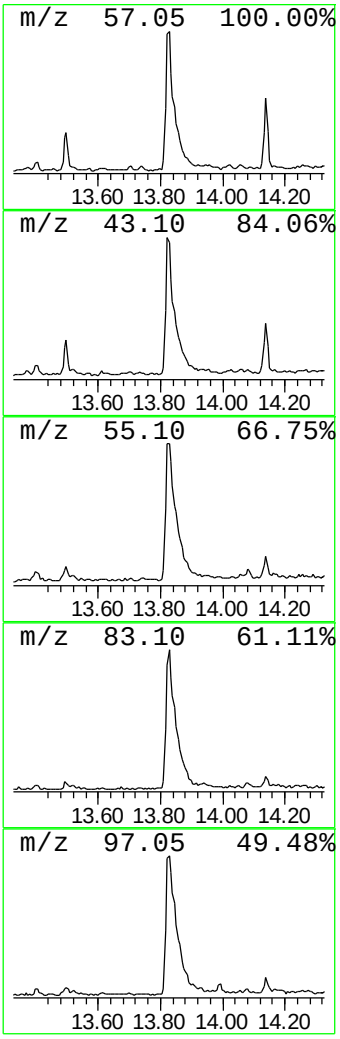
**********

Peak Number 4 1-Heneicosanol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.83 | 12.45 ng | 936570 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 2 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91 |
| 3 | Tricosyl pentafluoropropionate | 486 | C26H47F5O2 | 1000351-81-0 | 91 |
| 4 | Docosyl pentafluoropropionate | 472 | C25H45F5O2 | 1000351-80-9 | 91 |
| 5 | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

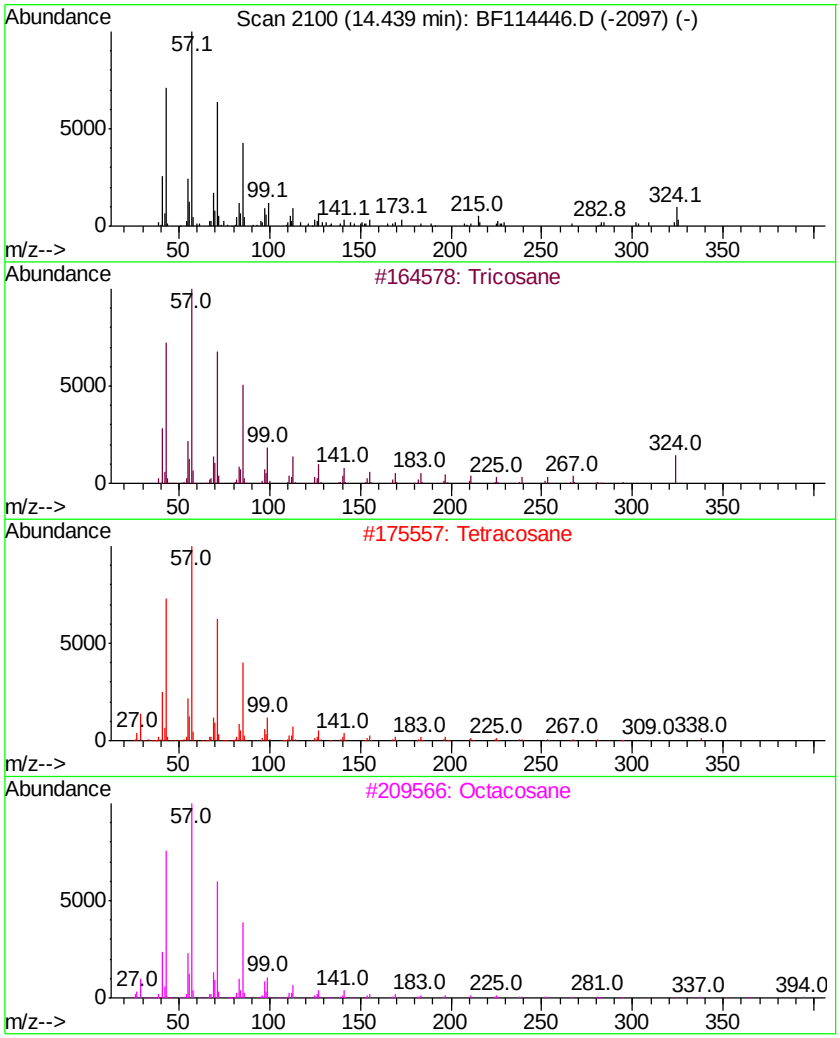
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

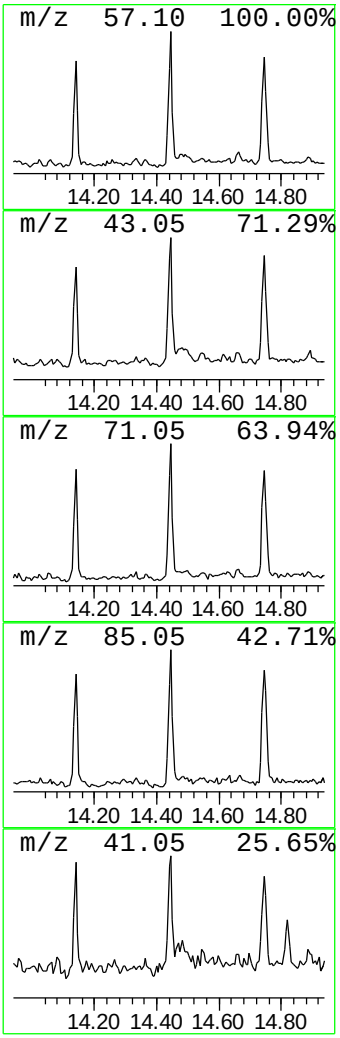
**********

Peak Number 5 Tricosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.44 | 2.26 ng | 169970 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricosane | 324 | C23H48 | 000638-67-5 | 95 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

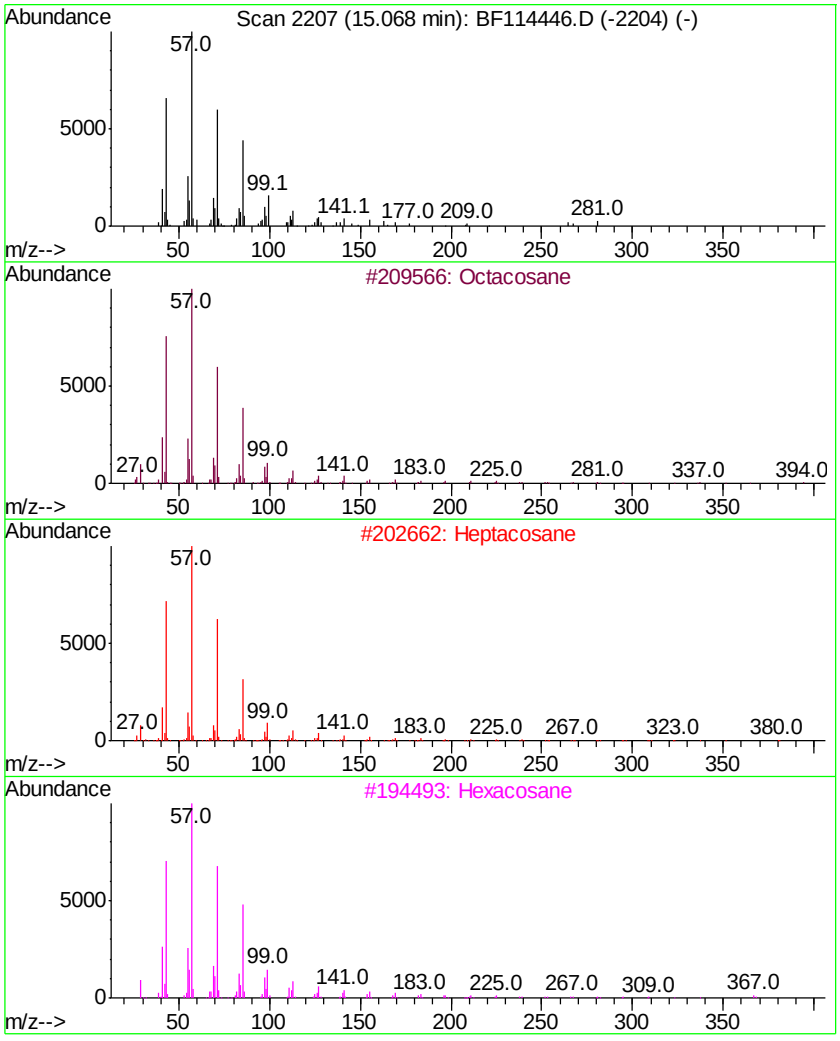
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

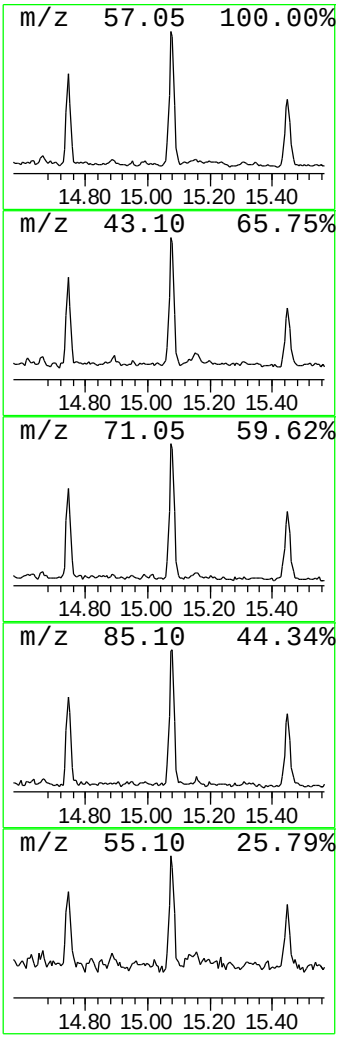
**********

Peak Number 6 Octacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.07 | 3.18 ng | 226375 | Perylene-d12 | 15.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 90 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 86 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

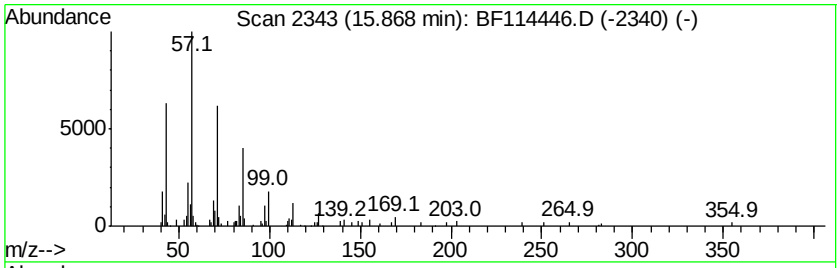
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

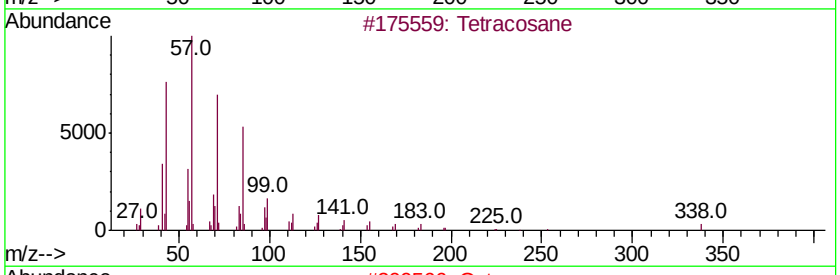
**********

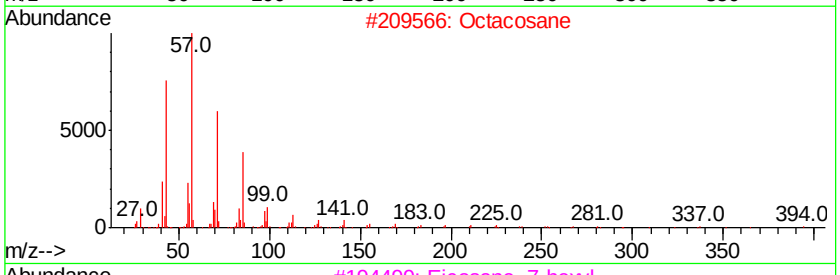
Peak Number 7 Tetracosane Concentration Rank 6

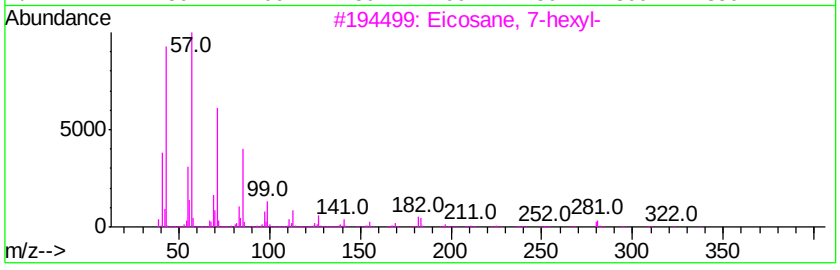
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.87 | 2.45 ng | 174889 | Perylene-d12 | 15.46 |

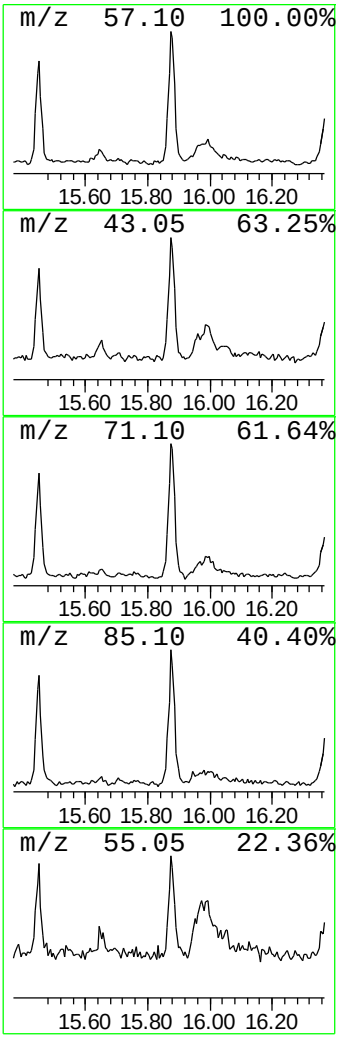
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 3 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 90 |
| 4 | Tridecanol, 2-ethyl-2-methyl- | 242 | C16H34O | 1000115-66-1 | 90 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052019\
Data File : BF114446.D
Acq On : 21 May 2019 3:09
Operator : JU/SJ
Sample : K2943-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** BUS-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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 |
| unknown6.60 | 6.60 | 88.5 | ng | 5609660 | 1 | 6.83 | 1267850 | 20.0 |
| n-Hexadecanoic acid | 11.87 | 4.4 | ng | 427602 | 4 | 11.35 | 1933710 | 20.0 |
| 1-Heneicosanol | 13.83 | 12.4 | ng | 936570 | 5 | 13.99 | 1504730 | 20.0 |
| Tricosane | 14.44 | 2.3 | ng | 169970 | 5 | 13.99 | 1504730 | 20.0 |
| Octacosane | 15.07 | 3.2 | ng | 226375 | 6 | 15.46 | 1425980 | 20.0 |
| Tetracosane | 15.87 | 2.5 | ng | 174889 | 6 | 15.46 | 1425980 | 20.0 |