LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

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-BF083019.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 | 5.457 | 569 | 573 | 583 | rBV | 1163802 | 995563 | 41.05% | 5.898% |
| 2 | 6.469 | 741 | 745 | 758 | rBV | 1397694 | 1142410 | 47.11% | 6.768% |
| 3 | 6.610 | 766 | 769 | 773 | rBV | 1252269 | 1120208 | 46.19% | 6.637% |
| 4 | 6.845 | 806 | 809 | 813 | rBV | 807292 | 626845 | 25.85% | 3.714% |
| 5 | 7.004 | 832 | 836 | 839 | rBV | 1022903 | 846030 | 34.89% | 5.012% |
| 6 | 7.398 | 899 | 903 | 912 | rBV | 828210 | 688803 | 28.40% | 4.081% |
| 7 | 8.128 | 1023 | 1027 | 1031 | rBV | 1103523 | 851781 | 35.12% | 5.047% |
| 8 | 9.198 | 1206 | 1209 | 1213 | rBV | 1700007 | 1446981 | 59.67% | 8.573% |
| 9 | 9.592 | 1273 | 1276 | 1281 | rBV | 130448 | 109498 | 4.52% | 0.649% |
| 10 | 9.880 | 1321 | 1325 | 1328 | rBV | 1255529 | 1012565 | 41.75% | 5.999% |
| 11 | 10.663 | 1454 | 1458 | 1468 | rBV | 1484444 | 1306012 | 53.85% | 7.738% |
| 12 | 11.363 | 1573 | 1577 | 1580 | rBV | 1196664 | 1021972 | 42.14% | 6.055% |
| 13 | 11.886 | 1662 | 1666 | 1670 | rBV | 101761 | 98296 | 4.05% | 0.582% |
| 14 | 12.668 | 1795 | 1799 | 1807 | rBV5 | 19226 | 27005 | 1.11% | 0.160% |
| 15 | 12.945 | 1841 | 1846 | 1849 | rBV | 2586402 | 2425164 | 100.00% | 14.368% |
| 16 | 13.421 | 1918 | 1927 | 1933 | rBV | 62583 | 100680 | 4.15% | 0.597% |
| 17 | 13.515 | 1937 | 1943 | 1946 | rBV2 | 46058 | 50165 | 2.07% | 0.297% |
| 18 | 13.833 | 1994 | 1997 | 2005 | rBV2 | 164565 | 240284 | 9.91% | 1.424% |
| 19 | 13.992 | 2020 | 2024 | 2028 | rVB | 1019127 | 873343 | 36.01% | 5.174% |
| 20 | 14.157 | 2049 | 2052 | 2056 | rBV | 79903 | 79759 | 3.29% | 0.473% |
| 21 | 14.462 | 2101 | 2104 | 2108 | rBV | 116415 | 103931 | 4.29% | 0.616% |
| 22 | 14.768 | 2152 | 2156 | 2159 | rVB | 128749 | 127877 | 5.27% | 0.758% |
| 23 | 15.098 | 2208 | 2212 | 2221 | rVB | 148150 | 183637 | 7.57% | 1.088% |
| 24 | 15.445 | 2266 | 2271 | 2274 | rBV | 715489 | 874639 | 36.07% | 5.182% |
| 25 | 15.480 | 2274 | 2277 | 2282 | rVB | 143265 | 179466 | 7.40% | 1.063% |
| 26 | 15.909 | 2345 | 2350 | 2354 | rBV | 108357 | 159419 | 6.57% | 0.945% |
| 27 | 16.409 | 2430 | 2435 | 2442 | rVB2 | 67234 | 121345 | 5.00% | 0.719% |
| 28 | 16.998 | 2531 | 2535 | 2542 | rVB4 | 35720 | 64779 | 2.67% | 0.384% |

Sum of corrected areas: 16878457

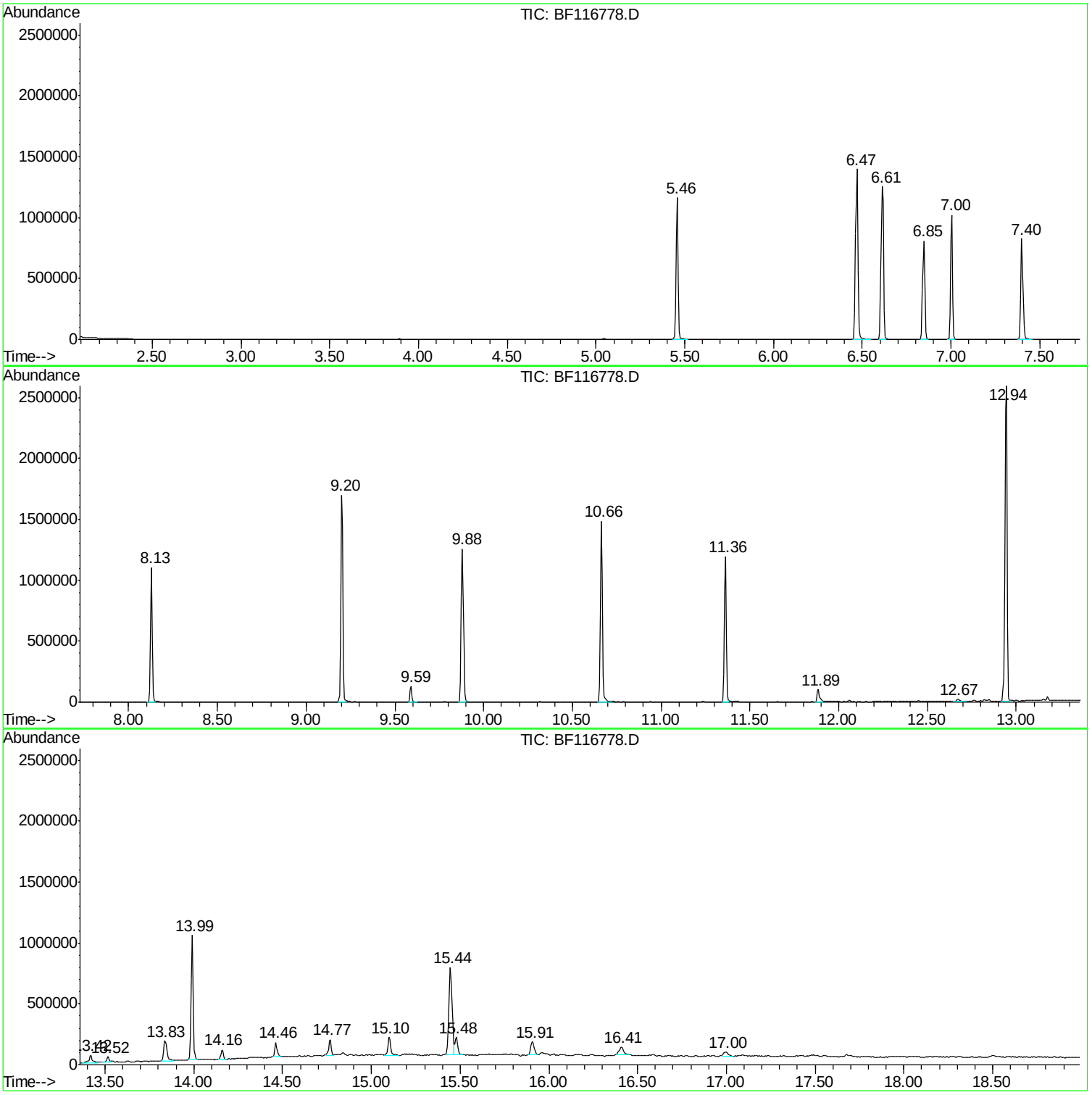
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

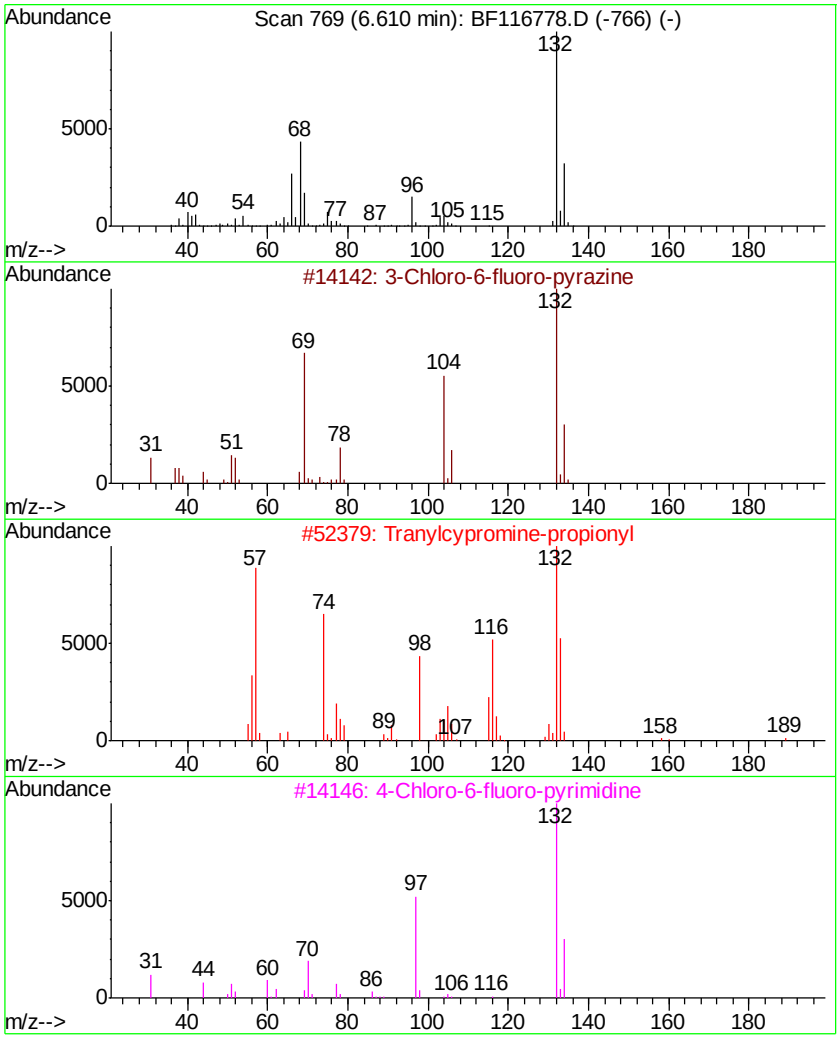
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

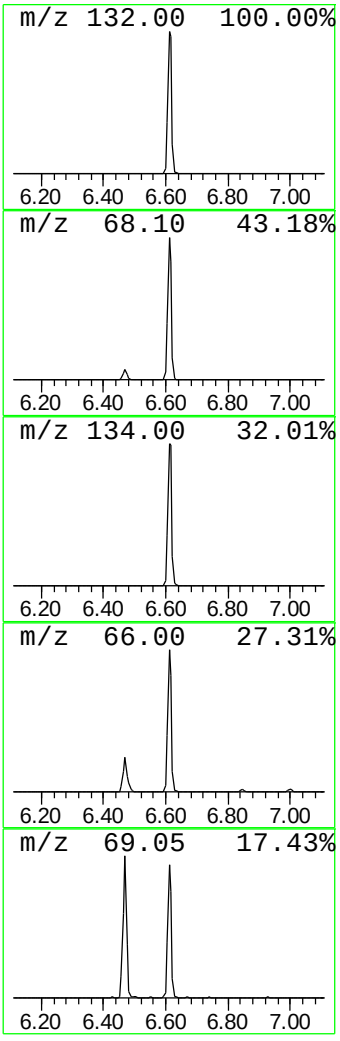
**********

Peak Number 1 unknown6.61 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.61 | 35.74 ng | 1120210 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

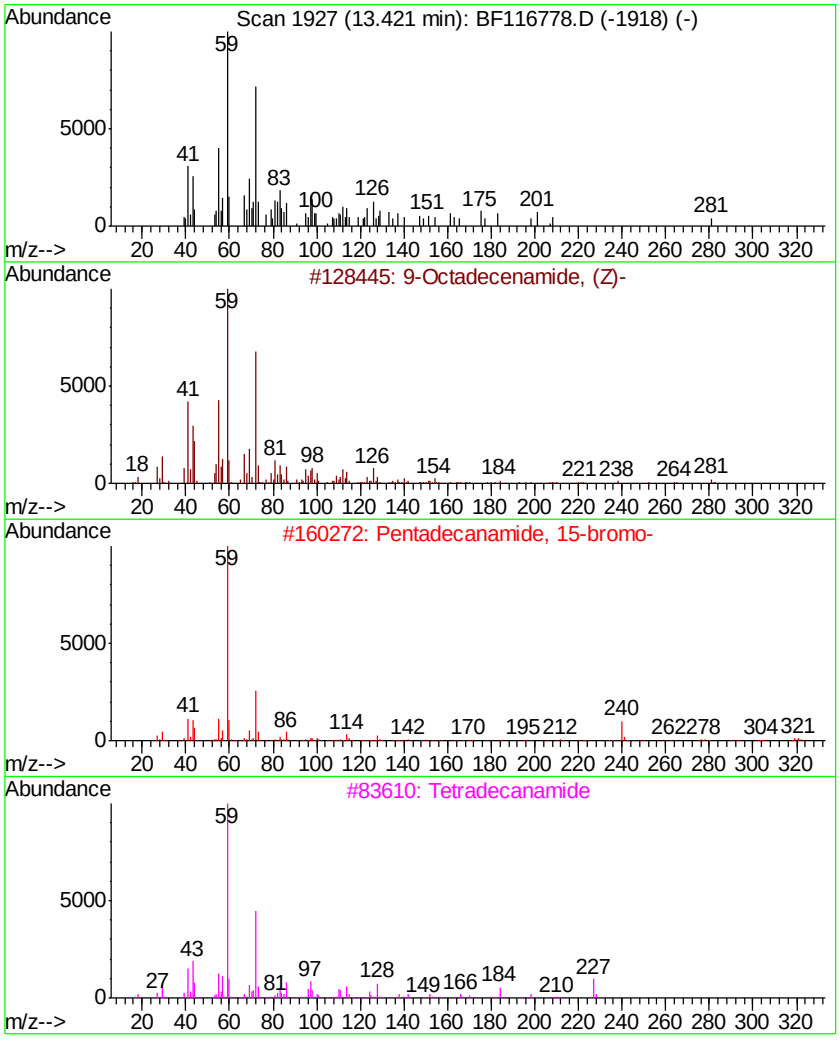
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

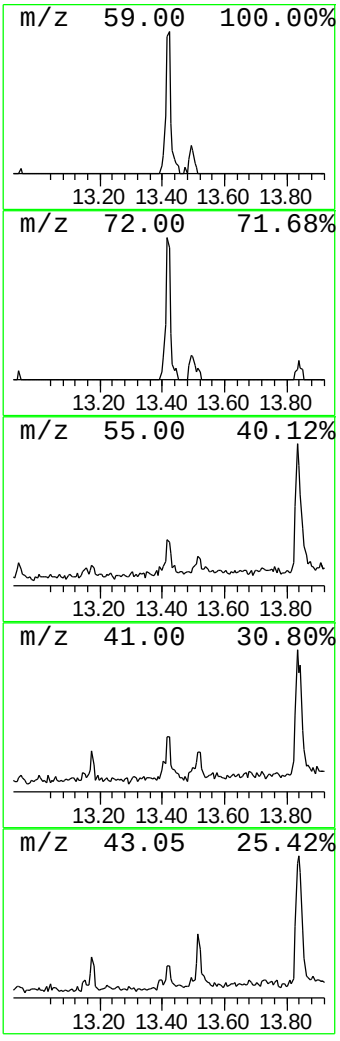
**********

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.42 | 2.31 ng | 100680 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 93 |
| 2 | Pentadecanamide, 15-bromo- | 319 | C15H30BrNO | 1000163-86-1 | 47 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 47 |
| 4 | 2-Hydroxy-2-methylundec-5-en-3-one | 198 | C12H22O2 | 1000191-46-2 | 43 |
| 5 | Heptanamide, 4-ethyl-5-methyl- | 171 | C10H21NO | 054789-40-1 | 40 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

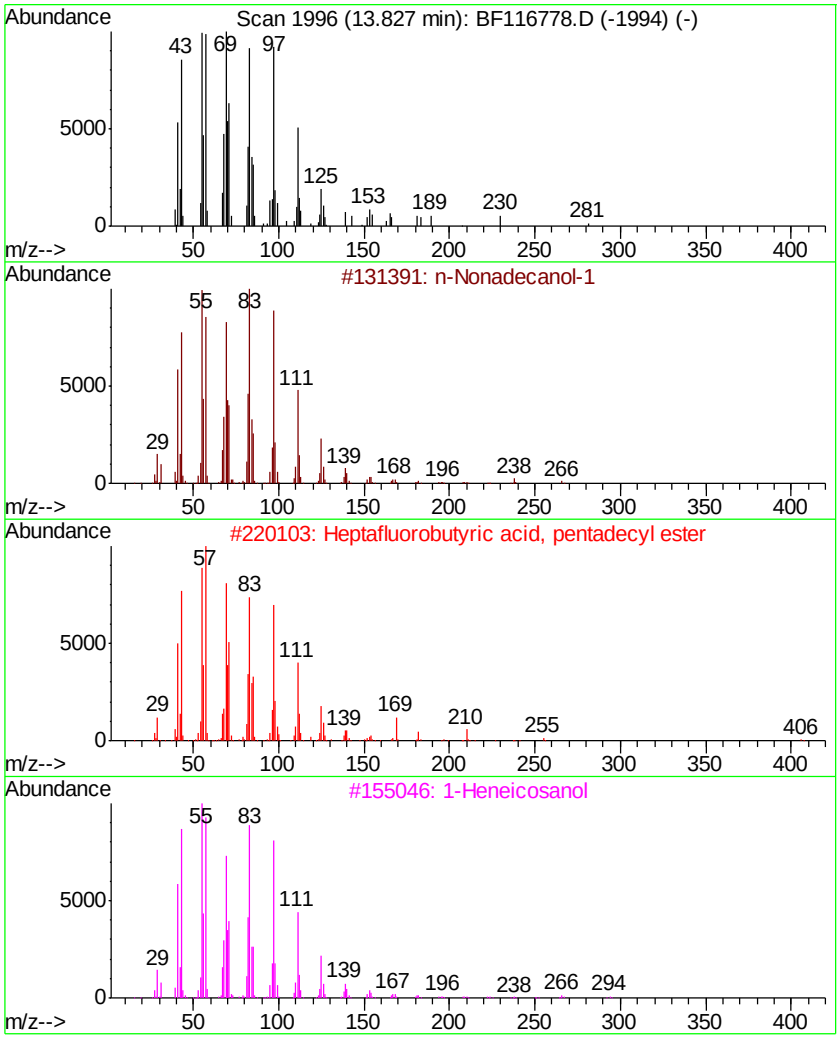
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

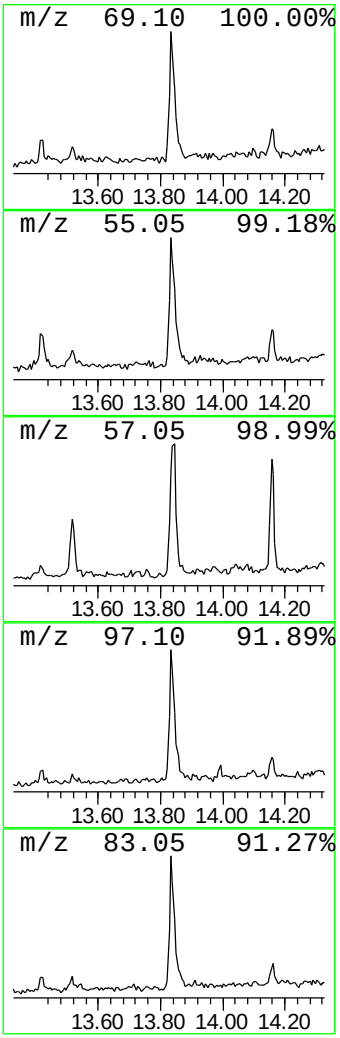
**********

Peak Number 4 n-Nonadecanol-1 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.83 | 5.50 ng | 240284 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 2 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 4 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 5 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

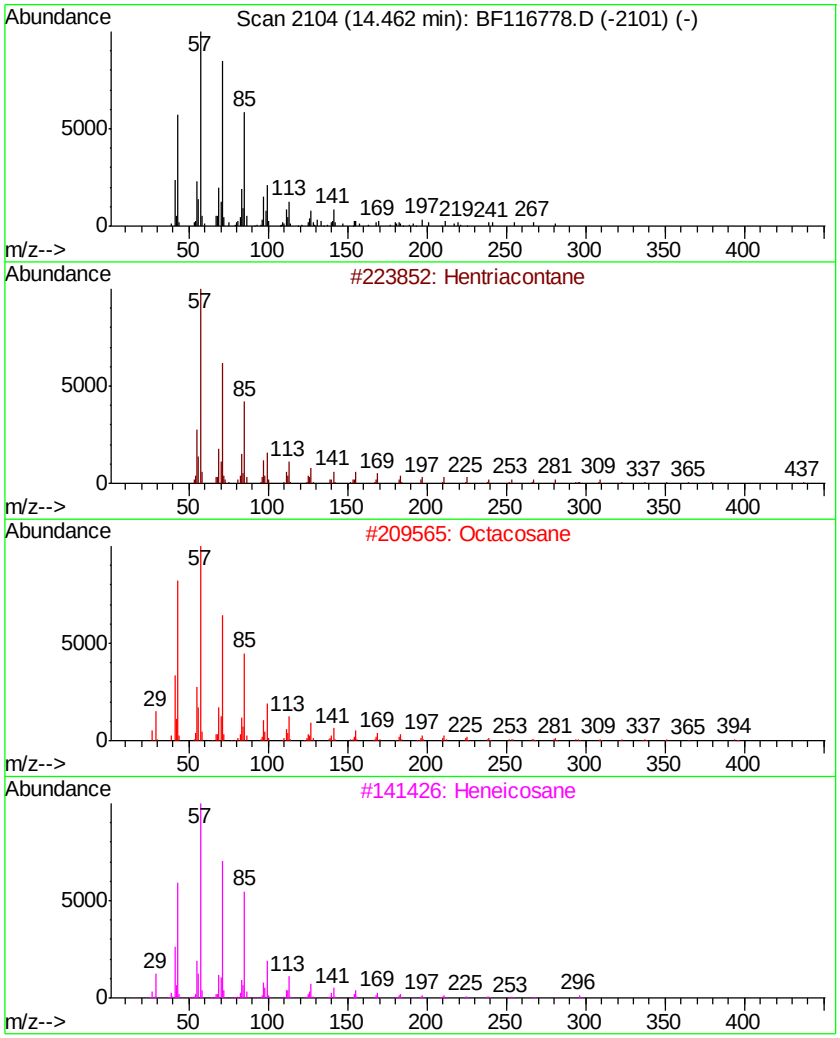
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

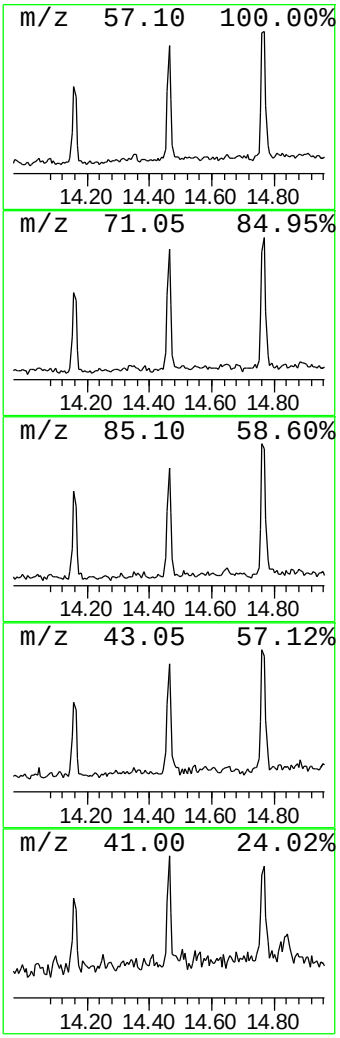
**********

Peak Number 5 Hentriacontane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.46 | 2.38 ng | 103931 | Chrysene-d12 | 13.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

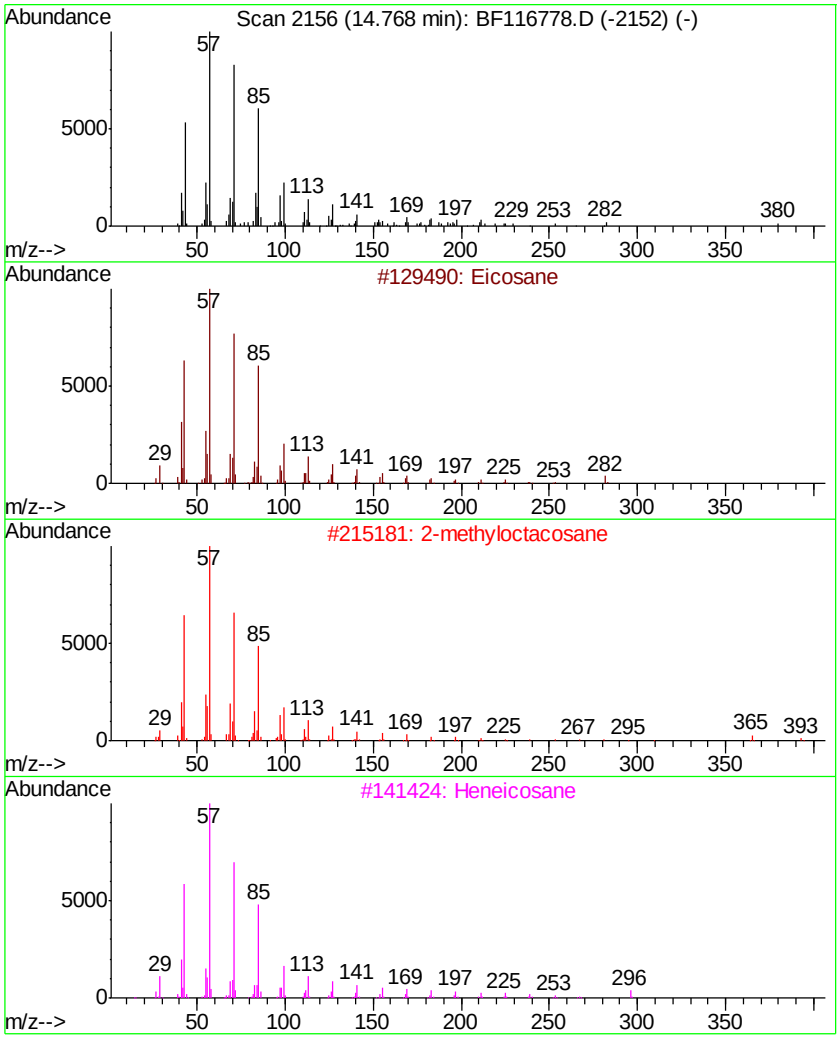
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

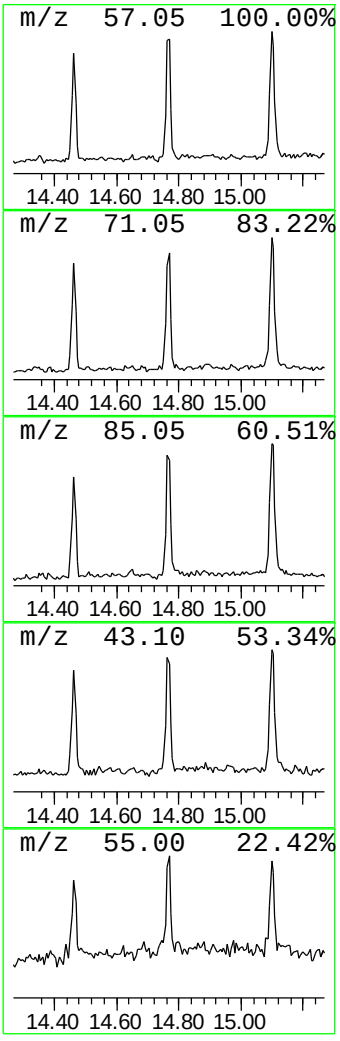
**********

Peak Number 6 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.77 | 2.92 ng | 127877 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 94 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 90 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

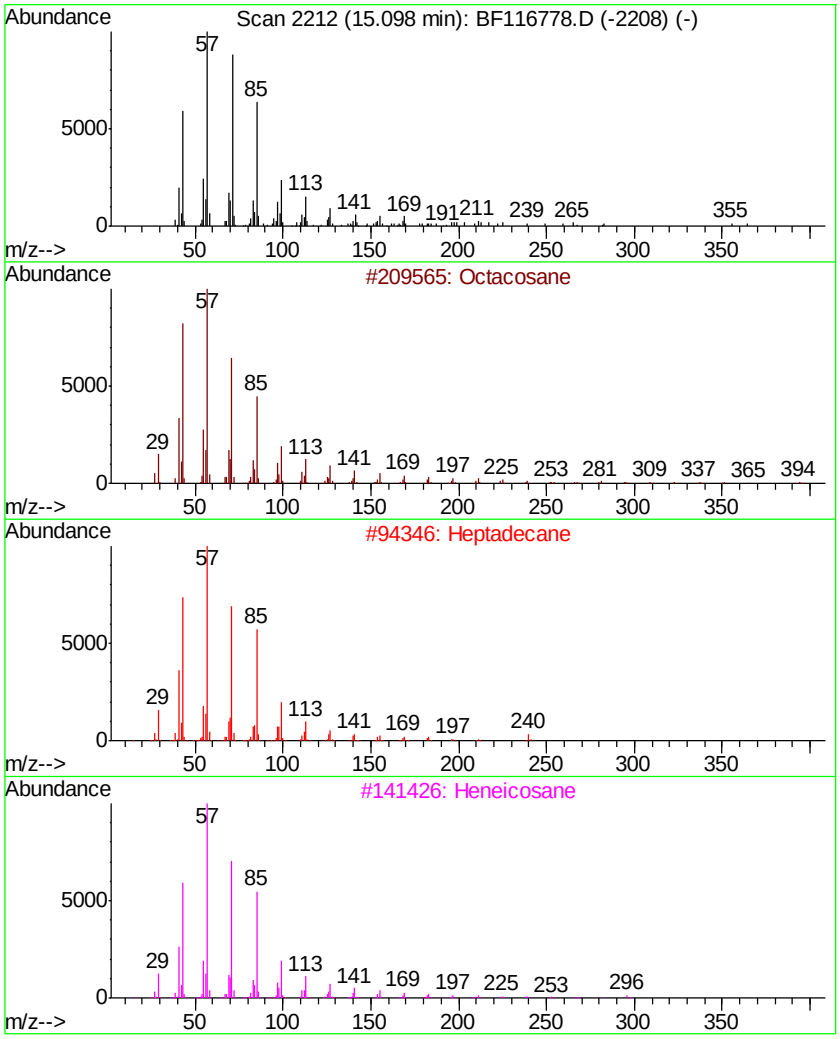
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

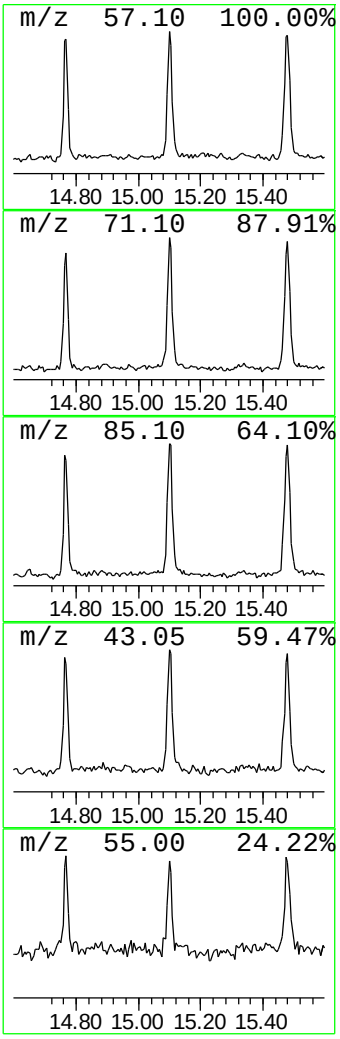
**********

Peak Number 7 Octacosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.10 | 4.20 ng | 183637 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 91 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

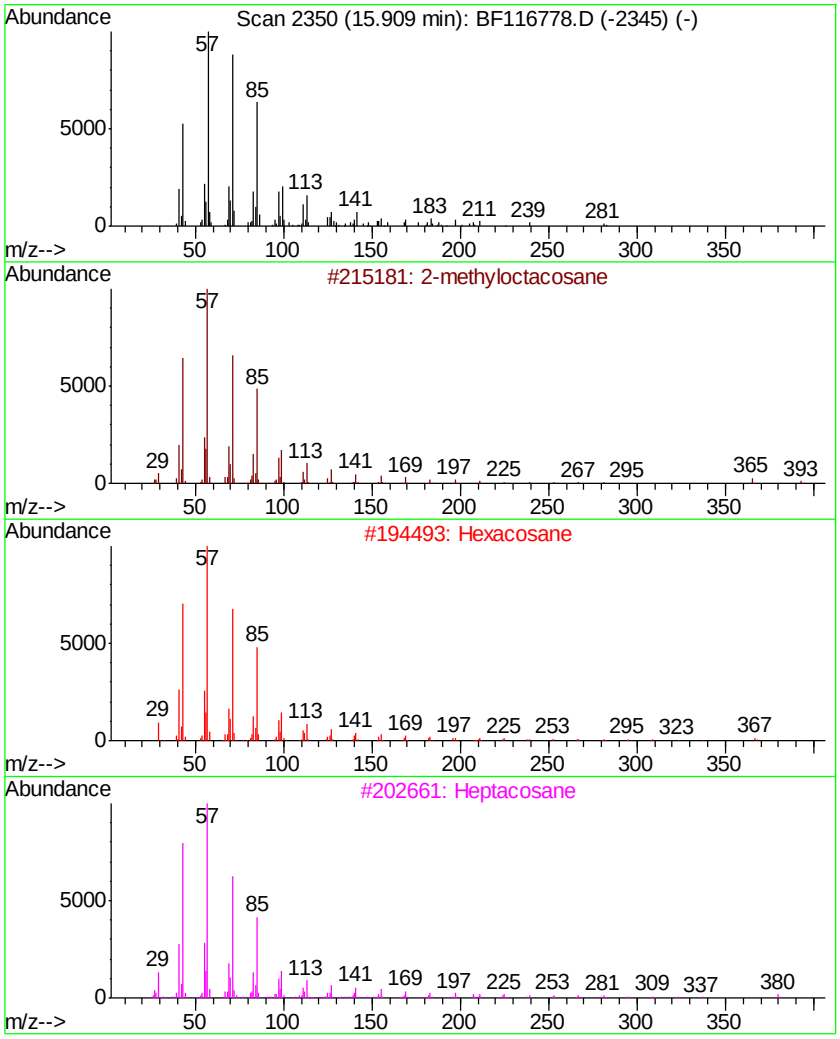
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

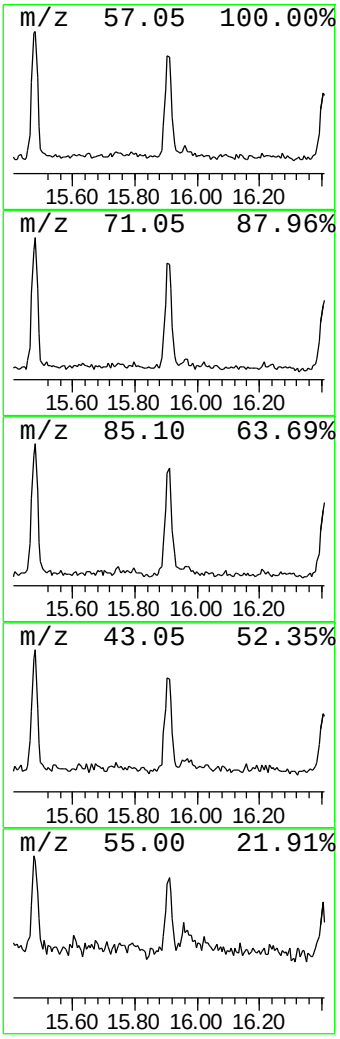
**********

Peak Number 8 2-methyloctacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.91 | 3.65 ng | 159419 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

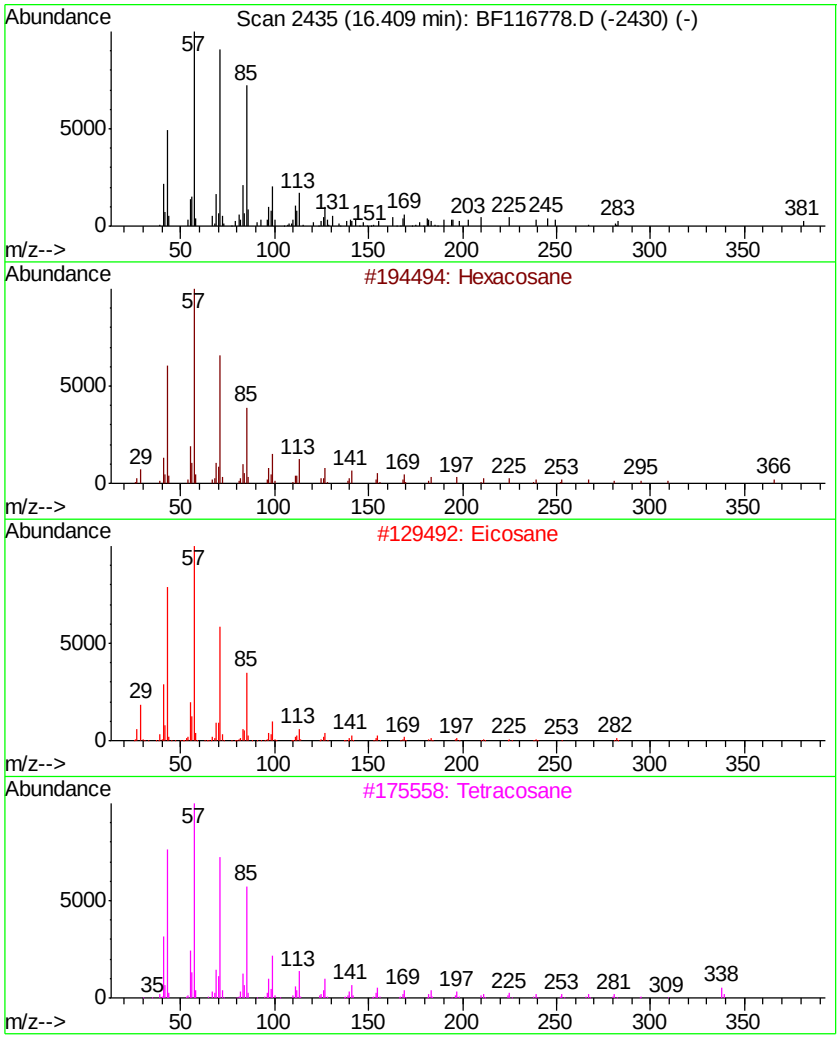
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

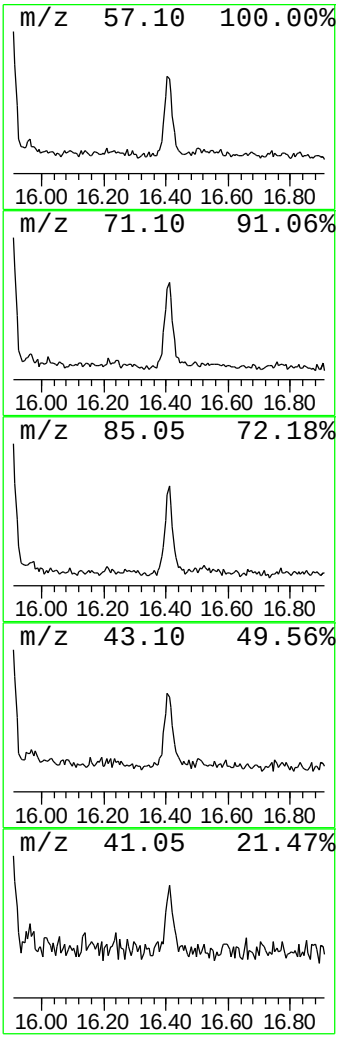
**********

Peak Number 9 Hexacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.41 | 2.77 ng | 121345 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 86 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 81 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 80 |
| 4 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 80 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 78 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090319\
Data File : BF116778.D
Acq On : 3 Sep 2019 17:52
Operator : HP/JU
Sample : K4554-27
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-6-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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 |
| unknown6.61 | 6.61 | 35.7 | ng | 1120210 | 1 | 6.85 | 626845 | 20.0 |
| 9-Octadecenamide,... | 13.42 | 2.3 | ng | 100680 | 5 | 13.99 | 873343 | 20.0 |
| n-Nonadecanol-1 | 13.83 | 5.5 | ng | 240284 | 5 | 13.99 | 873343 | 20.0 |
| Hentriacontane | 14.46 | 2.4 | ng | 103931 | 5 | 13.99 | 873343 | 20.0 |
| Eicosane | 14.77 | 2.9 | ng | 127877 | 6 | 15.44 | 874639 | 20.0 |
| Octacosane | 15.10 | 4.2 | ng | 183637 | 6 | 15.44 | 874639 | 20.0 |
| 2-methyloctacosane | 15.91 | 3.6 | ng | 159419 | 6 | 15.44 | 874639 | 20.0 |
| Hexacosane | 16.41 | 2.8 | ng | 121345 | 6 | 15.44 | 874639 | 20.0 |