LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

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:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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 | 2.299 | 30 | 36 | 44 | rVB | 118119 | 160997 | 4.11% | 0.458% |
| 2 | 5.222 | 528 | 533 | 544 | rBV | 164324 | 221078 | 5.64% | 0.629% |
| 3 | 5.598 | 592 | 597 | 600 | rBV | 3501433 | 3885934 | 99.19% | 11.061% |
| 4 | 6.598 | 761 | 767 | 770 | rBV | 3408090 | 3879319 | 99.02% | 11.042% |
| 5 | 6.745 | 787 | 792 | 795 | rBV | 3884904 | 3915031 | 99.93% | 11.143% |
| 6 | 6.975 | 827 | 831 | 834 | rBV | 1114984 | 910874 | 23.25% | 2.593% |
| 7 | 7.134 | 853 | 858 | 861 | rBV | 3234233 | 3027669 | 77.28% | 8.618% |
| 8 | 7.539 | 921 | 927 | 930 | rBV | 2458914 | 2475093 | 63.18% | 7.045% |
| 9 | 8.257 | 1045 | 1049 | 1052 | rBV | 1343264 | 1176908 | 30.04% | 3.350% |
| 10 | 8.745 | 1127 | 1132 | 1135 | rVB | 83364 | 65333 | 1.67% | 0.186% |
| 11 | 9.328 | 1227 | 1231 | 1234 | rBV | 4117586 | 3917615 | 100.00% | 11.151% |
| 12 | 9.669 | 1285 | 1289 | 1292 | rVB | 916409 | 745828 | 19.04% | 2.123% |
| 13 | 9.716 | 1294 | 1297 | 1302 | rBV | 318007 | 257006 | 6.56% | 0.732% |
| 14 | 9.927 | 1328 | 1333 | 1336 | rBV | 48658 | 40225 | 1.03% | 0.114% |
| 15 | 10.016 | 1344 | 1348 | 1360 | rVB | 1369336 | 1211539 | 30.93% | 3.448% |
| 16 | 10.404 | 1411 | 1414 | 1416 | rBV | 60871 | 48141 | 1.23% | 0.137% |
| 17 | 10.427 | 1416 | 1418 | 1421 | rVV | 61795 | 45428 | 1.16% | 0.129% |
| 18 | 10.480 | 1424 | 1427 | 1431 | rVB | 498061 | 465007 | 11.87% | 1.324% |
| 19 | 10.804 | 1478 | 1482 | 1486 | rBV | 2107179 | 2111416 | 53.90% | 6.010% |
| 20 | 10.904 | 1495 | 1499 | 1504 | rBV | 51718 | 60164 | 1.54% | 0.171% |
| 21 | 11.351 | 1572 | 1575 | 1578 | rBV | 51392 | 40090 | 1.02% | 0.114% |
| 22 | 11.510 | 1598 | 1602 | 1605 | rBV | 1032698 | 990965 | 25.30% | 2.821% |
| 23 | 11.710 | 1633 | 1636 | 1644 | rBV3 | 49219 | 55023 | 1.40% | 0.157% |
| 24 | 12.186 | 1714 | 1717 | 1720 | rBV2 | 47509 | 40570 | 1.04% | 0.115% |
| 25 | 12.533 | 1773 | 1776 | 1780 | rBV | 130960 | 107987 | 2.76% | 0.307% |
| 26 | 12.592 | 1780 | 1786 | 1788 | rBV3 | 86254 | 109089 | 2.78% | 0.311% |
| 27 | 12.721 | 1805 | 1808 | 1813 | rBV | 43327 | 49341 | 1.26% | 0.140% |
| 28 | 12.957 | 1844 | 1848 | 1850 | rBV2 | 47237 | 44045 | 1.12% | 0.125% |
| 29 | 13.098 | 1867 | 1872 | 1875 | rBV | 3056708 | 2954961 | 75.43% | 8.411% |
| 30 | 13.510 | 1939 | 1942 | 1944 | rBV2 | 48399 | 47665 | 1.22% | 0.136% |
| 31 | 13.974 | 2018 | 2021 | 2029 | rVB | 146390 | 156928 | 4.01% | 0.447% |
| 32 | 14.157 | 2048 | 2052 | 2056 | rBV | 954063 | 973478 | 24.85% | 2.771% |
| 33 | 15.015 | 2196 | 2198 | 2203 | rVB | 58216 | 55436 | 1.42% | 0.158% |
| 34 | 15.704 | 2310 | 2315 | 2325 | rVB | 646378 | 886990 | 22.64% | 2.525% |

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PIT-A-0-5

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:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

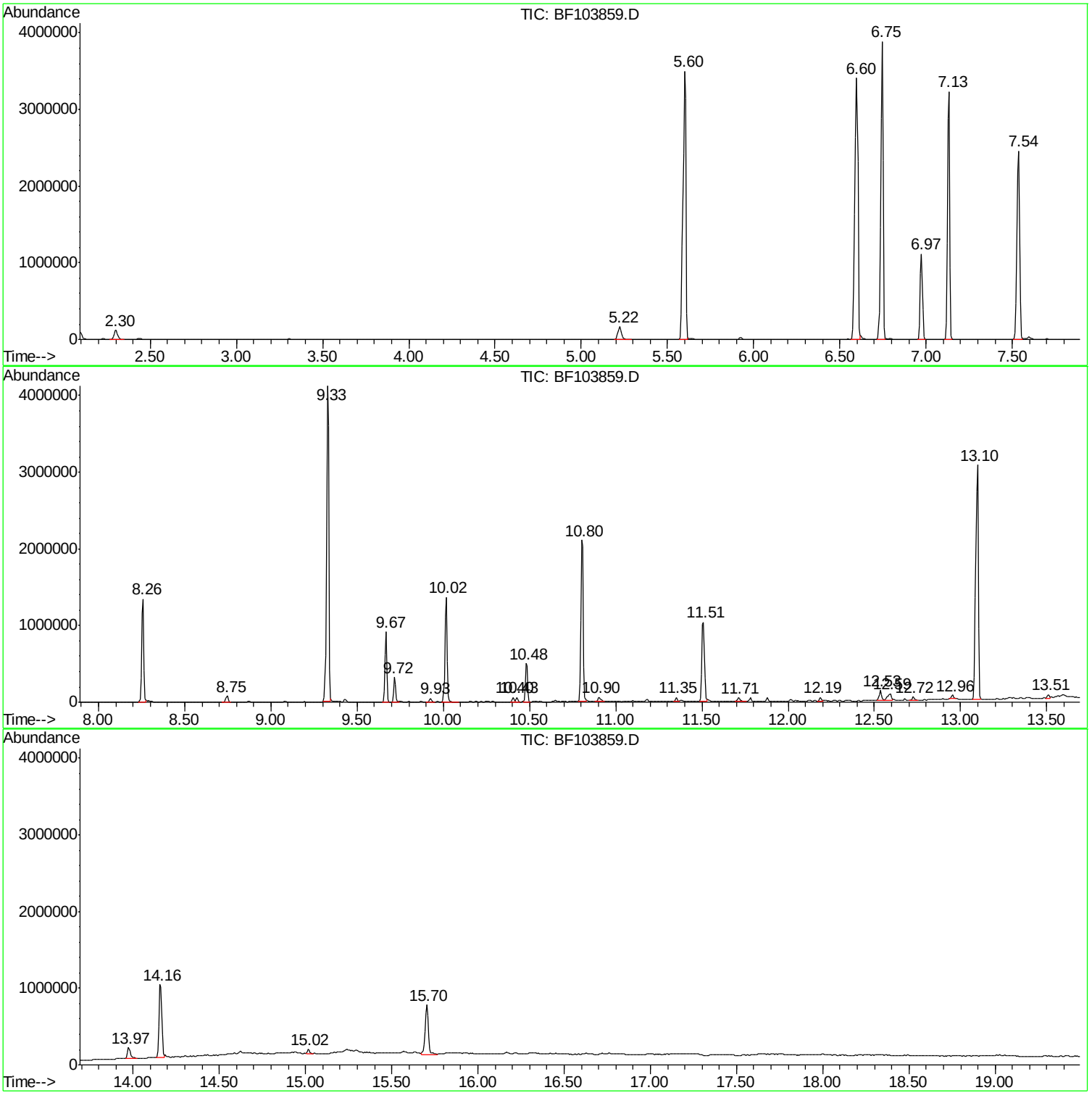
Sum of corrected areas: 35133173

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

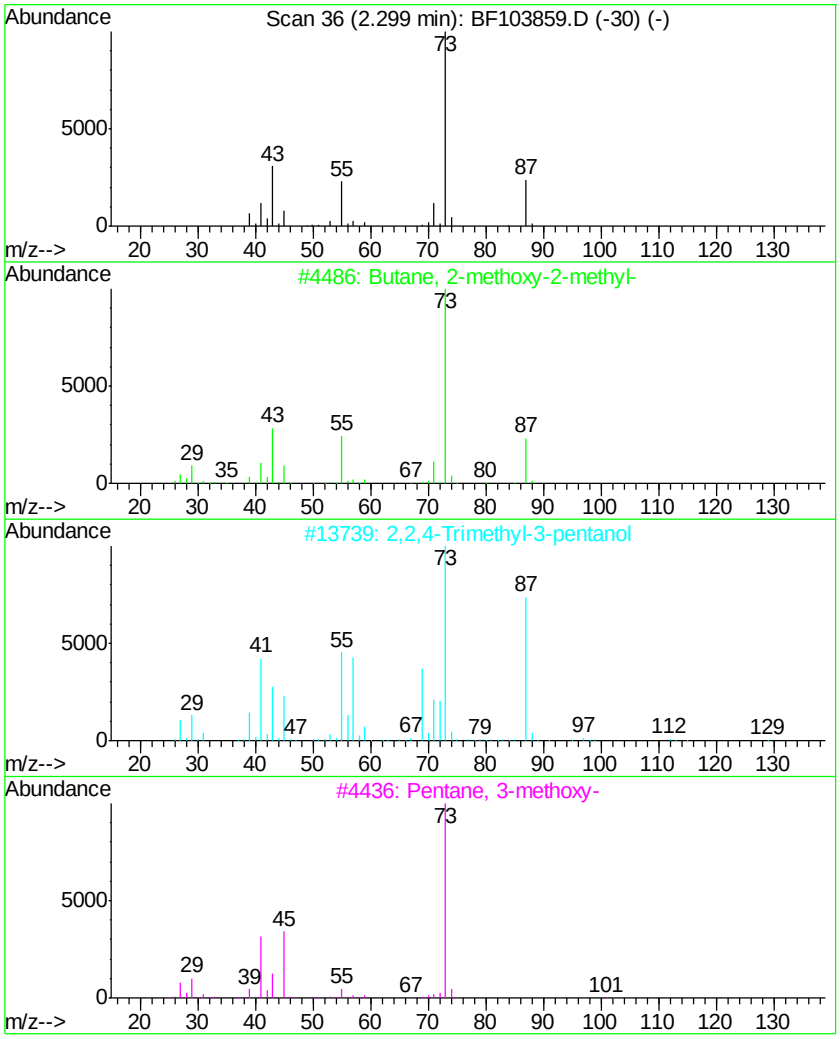
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

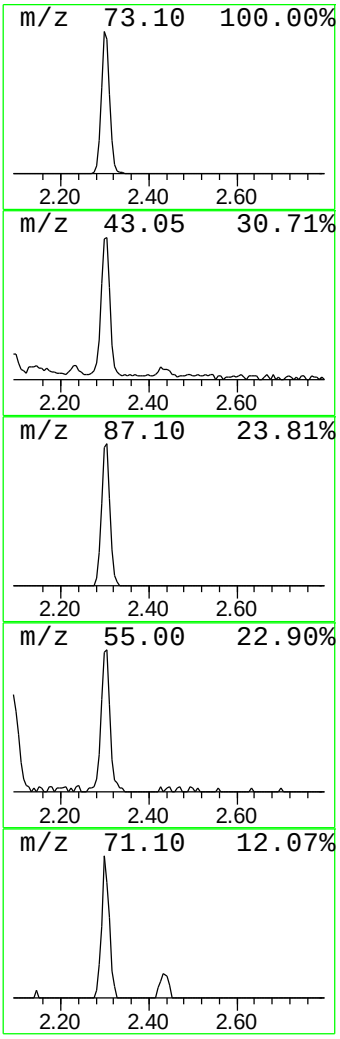
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.30 | 3.54 ng | 160997 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 4 | 3-Hexanol, 2-methyl- | 116 | C7H16O | 000617-29-8 | 17 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

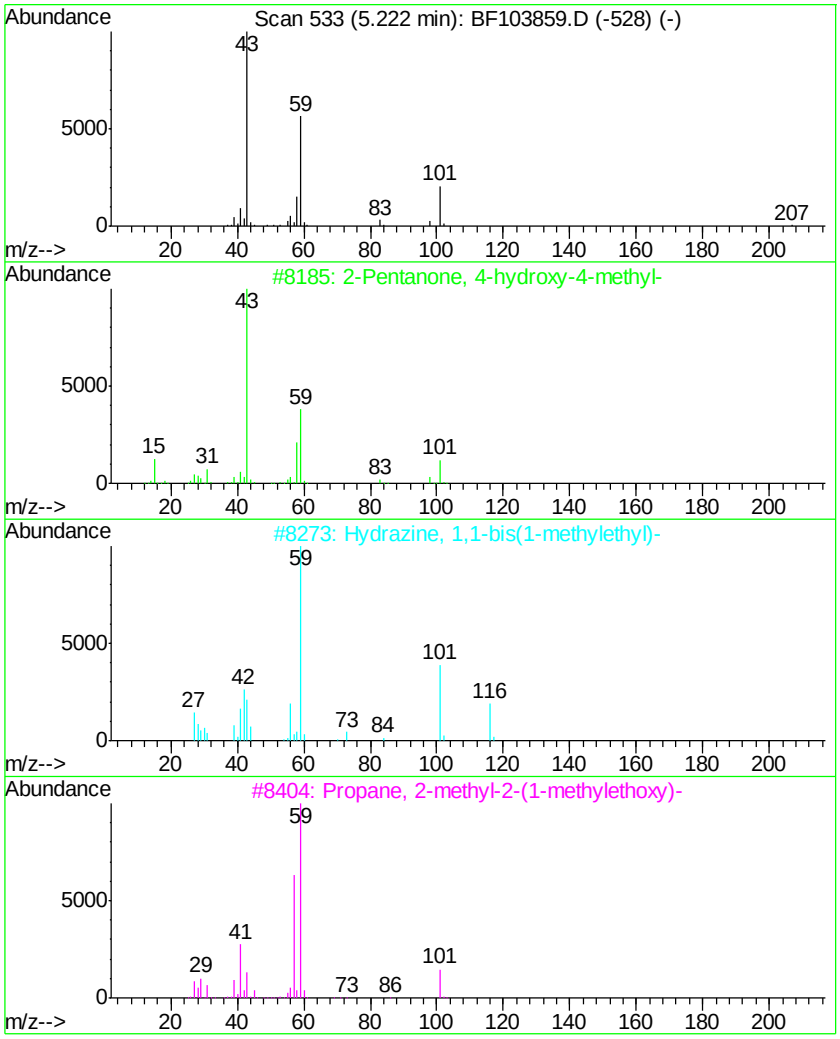
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

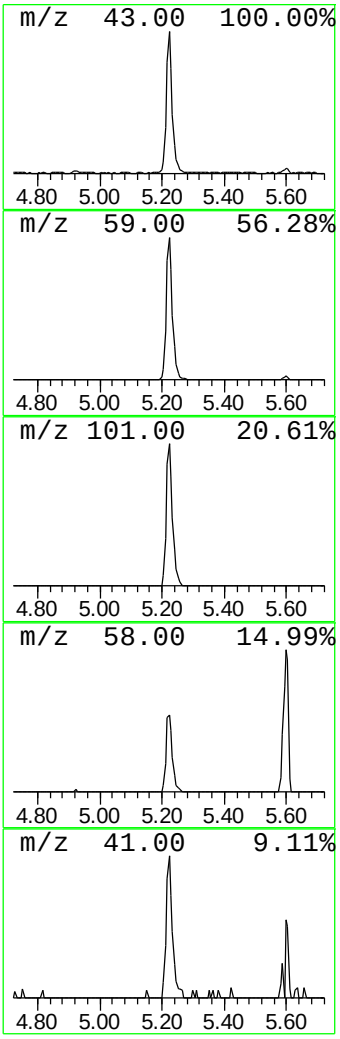
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.22 | 4.85 ng | 221078 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 28 |
| 3 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 28 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

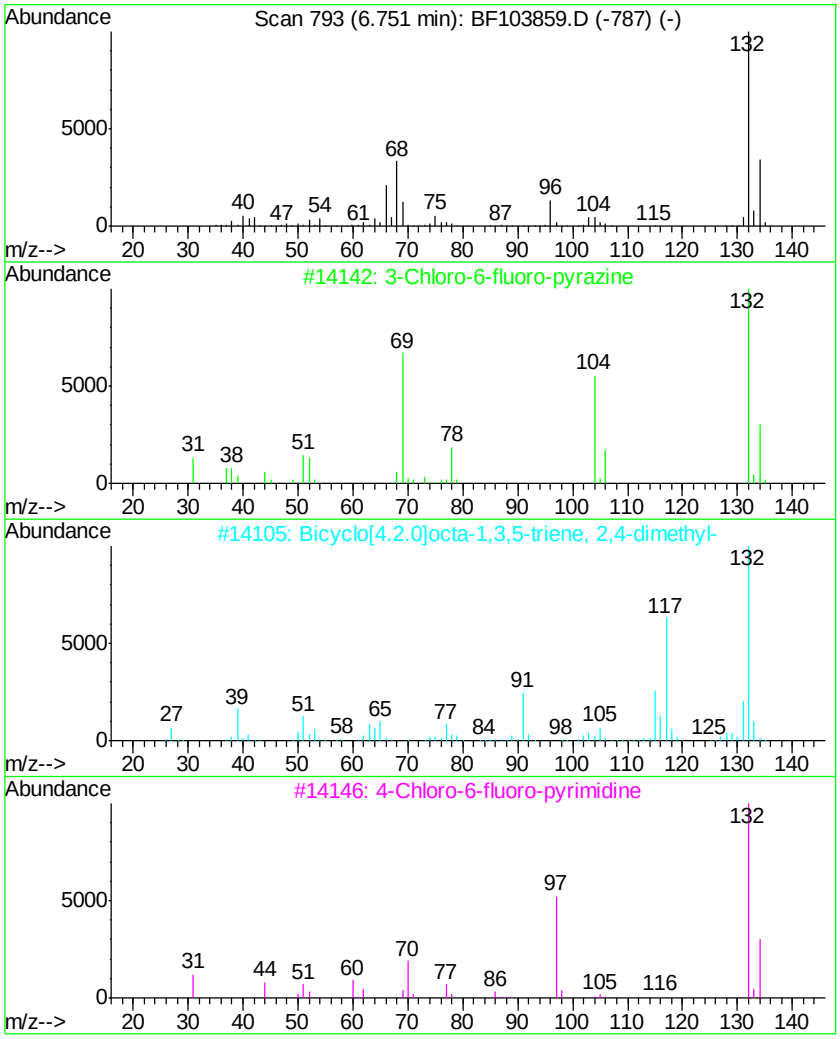
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

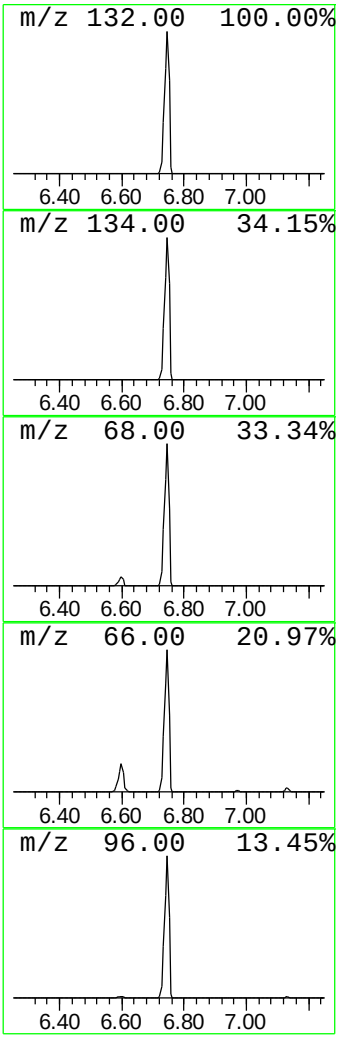
**********

Peak Number 3 unknown6.75 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.75 | 85.96 ng | 3915030 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

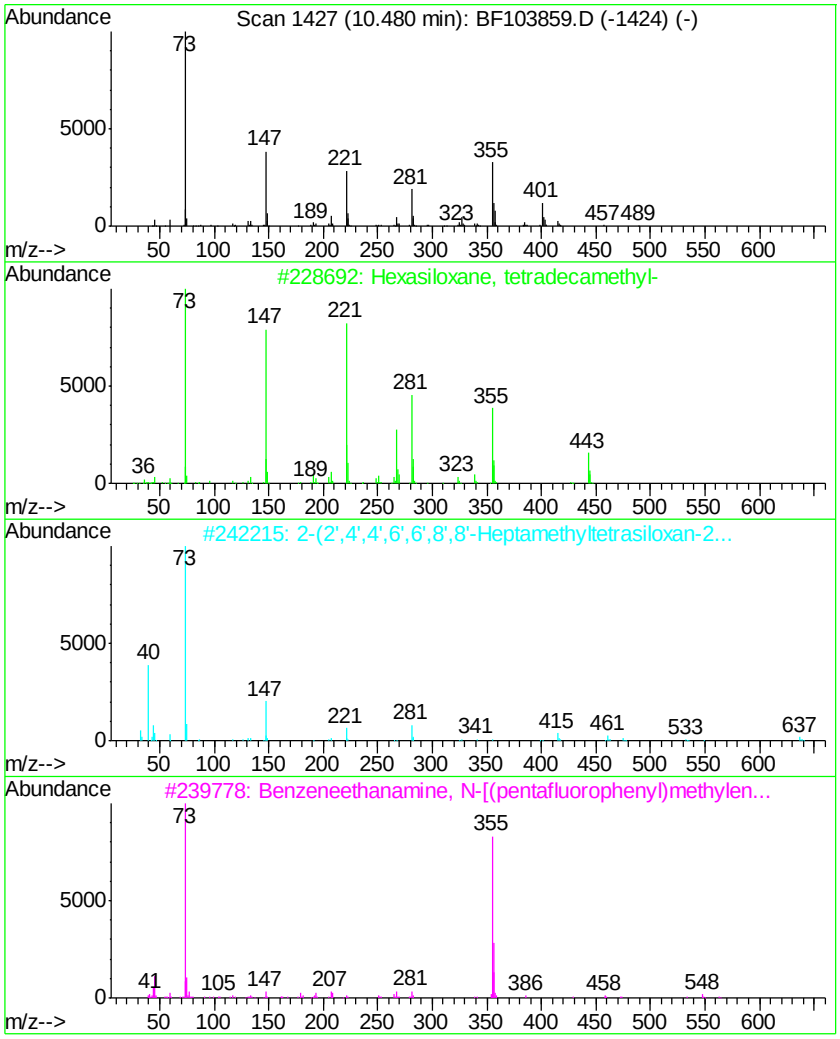
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

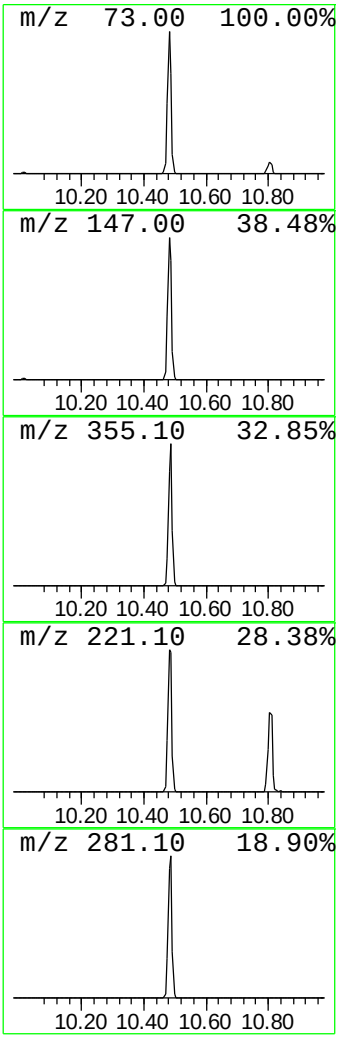
**********

Peak Number 5 unknown10.48 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.48 | 7.68 ng | 465007 | Acenaphthene-d10 | 10.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexasiloxane, tetradecamethyl- | 458 | C14H42O5Si6 | 000107-52-8 | 40 |
| 2 | 2-(2',4',4',6',6',8',8'-Heptamet... | 652 | C16H48O10Si9 | 145344-72-5 | 25 |
| 3 | Benzeneethanamine, N-[(pentafluo... | 563 | C24H34F5NO3Si3 | 055429-13-5 | 22 |
| 4 | 3-Amino-2-phenazinol ditms | 355 | C18H25N3OSi2 | 1000332-15-5 | 22 |
| 5 | Benzoic acid, 2,6-bis[(trimethyl... | 370 | C16H30O4Si3 | 003782-85-2 | 17 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

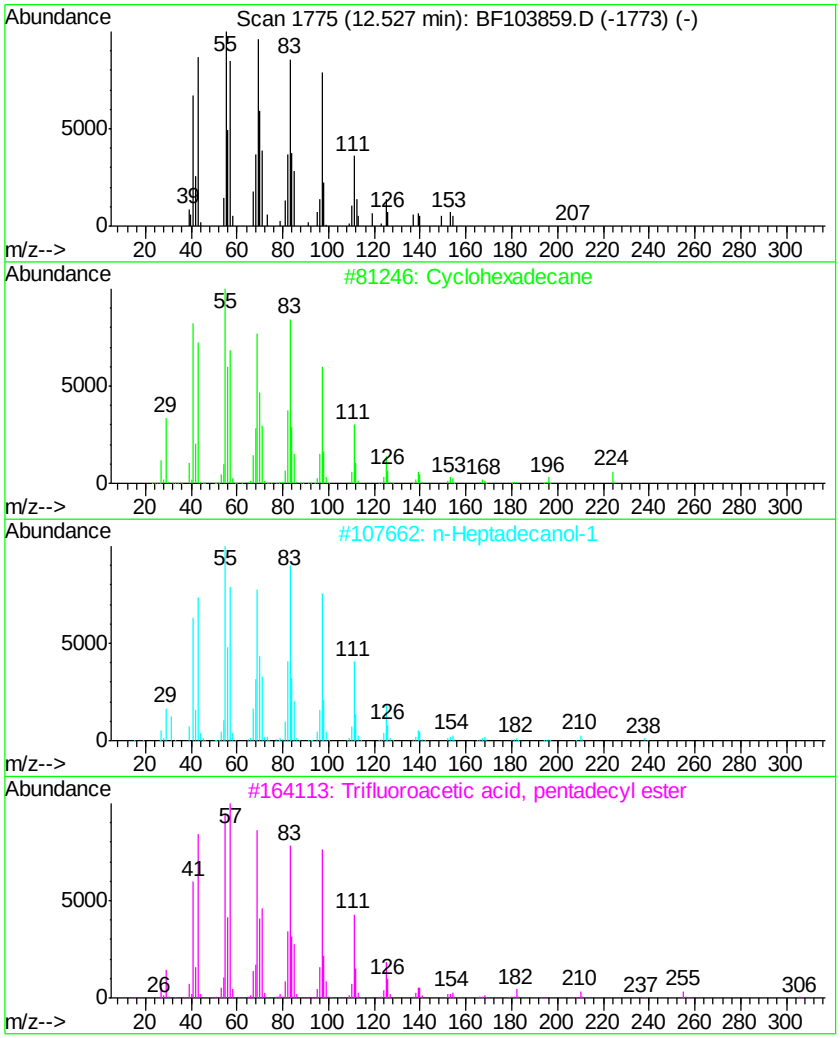
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

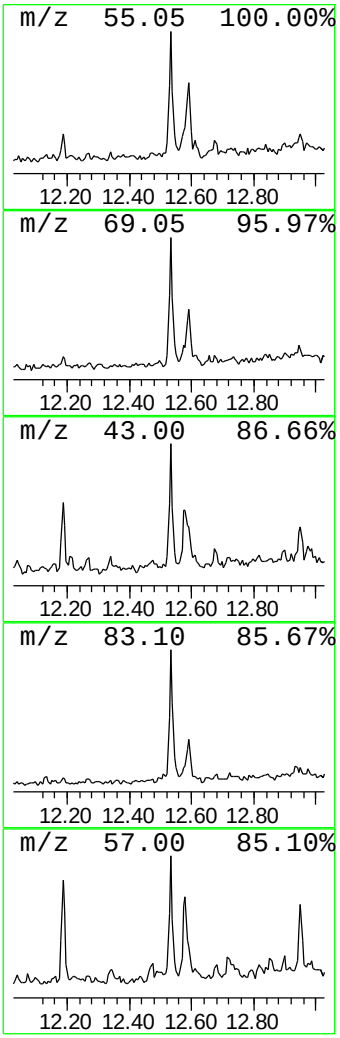
**********

Peak Number 6 Cyclohexadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.53 | 2.18 ng | 107987 | Phenanthrene-d10 | 11.51 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 95 |
| 2 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 95 |
| 3 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |
| 4 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 93 |
| 5 | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 93 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

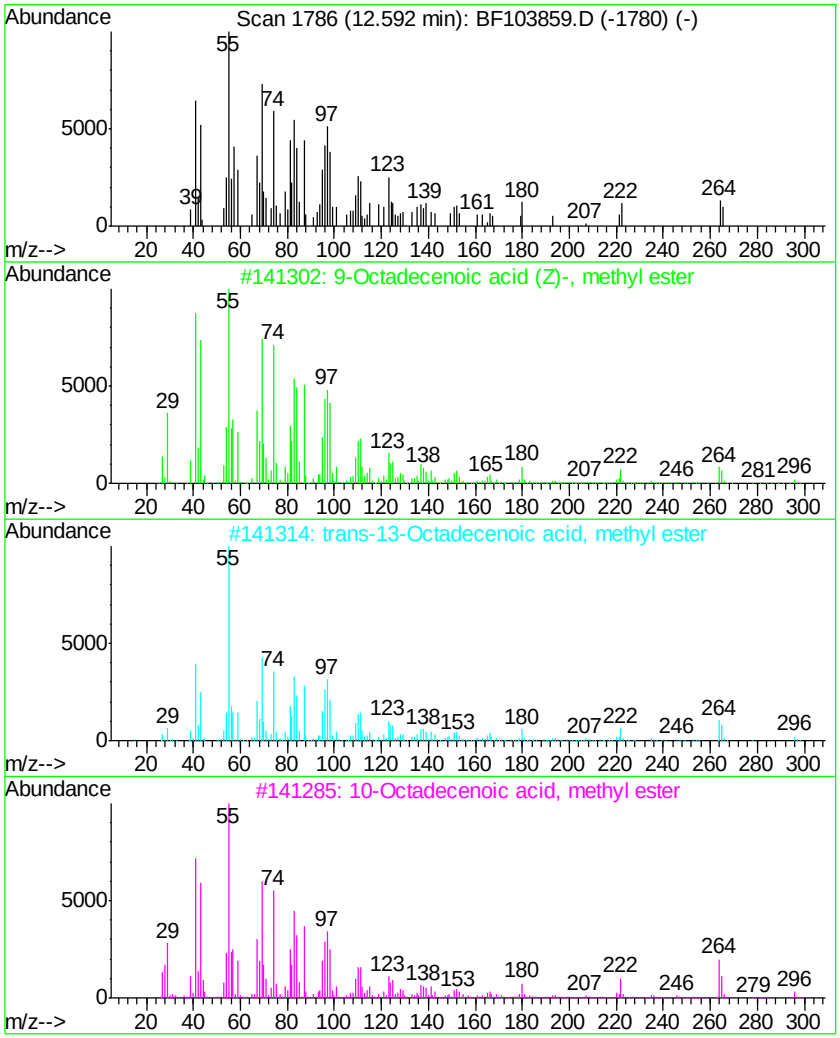
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

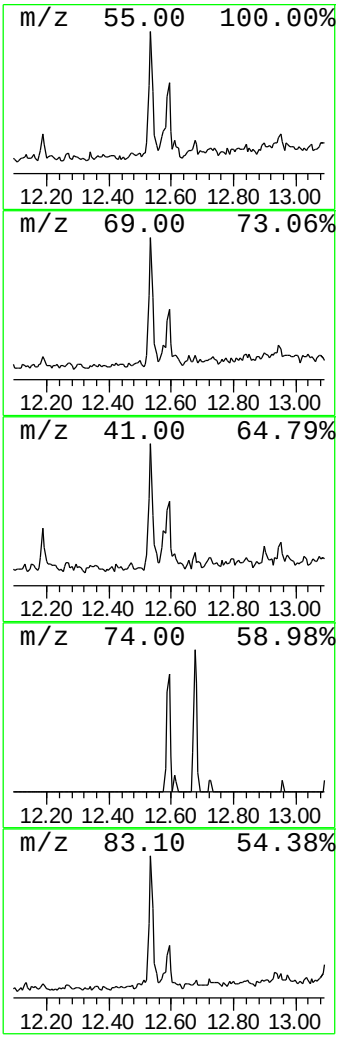
**********

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.59 | 2.20 ng | 109089 | Phenanthrene-d10 | 11.51 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 95 |
| 2 | trans-13-Octadecenoic acid, meth... | 296 | C19H36O2 | 1000333-61-3 | 91 |
| 3 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 91 |
| 4 | 6-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052355-31-4 | 87 |
| 5 | 14-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-48-4 | 87 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

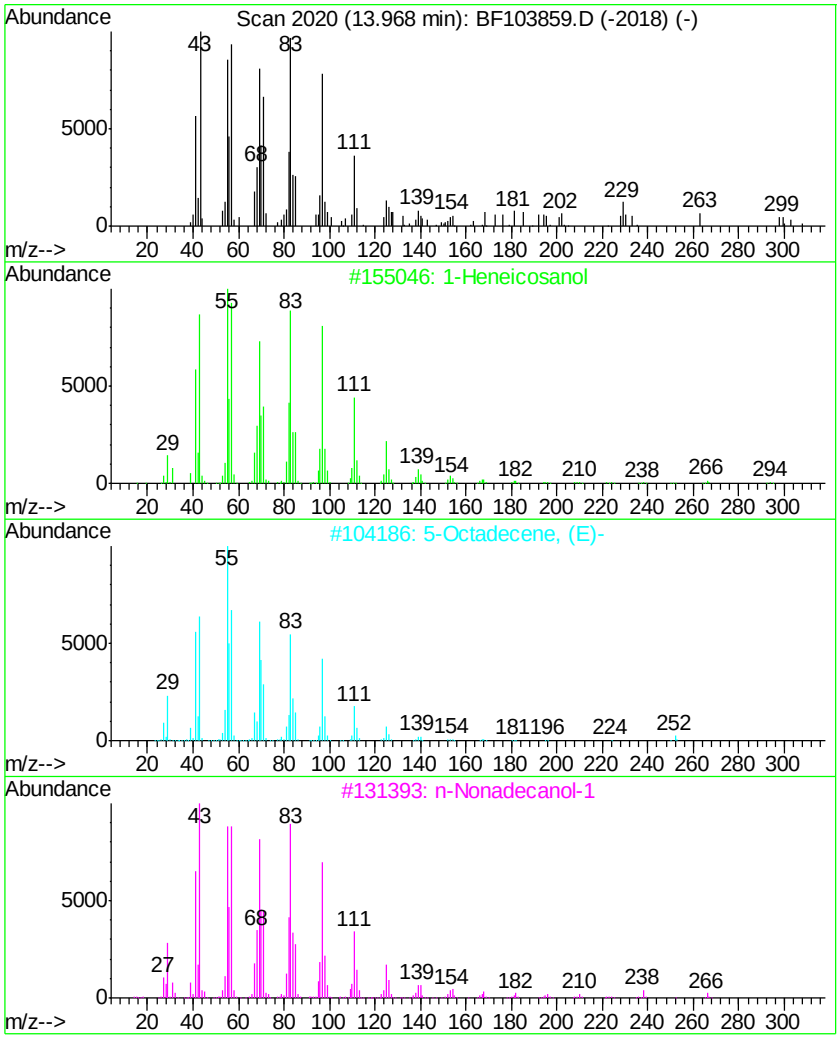
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

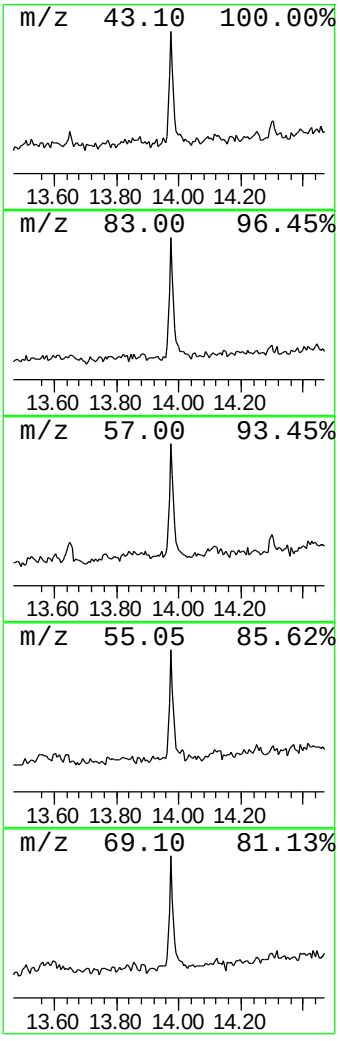
**********

Peak Number 8 1-Heneicosanol Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.97 | 3.22 ng | 156928 | Chrysene-d12 | 14.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 95 |
| 3 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 4 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 95 |
| 5 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103859.D
Acq On : 22 Mar 2018 18:32
Operator : JU/SJ
Sample : J1995-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** PIT-A-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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... | 2.30 | 3.5 | ng | 160997 | 1 | 6.97 | 910874 | 20.0 |
| 2-Pentanone, 4-hy... | 5.22 | 4.8 | ng | 221078 | 1 | 6.97 | 910874 | 20.0 |
| unknown6.75 | 6.75 | 86.0 | ng | 3915030 | 1 | 6.97 | 910874 | 20.0 |
| unknown10.48 | 10.48 | 7.7 | ng | 465007 | 3 | 10.02 | 1211540 | 20.0 |
| Cyclohexadecane | 12.53 | 2.2 | ng | 107987 | 4 | 11.51 | 990965 | 20.0 |
| 9-Octadecenoic ac... | 12.59 | 2.2 | ng | 109089 | 4 | 11.51 | 990965 | 20.0 |
| 1-Heneicosanol | 13.97 | 3.2 | ng | 156928 | 5 | 14.16 | 973478 | 20.0 |