LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

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-BF110818.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 | 2.222 | 19 | 23 | 29 | rVB | 64948 | 88121 | 6.58% | 0.782% |
| 2 | 5.169 | 521 | 524 | 538 | rBV | 29508 | 44928 | 3.36% | 0.399% |
| 3 | 5.557 | 586 | 590 | 609 | rBV | 1089029 | 1126714 | 84.18% | 10.002% |
| 4 | 6.563 | 757 | 761 | 775 | rBV | 1165547 | 1221326 | 91.25% | 10.842% |
| 5 | 6.710 | 782 | 786 | 798 | rVB | 1361208 | 1216815 | 90.91% | 10.802% |
| 6 | 6.939 | 821 | 825 | 832 | rBV | 409502 | 354172 | 26.46% | 3.144% |
| 7 | 7.092 | 848 | 851 | 864 | rBV | 1060878 | 935709 | 69.91% | 8.307% |
| 8 | 7.504 | 917 | 921 | 938 | rBV | 761761 | 734259 | 54.86% | 6.518% |
| 9 | 8.222 | 1040 | 1043 | 1064 | rBV | 461612 | 452640 | 33.82% | 4.018% |
| 10 | 9.292 | 1222 | 1225 | 1242 | rBV | 1367843 | 1338473 | 100.00% | 11.882% |
| 11 | 9.692 | 1289 | 1293 | 1306 | rBV | 100585 | 97091 | 7.25% | 0.862% |
| 12 | 9.980 | 1339 | 1342 | 1355 | rBV | 479908 | 454790 | 33.98% | 4.037% |
| 13 | 10.775 | 1474 | 1477 | 1491 | rBV | 637765 | 640294 | 47.84% | 5.684% |
| 14 | 11.480 | 1593 | 1597 | 1607 | rBV | 383482 | 384965 | 28.76% | 3.417% |
| 15 | 11.980 | 1679 | 1682 | 1690 | rBV | 28656 | 33598 | 2.51% | 0.298% |
| 16 | 13.057 | 1861 | 1865 | 1869 | rBV | 1176228 | 1044905 | 78.07% | 9.276% |
| 17 | 13.933 | 2011 | 2014 | 2021 | rBV | 54841 | 68110 | 5.09% | 0.605% |
| 18 | 14.133 | 2044 | 2048 | 2056 | rBV | 411241 | 420469 | 31.41% | 3.733% |
| 19 | 14.251 | 2065 | 2068 | 2074 | rBV | 18600 | 20883 | 1.56% | 0.185% |
| 20 | 14.557 | 2117 | 2120 | 2124 | rBV | 30215 | 35883 | 2.68% | 0.319% |
| 21 | 14.874 | 2170 | 2174 | 2179 | rBV | 39788 | 41225 | 3.08% | 0.366% |
| 22 | 15.221 | 2230 | 2233 | 2238 | rVB | 42941 | 53060 | 3.96% | 0.471% |
| 23 | 15.621 | 2297 | 2301 | 2303 | rBV | 42765 | 53701 | 4.01% | 0.477% |
| 24 | 15.657 | 2303 | 2307 | 2318 | rVB | 192671 | 299020 | 22.34% | 2.654% |
| 25 | 16.074 | 2373 | 2378 | 2382 | rVB2 | 41359 | 61155 | 4.57% | 0.543% |
| 26 | 16.604 | 2463 | 2468 | 2472 | rVB2 | 22964 | 42458 | 3.17% | 0.377% |

Sum of corrected areas: 11264764

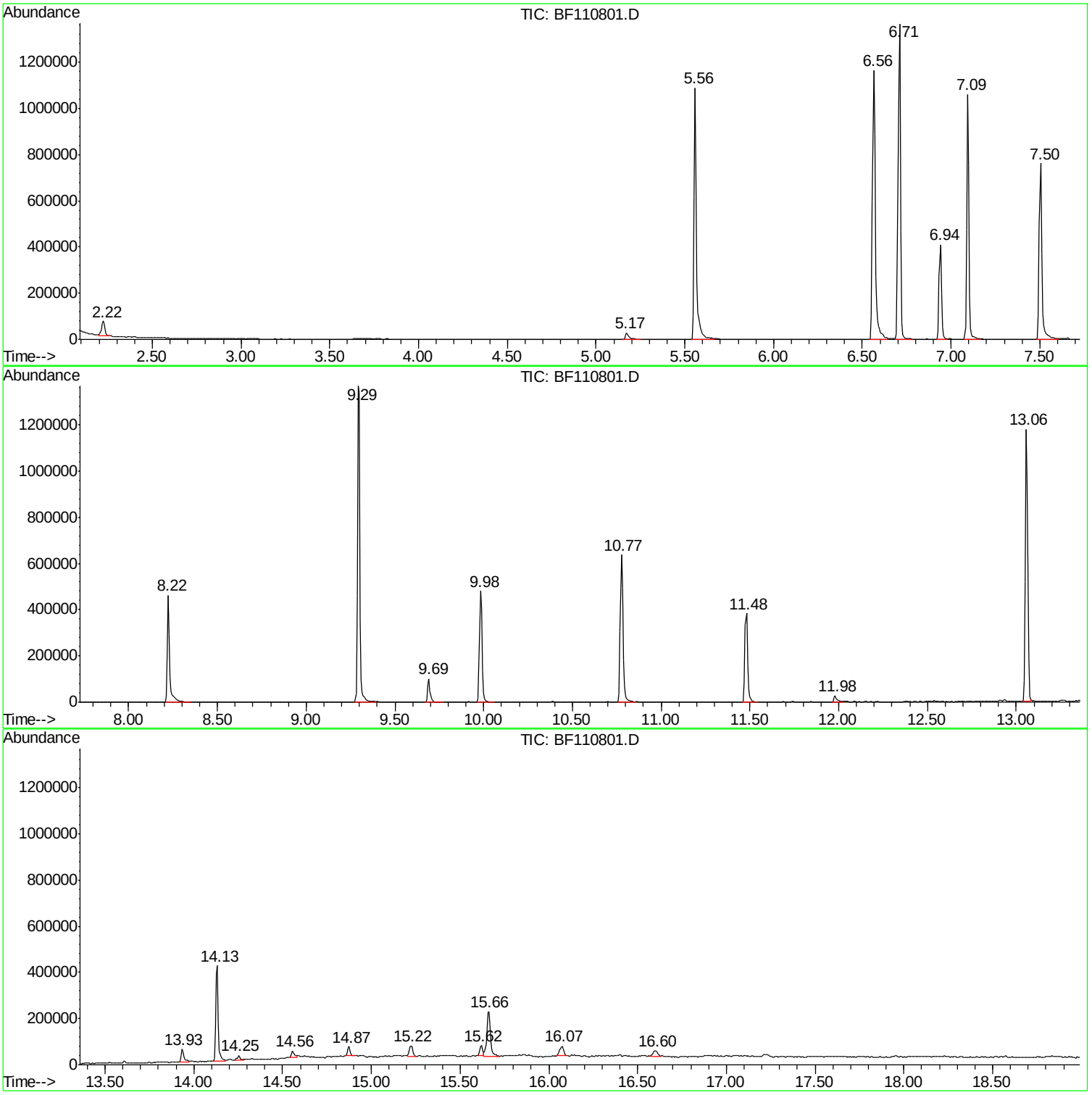
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

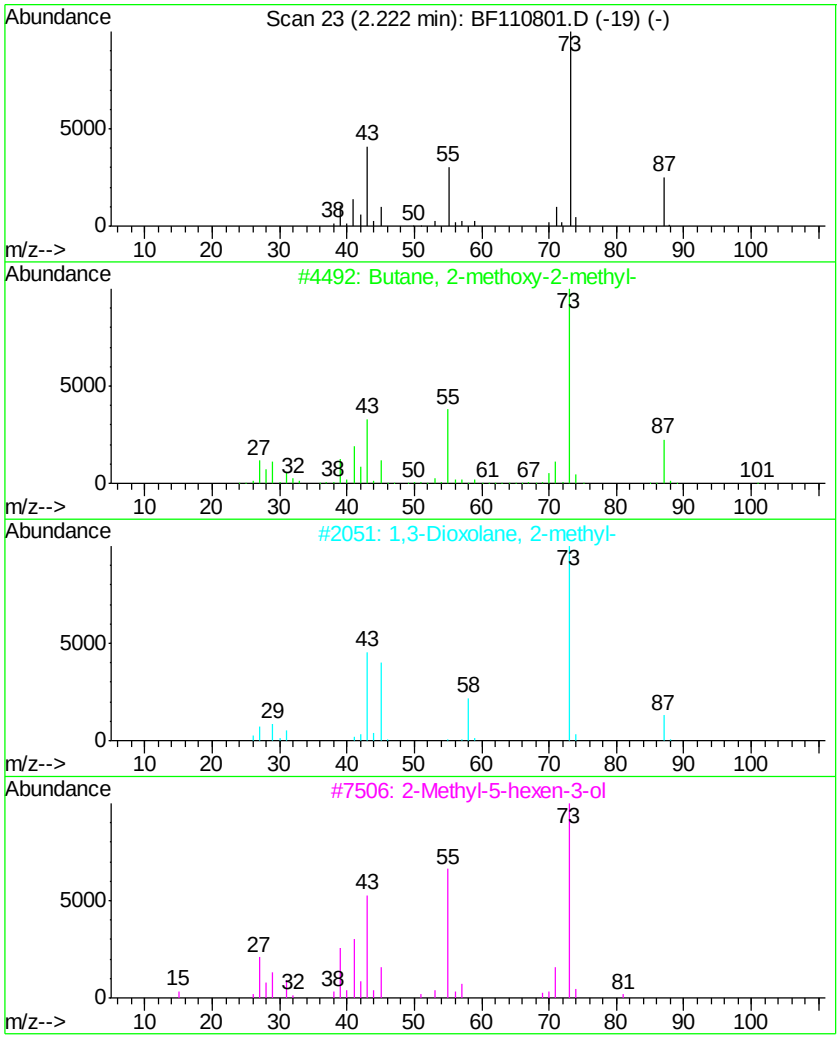
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

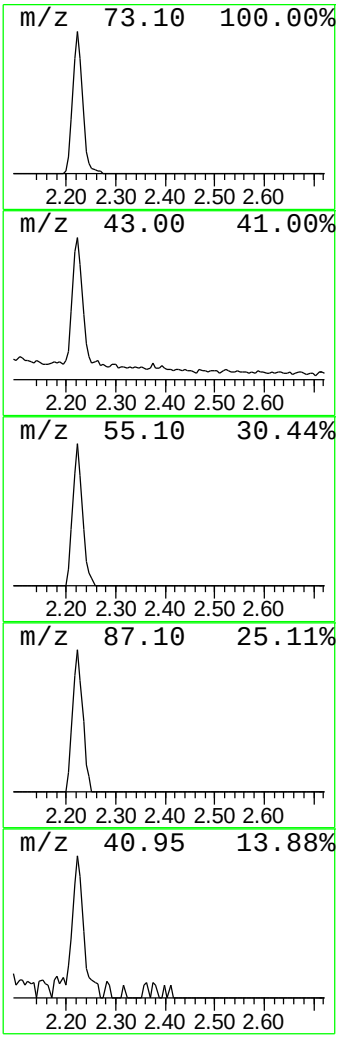
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.22 | 4.98 ng | 88121 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 37 |
| 3 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 25 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 12 |
| 5 | 1-Propene-1-thiol | 74 | C3H6S | 000925-89-3 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

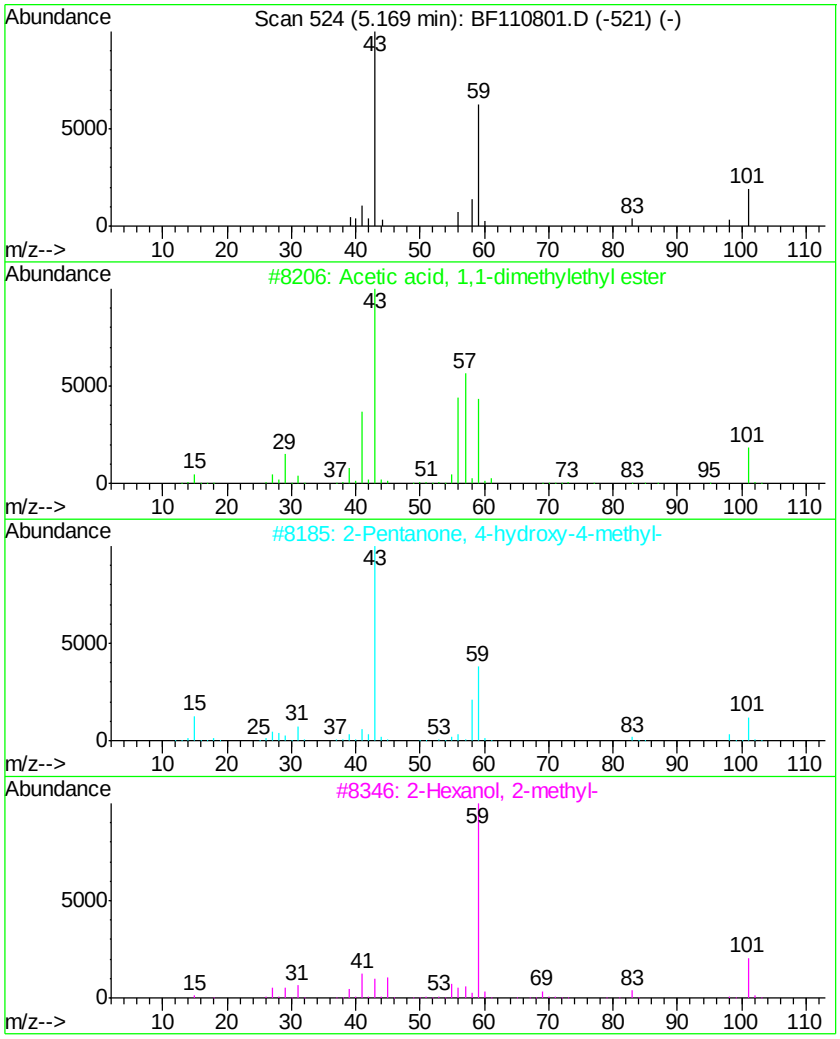
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

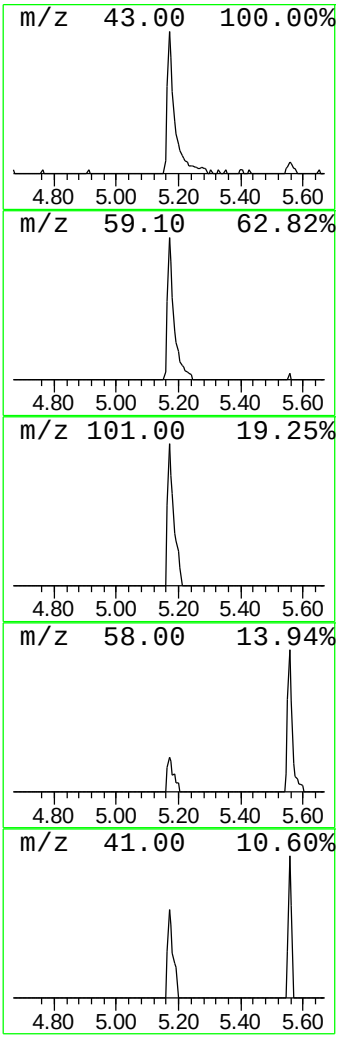
**********

Peak Number 2 unknown5.17 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 2.54 ng | 44928 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 2 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 36 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 36 |
| 4 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 28 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

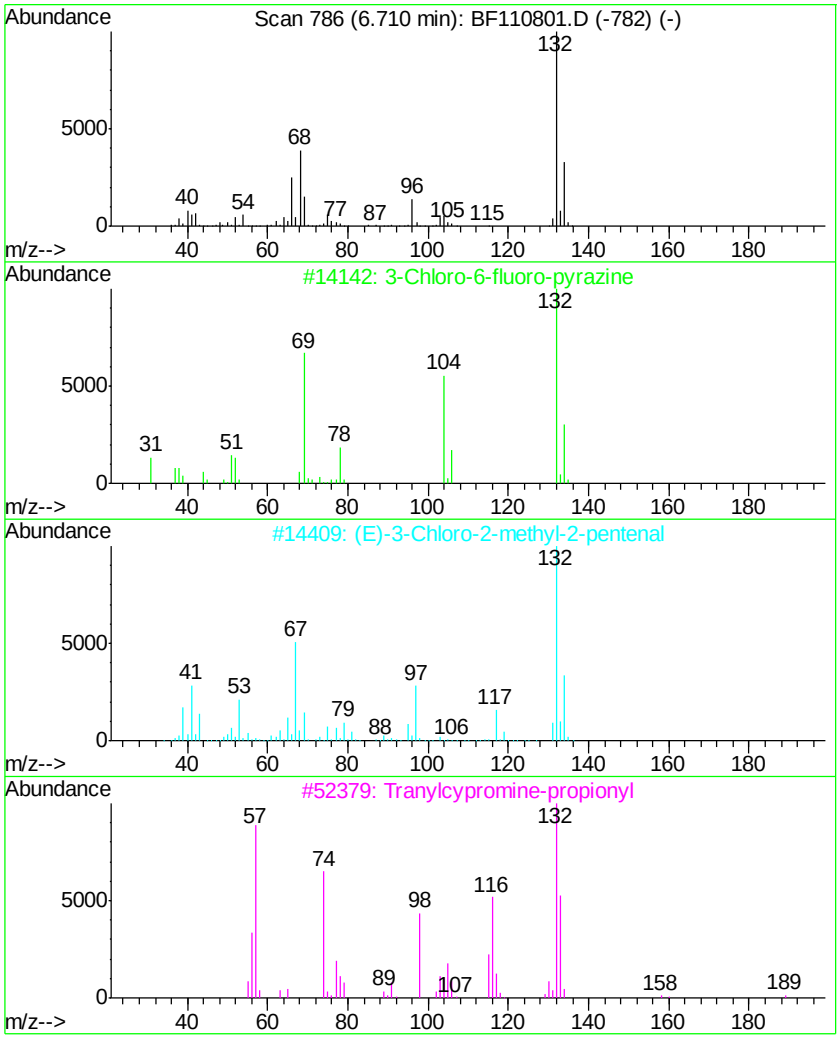
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

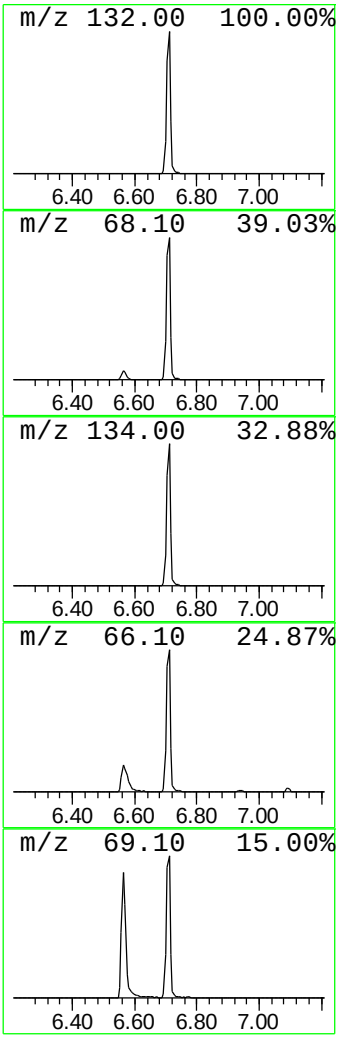
**********

Peak Number 3 unknown6.71 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.71 | 68.71 ng | 1216820 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

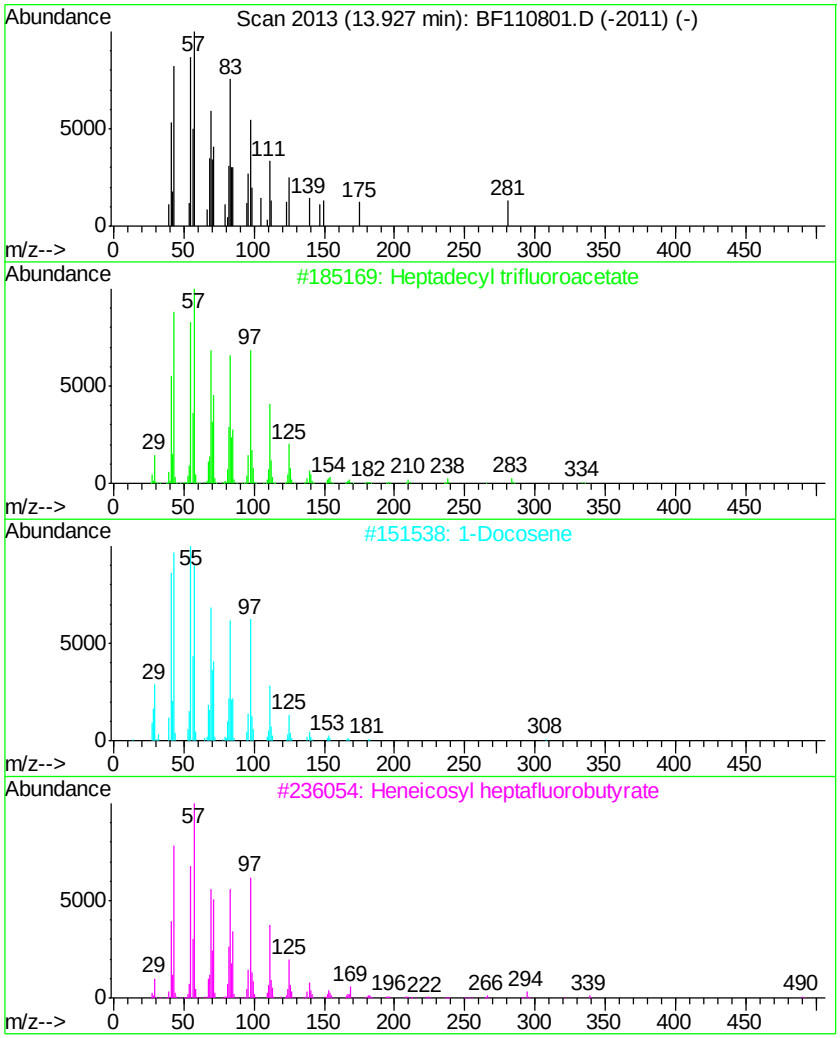
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

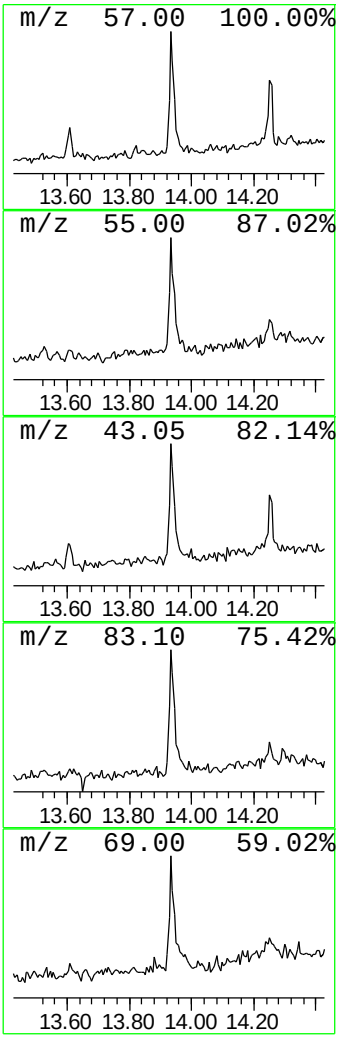
**********

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.93 | 3.24 ng | 68110 | Chrysene-d12 | 14.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 91 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91 |
| 4 | Tricosyl trifluoroacetate | 436 | C25H47F3O2 | 1000351-75-1 | 91 |
| 5 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111518\
Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

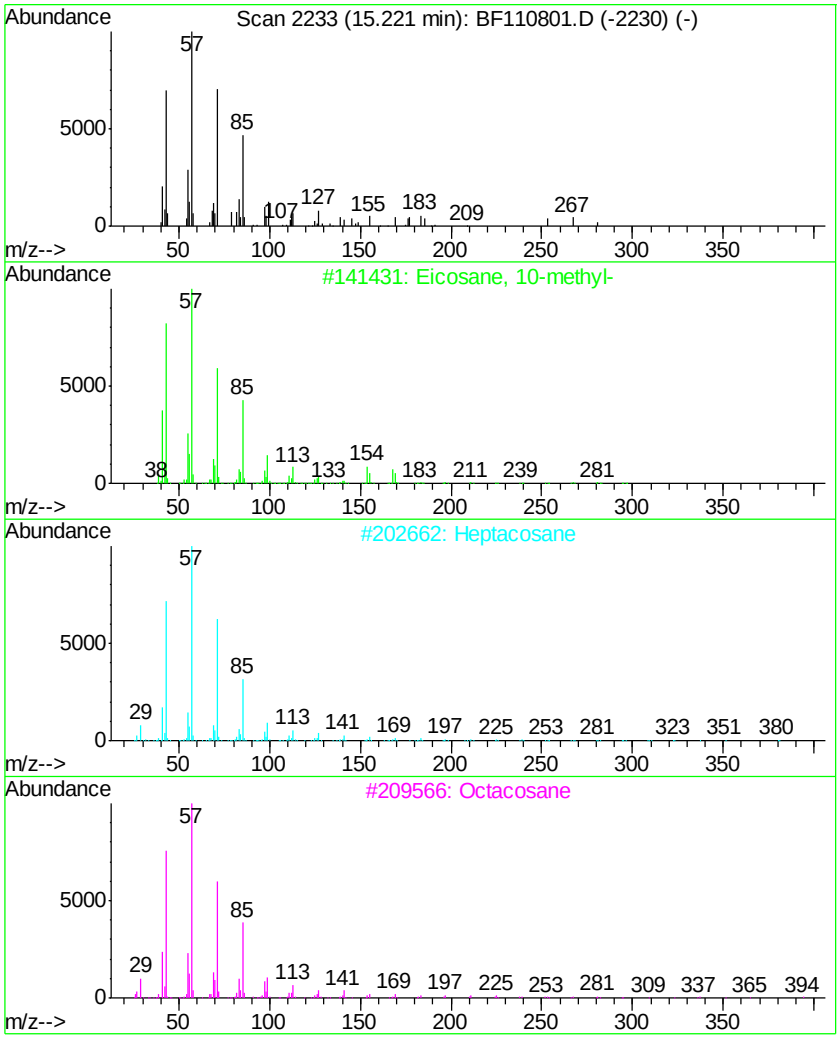
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

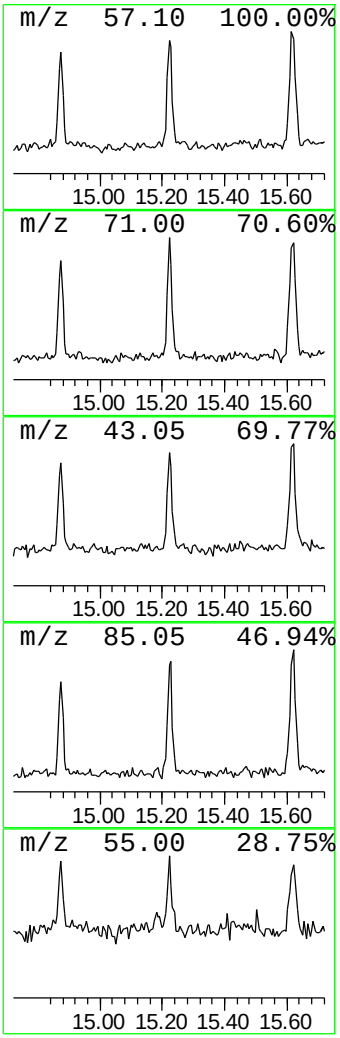
**********

Peak Number 6 Eicosane, 10-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.22 | 3.55 ng | 53060 | Perylene-d12 | 15.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 83 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 80 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 80 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 80 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |



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Data File : BF110801.D
Acq On : 15 Nov 2018 21:07
Operator : JU/SJ
Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

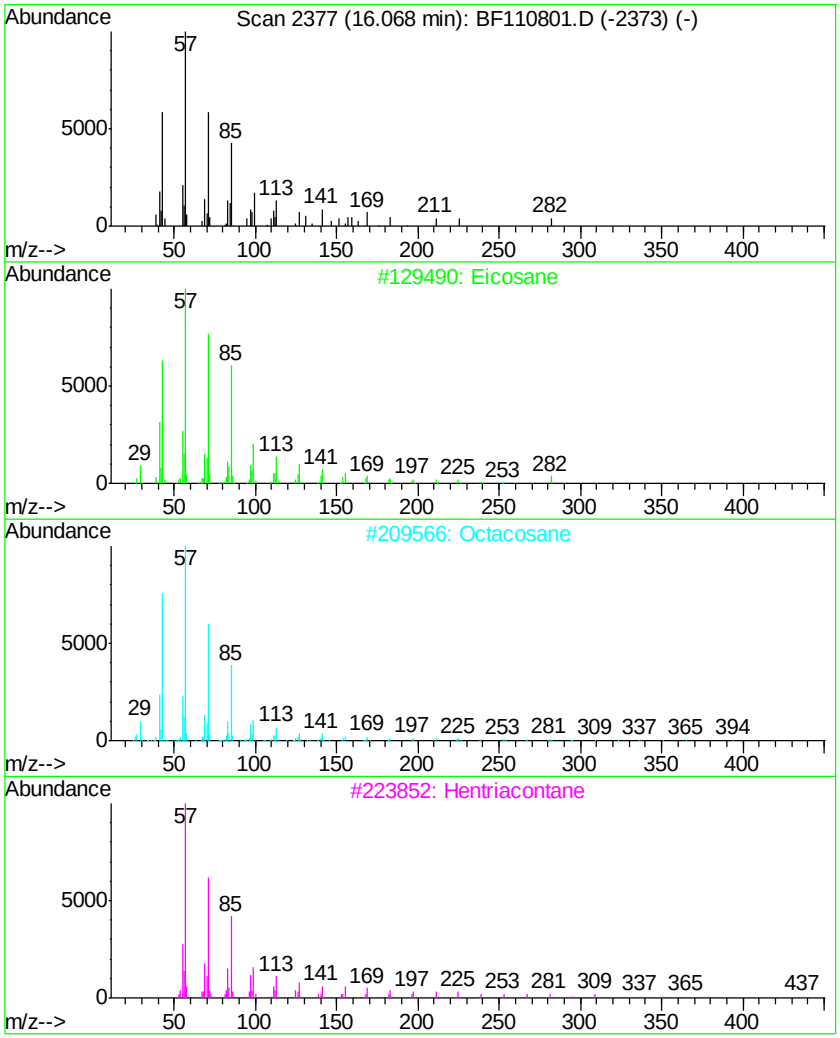
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

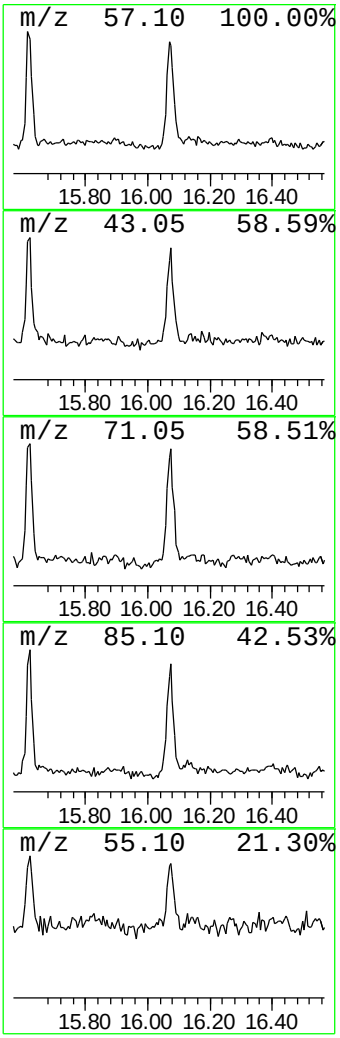
**********

Peak Number 7 Eicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.07 | 4.09 ng | 61155 | Perylene-d12 | 15.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 93 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 90 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |



# Library Search Compound Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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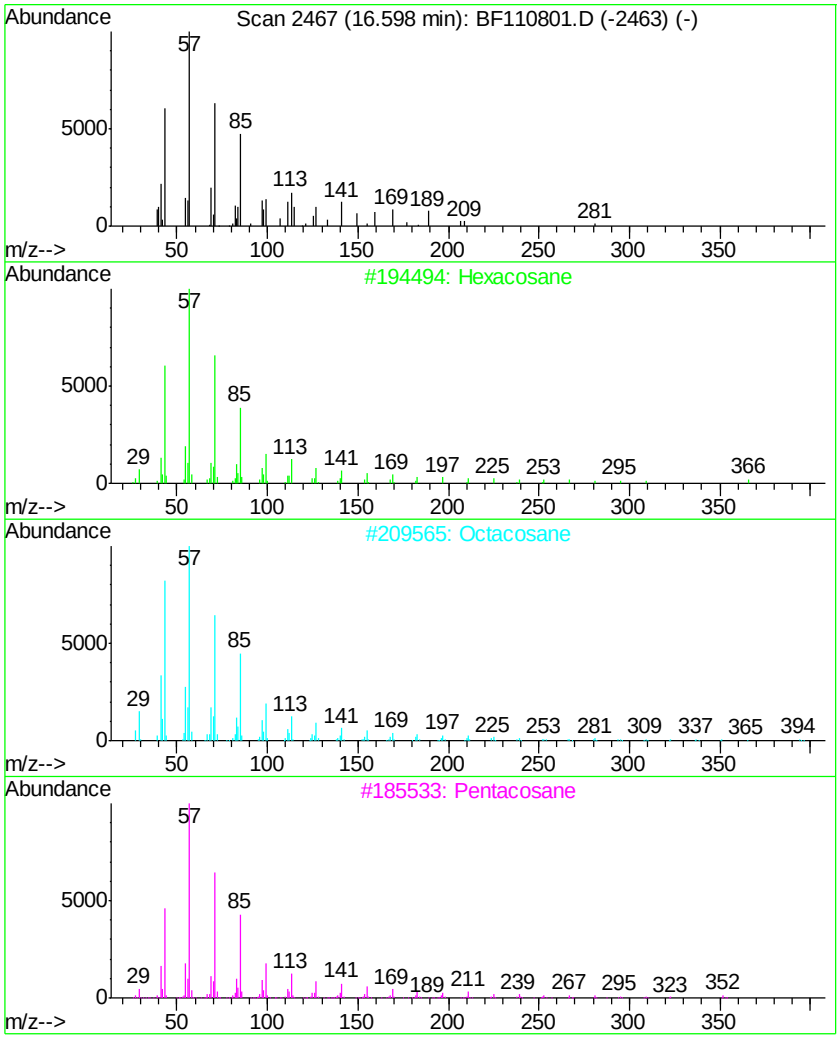
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

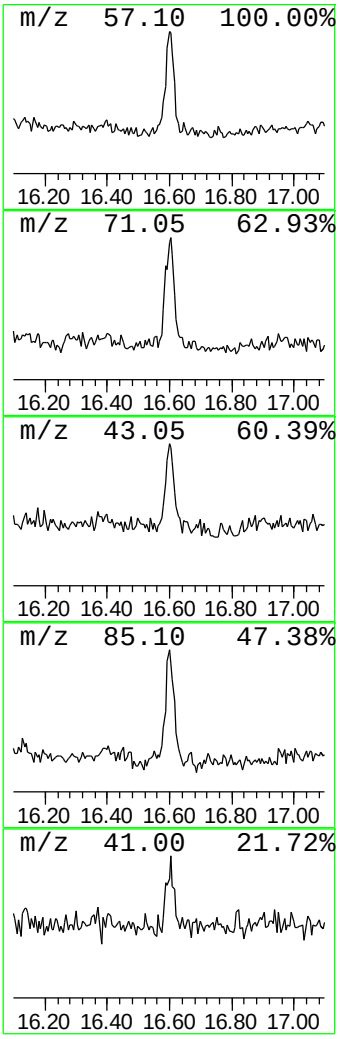
**********

Peak Number 8 Hexacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.60 | 2.84 ng | 42458 | Perylene-d12 | 15.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 72 |
| 3 | Pentacosane | 352 | C25H52 | 000629-99-2 | 72 |
| 4 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 72 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 64 |



Tentatively Identified Compound (LSC) summary

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Sample : J5942-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VW-F2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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 | 5.0 | ng | 88121 | 1 | 6.94 | 354172 | 20.0 |
| unknown5.17 | 5.17 | 2.5 | ng | 44928 | 1 | 6.94 | 354172 | 20.0 |
| unknown6.71 | 6.71 | 68.7 | ng | 1216820 | 1 | 6.94 | 354172 | 20.0 |
| Heptadecyl triflu... | 13.93 | 3.2 | ng | 68110 | 5 | 14.13 | 420469 | 20.0 |
| Eicosane, 10-methyl- | 15.22 | 3.5 | ng | 53060 | 6 | 15.66 | 299020 | 20.0 |
| Eicosane | 16.07 | 4.1 | ng | 61155 | 6 | 15.66 | 299020 | 20.0 |
| Hexacosane | 16.60 | 2.8 | ng | 42458 | 6 | 15.66 | 299020 | 20.0 |