LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-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-BF042219.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 | 2.216 | 16 | 22 | 27 | rVB | 48457 | 70669 | 1.89% | 0.233% |
| 2 | 5.522 | 579 | 584 | 587 | rBV | 2995131 | 2954524 | 78.92% | 9.757% |
| 3 | 6.522 | 749 | 754 | 757 | rBV | 2669102 | 3054081 | 81.58% | 10.086% |
| 4 | 6.669 | 774 | 779 | 782 | rBV | 3329371 | 3222786 | 86.09% | 10.643% |
| 5 | 6.892 | 814 | 817 | 821 | rBV | 791622 | 693556 | 18.53% | 2.290% |
| 6 | 7.051 | 840 | 844 | 848 | rBV | 2821859 | 2605168 | 69.59% | 8.604% |
| 7 | 7.451 | 907 | 912 | 915 | rBV | 1923664 | 1982176 | 52.95% | 6.546% |
| 8 | 8.175 | 1031 | 1035 | 1050 | rBV | 1011221 | 871997 | 23.29% | 2.880% |
| 9 | 9.251 | 1213 | 1218 | 1221 | rBV | 4269988 | 3743659 | 100.00% | 12.363% |
| 10 | 9.639 | 1280 | 1284 | 1289 | rBV | 374904 | 319700 | 8.54% | 1.056% |
| 11 | 9.927 | 1329 | 1333 | 1345 | rVB | 1022721 | 1015504 | 27.13% | 3.354% |
| 12 | 10.716 | 1463 | 1467 | 1483 | rBV | 2343970 | 2262770 | 60.44% | 7.473% |
| 13 | 11.416 | 1582 | 1586 | 1593 | rBV | 1130548 | 1026880 | 27.43% | 3.391% |
| 14 | 11.939 | 1671 | 1675 | 1685 | rBV2 | 107436 | 130970 | 3.50% | 0.433% |
| 15 | 12.721 | 1804 | 1808 | 1820 | rBV | 91298 | 110976 | 2.96% | 0.366% |
| 16 | 12.998 | 1851 | 1855 | 1858 | rBV | 3899489 | 3512874 | 93.84% | 11.601% |
| 17 | 14.057 | 2025 | 2035 | 2051 | rBV | 917443 | 1151397 | 30.76% | 3.803% |
| 18 | 14.227 | 2061 | 2064 | 2070 | rVB | 52693 | 51895 | 1.39% | 0.171% |
| 19 | 14.539 | 2112 | 2117 | 2120 | rBV | 81518 | 77389 | 2.07% | 0.256% |
| 20 | 14.857 | 2167 | 2171 | 2174 | rVB | 96853 | 94184 | 2.52% | 0.311% |
| 21 | 15.198 | 2225 | 2229 | 2235 | rVB | 102966 | 118138 | 3.16% | 0.390% |
| 22 | 15.551 | 2284 | 2289 | 2293 | rBV | 699956 | 886638 | 23.68% | 2.928% |
| 23 | 15.586 | 2293 | 2295 | 2304 | rVB | 100589 | 128862 | 3.44% | 0.426% |
| 24 | 16.033 | 2366 | 2371 | 2377 | rBV | 76294 | 113365 | 3.03% | 0.374% |
| 25 | 16.551 | 2455 | 2459 | 2469 | rVB3 | 42026 | 79841 | 2.13% | 0.264% |

Sum of corrected areas: 30279999

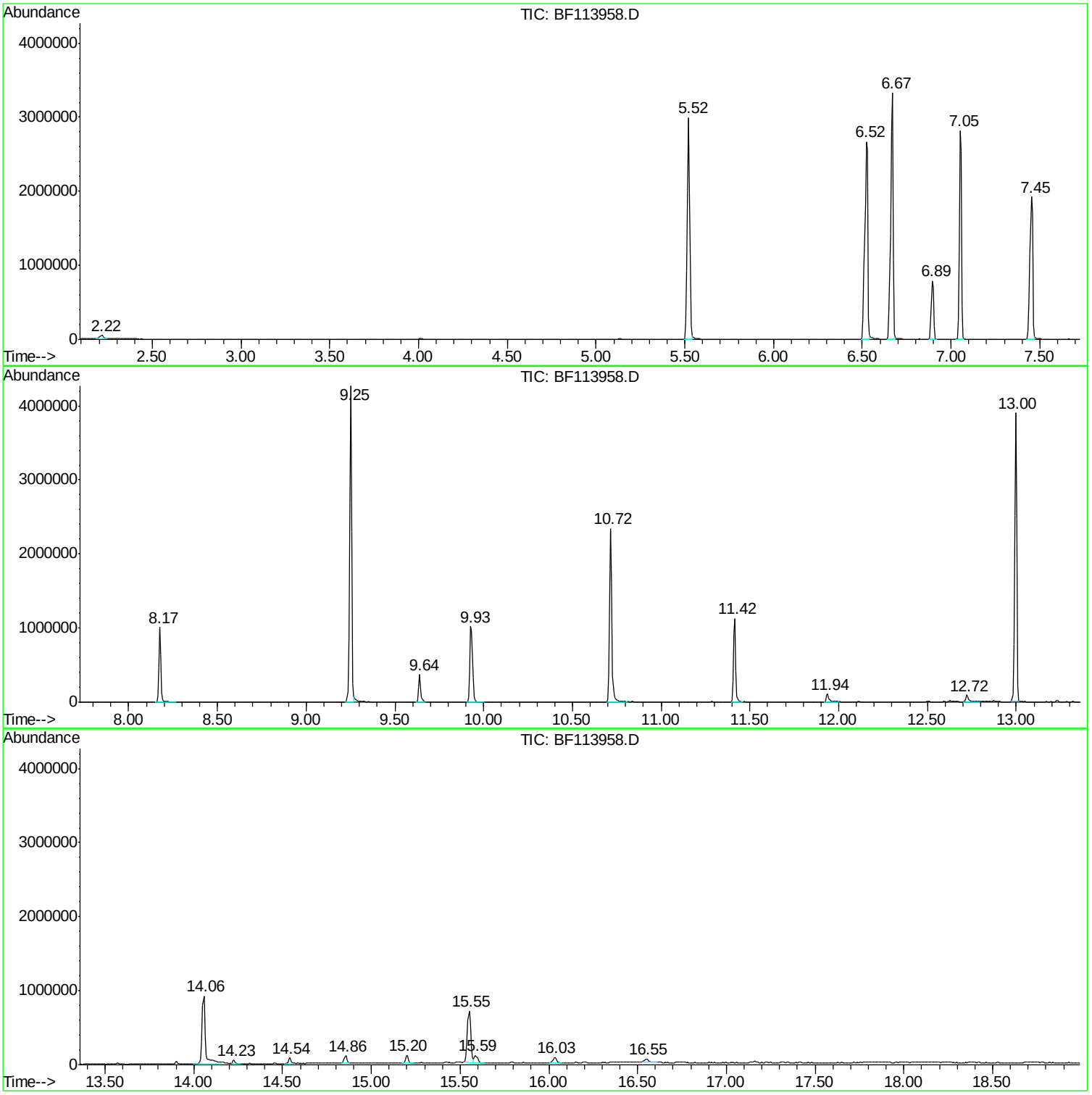
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

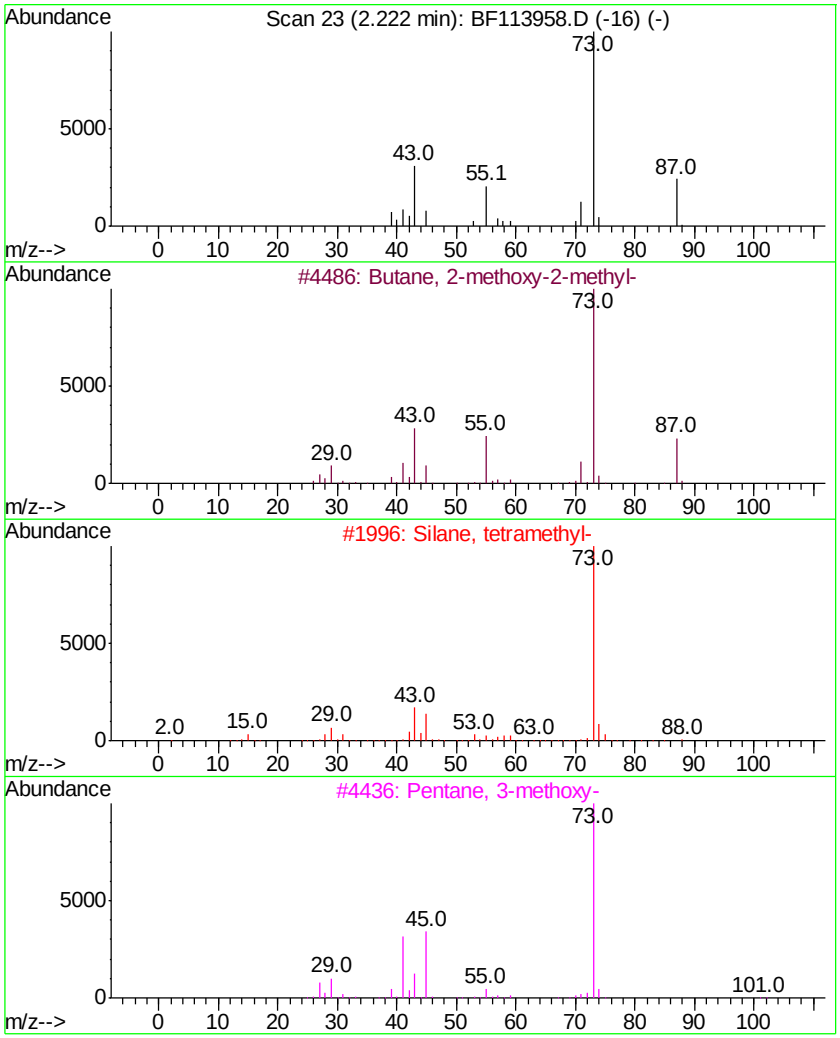
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

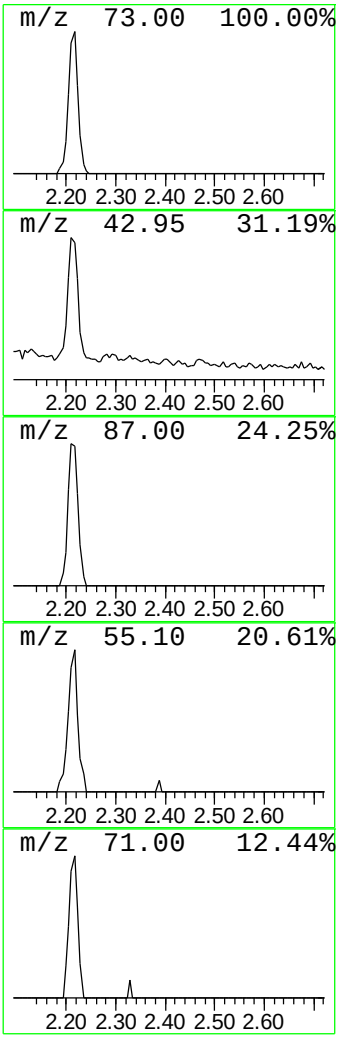
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.22 | 2.04 ng | 70669 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 27 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 25 |
| 4 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 25 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

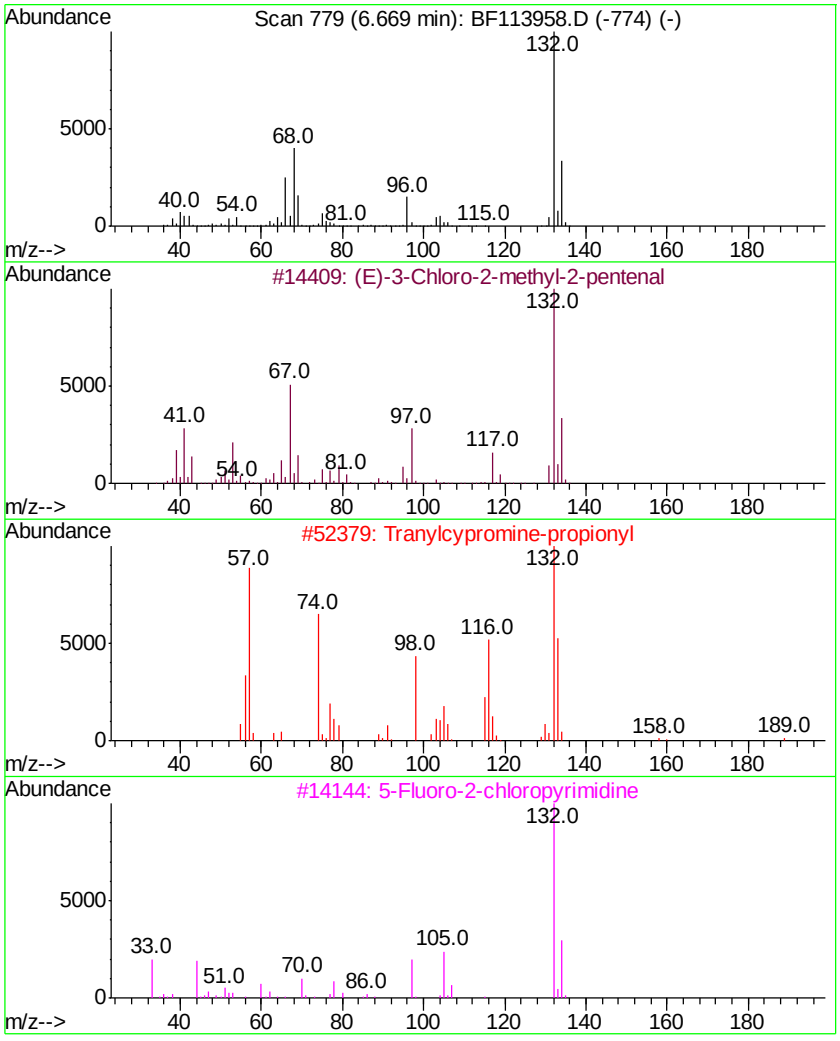
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

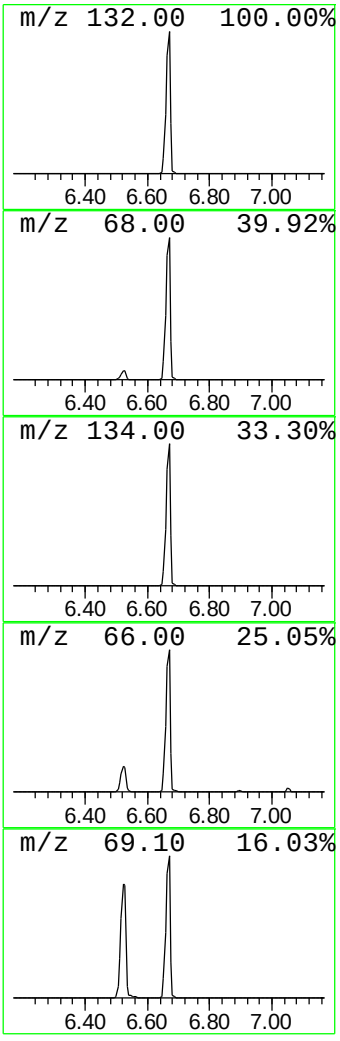
**********

Peak Number 2 unknown6.67 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 92.94 ng | 3222790 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

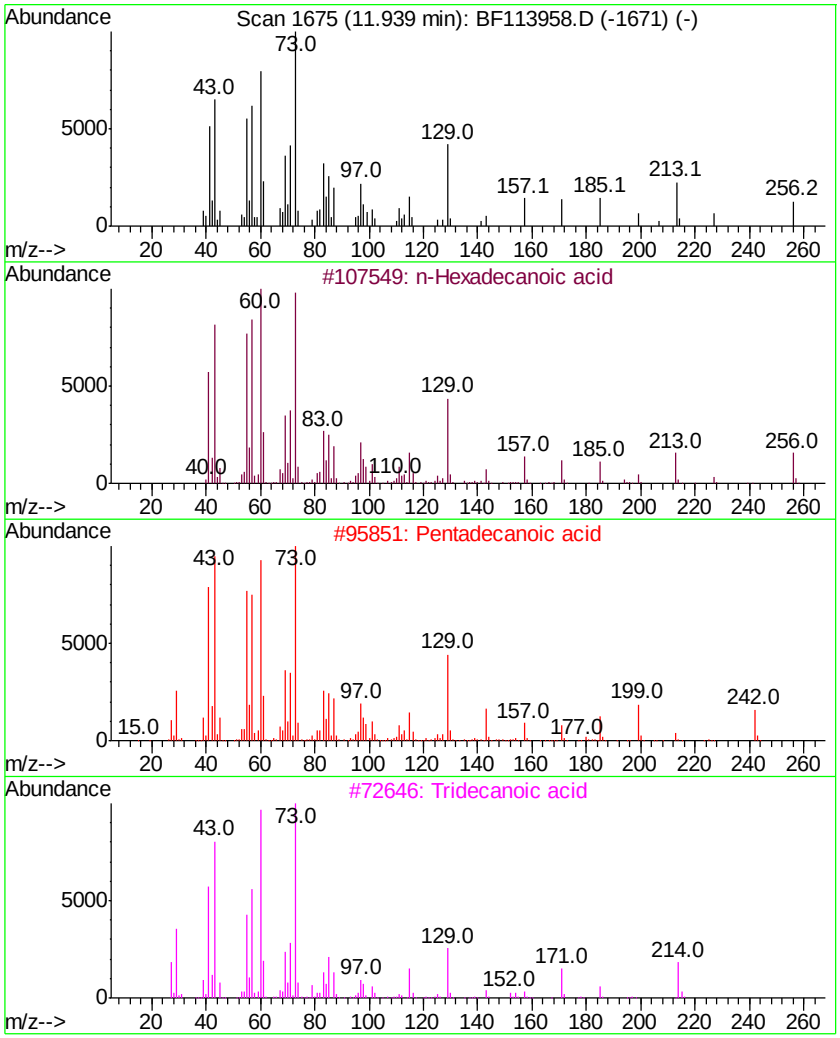
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

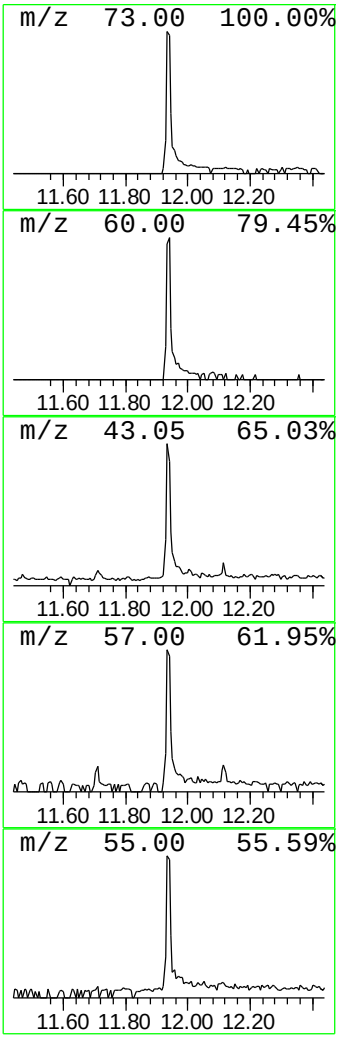
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.94 | 2.55 ng | 130970 | Phenanthrene-d10 | 11.42 |

| 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 | 74 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 68 |
| 4 | Sulfurous acid, 2-propyl tetrade... | 320 | C17H36O3S | 1000309-12-5 | 11 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 11 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

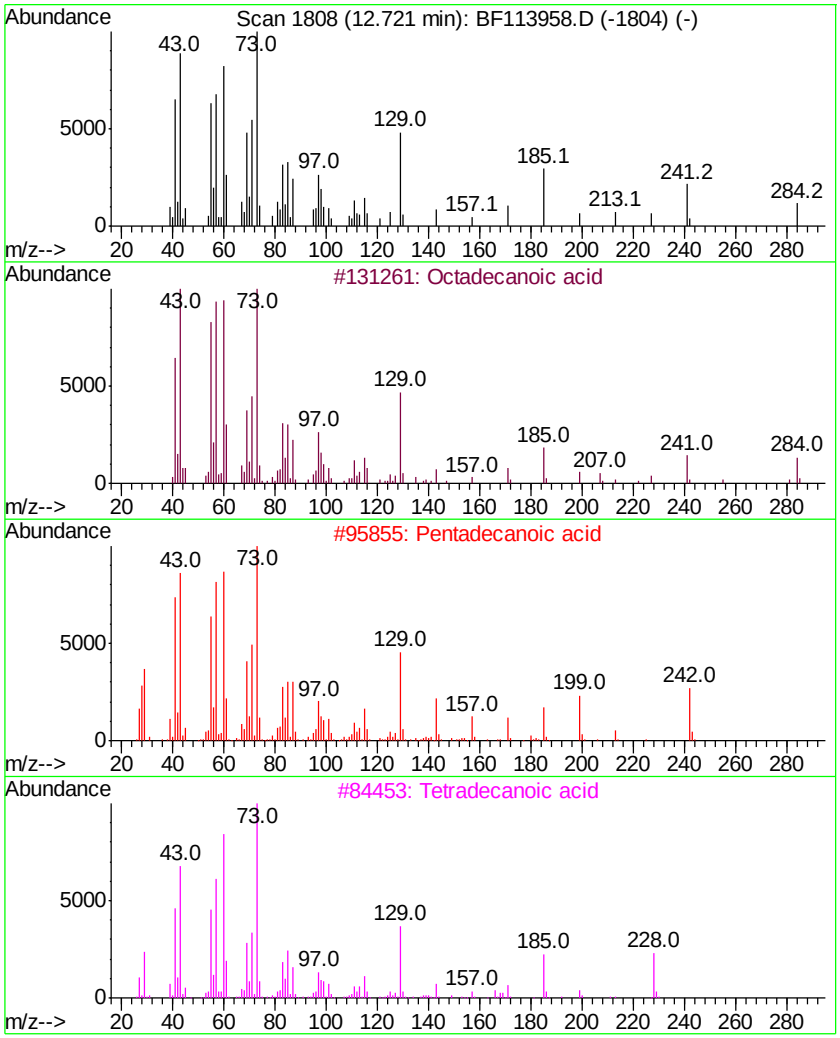
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

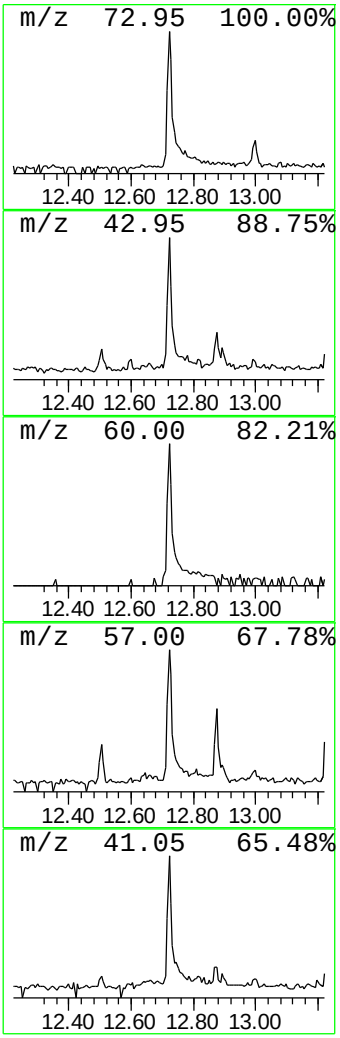
**********

Peak Number 5 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.72 | 2.16 ng | 110976 | Phenanthrene-d10 | 11.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 4 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 58 |
| 5 | Oxalic acid, propyl tetradecyl e... | 328 | C19H36O4 | 1000309-26-7 | 38 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

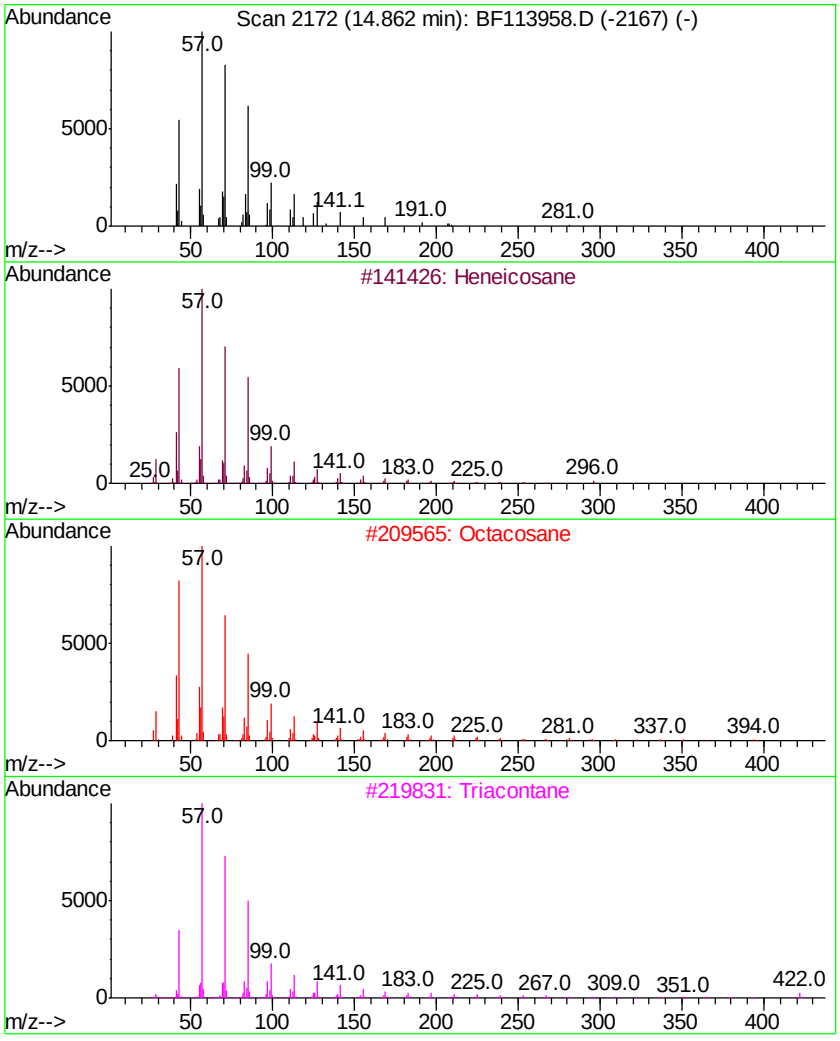
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

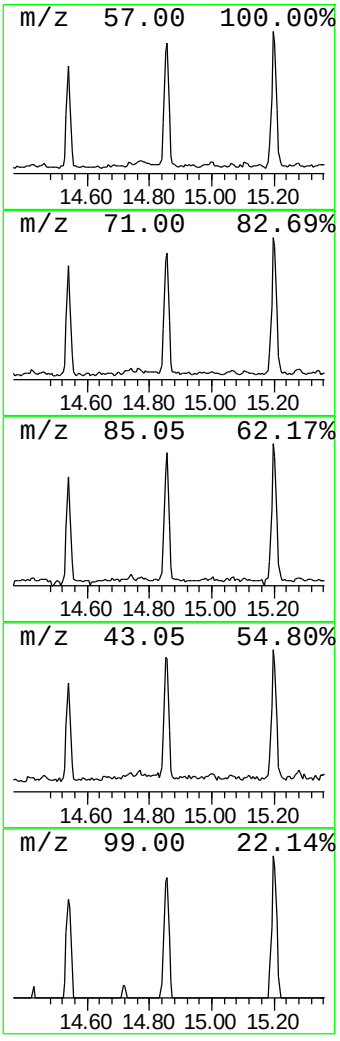
**********

Peak Number 6 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.86 | 2.12 ng | 94184 | Perylene-d12 | 15.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Triacontane | 422 | C30H62 | 000638-68-6 | 91 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 91 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

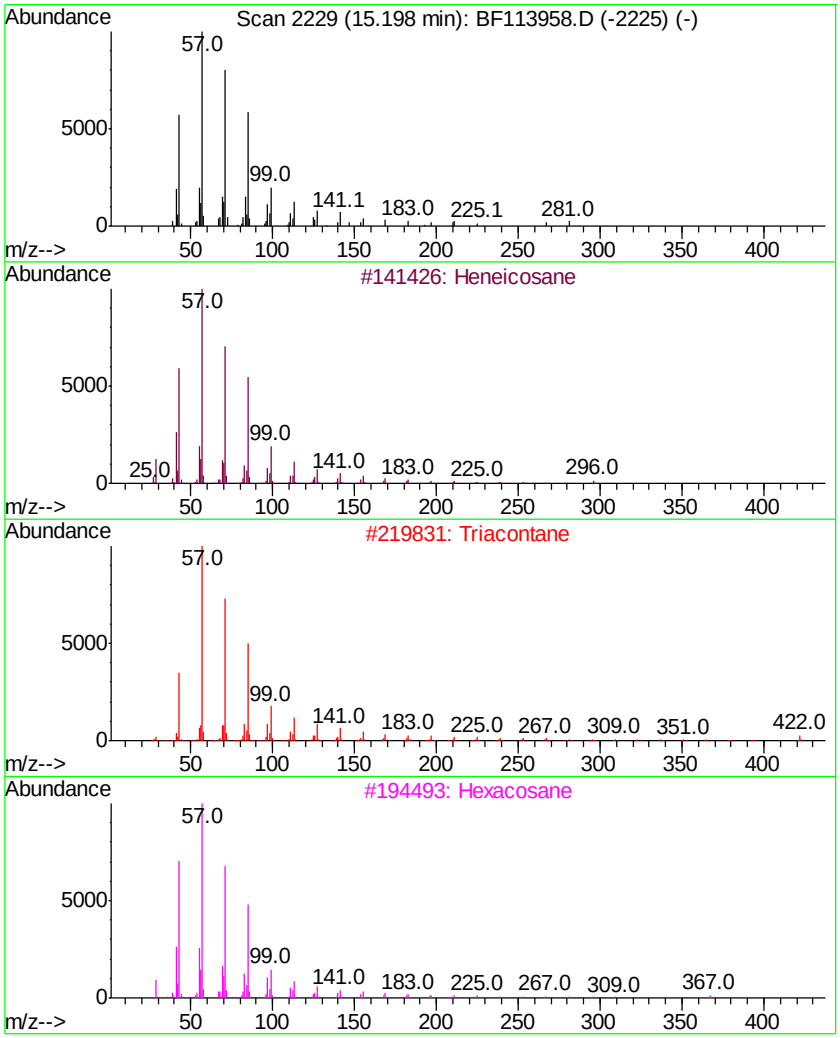
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

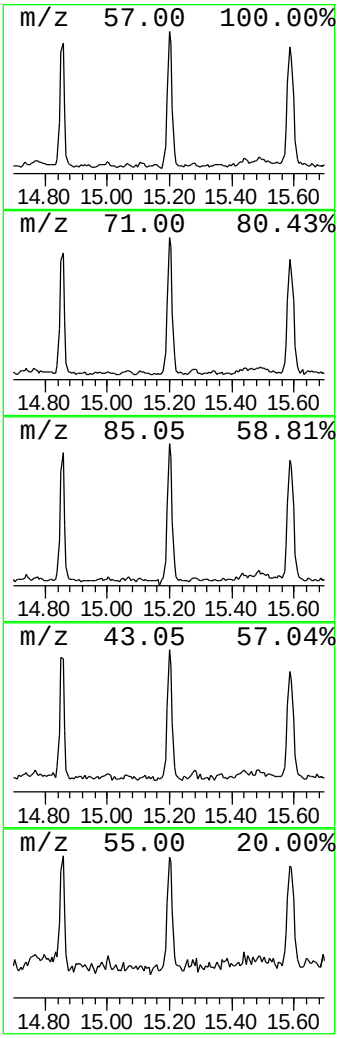
**********

Peak Number 7 Triacontane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.20 | 2.66 ng | 118138 | Perylene-d12 | 15.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Triacontane | 422 | C30H62 | 000638-68-6 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 4 | Pentacosane | 352 | C25H52 | 000629-99-2 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

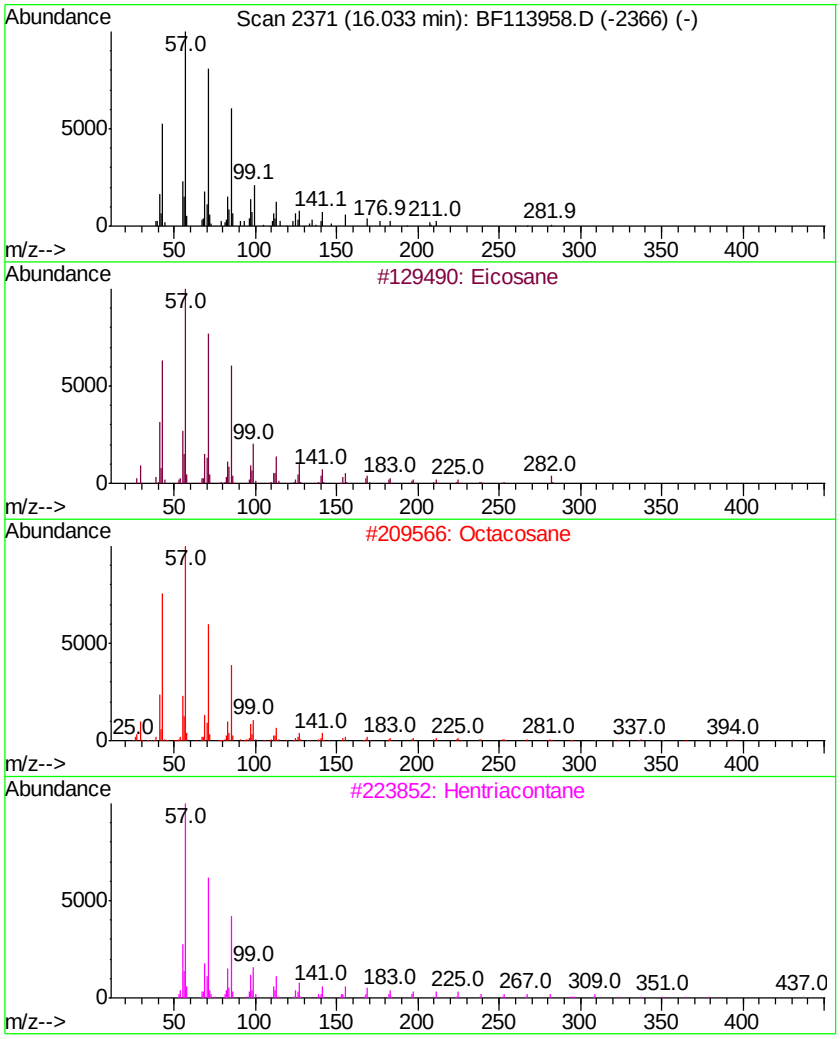
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

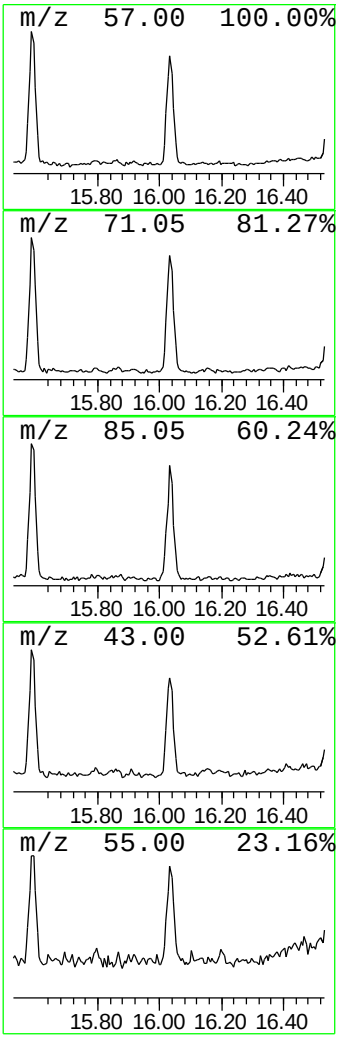
**********

Peak Number 8 Eicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.03 | 2.56 ng | 113365 | Perylene-d12 | 15.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042419\
Data File : BF113958.D
Acq On : 24 Apr 2019 13:51
Operator : JU/SJ
Sample : K2542-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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 |
| Butane, 2-methoxy... | 2.22 | 2.0 | ng | 70669 | 1 | 6.89 | 693556 | 20.0 |
| unknown6.67 | 6.67 | 92.9 | ng | 3222790 | 1 | 6.89 | 693556 | 20.0 |
| n-Hexadecanoic acid | 11.94 | 2.5 | ng | 130970 | 4 | 11.42 | 1026880 | 20.0 |
| Octadecanoic acid | 12.72 | 2.2 | ng | 110976 | 4 | 11.42 | 1026880 | 20.0 |
| Heneicosane | 14.86 | 2.1 | ng | 94184 | 6 | 15.55 | 886638 | 20.0 |
| Triacontane | 15.20 | 2.7 | ng | 118138 | 6 | 15.55 | 886638 | 20.0 |
| Eicosane | 16.03 | 2.6 | ng | 113365 | 6 | 15.55 | 886638 | 20.0 |