LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

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-BF110817.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 | 2.134 | 6 | 8 | 27 | rVB | 66505 | 175602 | 7.87% | 1.418% |
| 2 | 5.069 | 504 | 507 | 517 | rBB | 111848 | 113865 | 5.10% | 0.919% |
| 3 | 5.469 | 571 | 575 | 579 | rBV | 627953 | 556045 | 24.93% | 4.489% |
| 4 | 6.481 | 743 | 747 | 756 | rBB | 408145 | 383322 | 17.18% | 3.095% |
| 5 | 6.628 | 767 | 772 | 775 | rBV | 1137780 | 1042112 | 46.72% | 8.413% |
| 6 | 6.857 | 807 | 811 | 814 | rBV | 523177 | 398098 | 17.85% | 3.214% |
| 7 | 7.016 | 833 | 838 | 841 | rBV | 1706015 | 1466743 | 65.75% | 11.841% |
| 8 | 7.422 | 902 | 907 | 910 | rBV | 1153520 | 1180459 | 52.92% | 9.530% |
| 9 | 8.139 | 1025 | 1029 | 1032 | rBV | 655534 | 524460 | 23.51% | 4.234% |
| 10 | 9.216 | 1207 | 1212 | 1215 | rBV | 2419590 | 2230647 | 100.00% | 18.008% |
| 11 | 9.604 | 1275 | 1278 | 1281 | rBV | 35877 | 27758 | 1.24% | 0.224% |
| 12 | 9.892 | 1322 | 1327 | 1331 | rBV | 617256 | 579229 | 25.97% | 4.676% |
| 13 | 10.680 | 1458 | 1461 | 1465 | rBV | 854253 | 783996 | 35.15% | 6.329% |
| 14 | 10.786 | 1476 | 1479 | 1485 | rVB | 27373 | 26710 | 1.20% | 0.216% |
| 15 | 11.380 | 1576 | 1580 | 1584 | rBV | 621653 | 506368 | 22.70% | 4.088% |
| 16 | 12.968 | 1845 | 1850 | 1853 | rBV | 1698045 | 1577310 | 70.71% | 12.734% |
| 17 | 13.851 | 1995 | 2000 | 2004 | rBV | 39262 | 40801 | 1.83% | 0.329% |
| 18 | 14.021 | 2025 | 2029 | 2032 | rBV | 389585 | 353029 | 15.83% | 2.850% |
| 19 | 14.857 | 2166 | 2171 | 2175 | rBV | 31498 | 30004 | 1.35% | 0.242% |
| 20 | 15.492 | 2273 | 2279 | 2290 | rVB | 311462 | 390308 | 17.50% | 3.151% |

Sum of corrected areas: 12386866

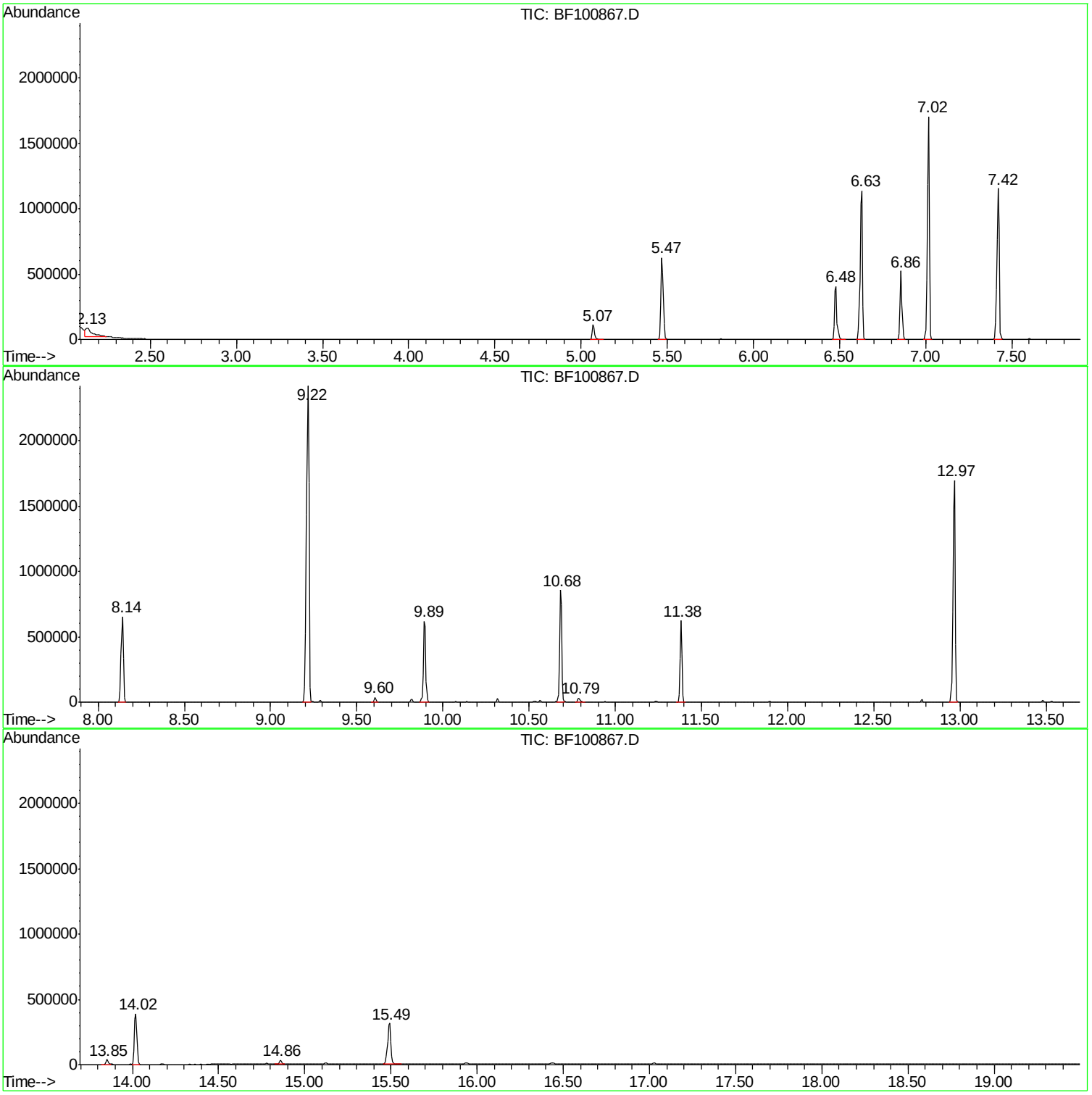
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

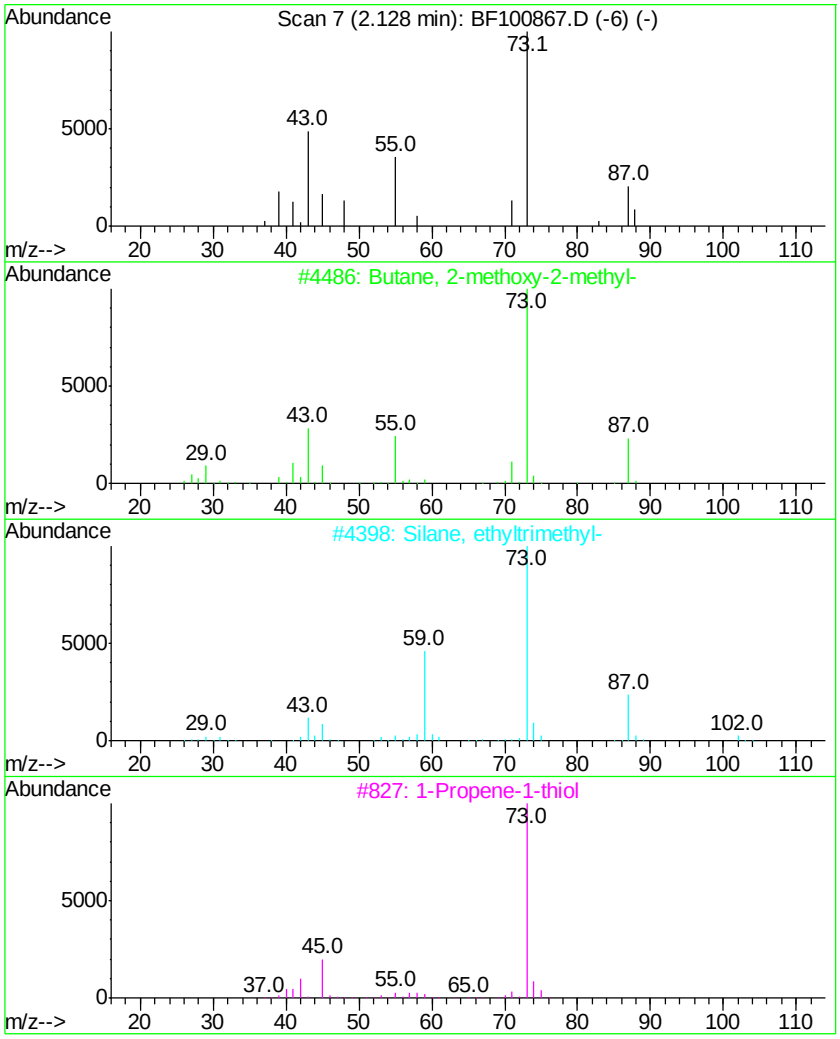
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

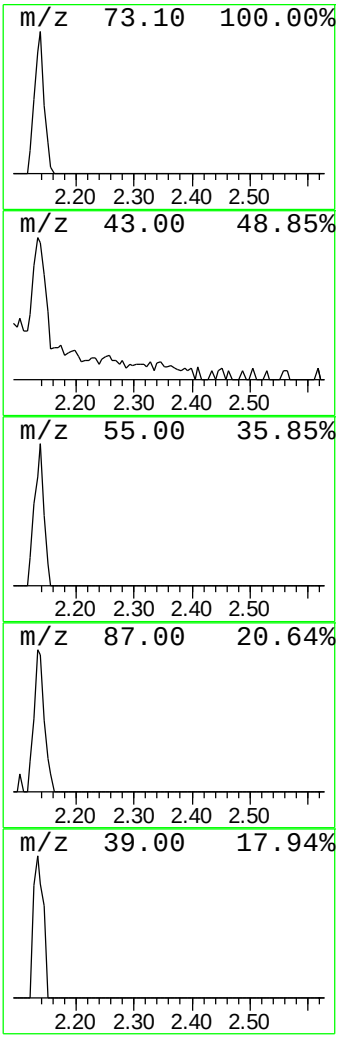
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.13 | 8.82 ng | 175602 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 56 |
| 2 | Silane, ethyltrimethyl- | 102 | C5H14Si | 003439-38-1 | 9 |
| 3 | 1-Propene-1-thiol | 74 | C3H6S | 000925-89-3 | 5 |
| 4 | 1,4-Butanediamine | 88 | C4H12N2 | 000110-60-1 | 5 |
| 5 | 1-Pentanamine | 87 | C5H13N | 000110-58-7 | 5 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

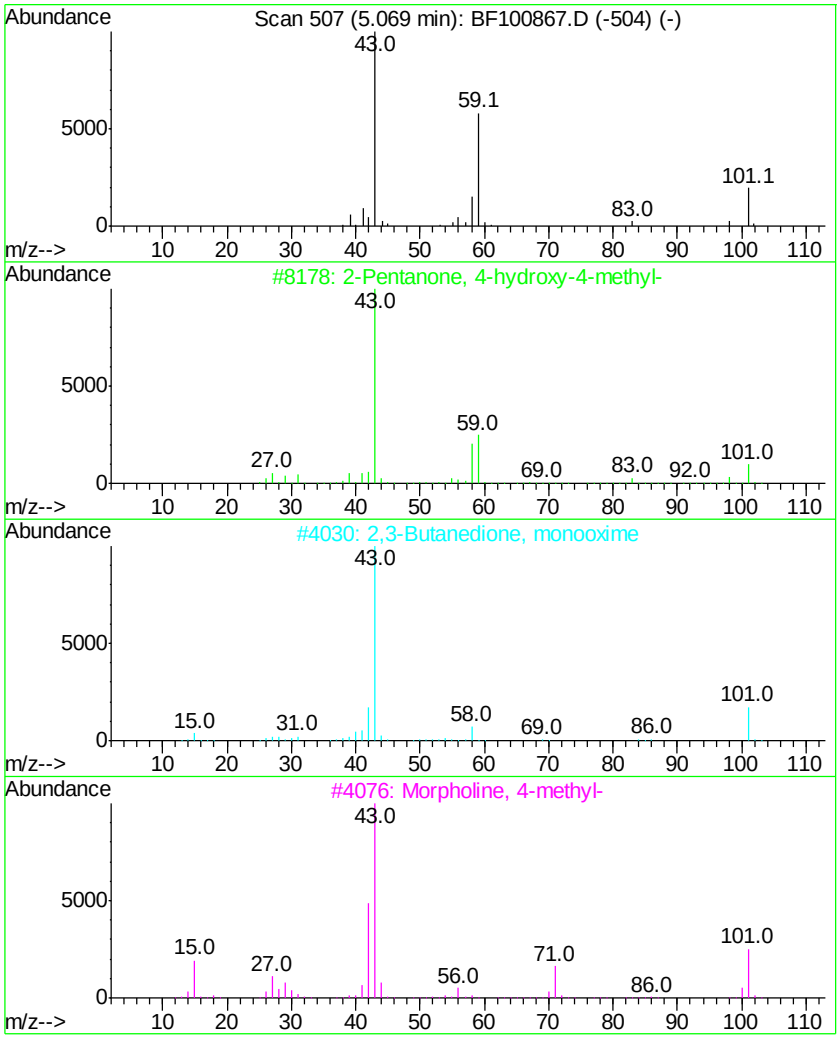
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

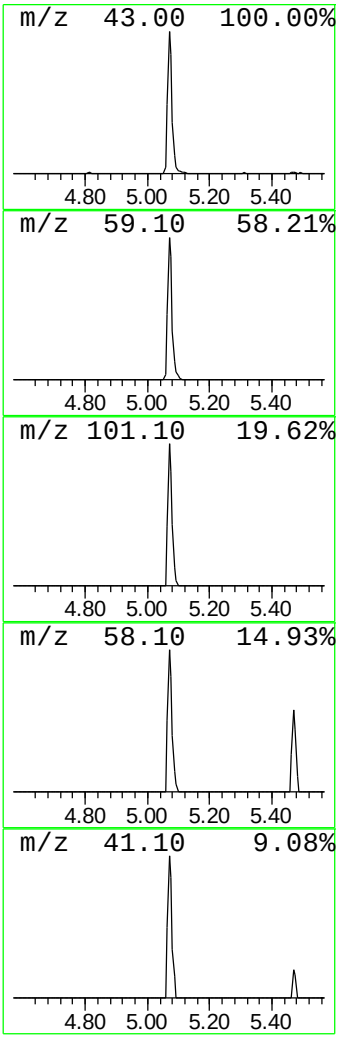
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.07 | 5.72 ng | 113865 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 35 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | Butanamide, 2-hydroxy-2,N-dimethyl- | 117 | C5H11NO2 | 039961-72-3 | 9 |
| 5 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

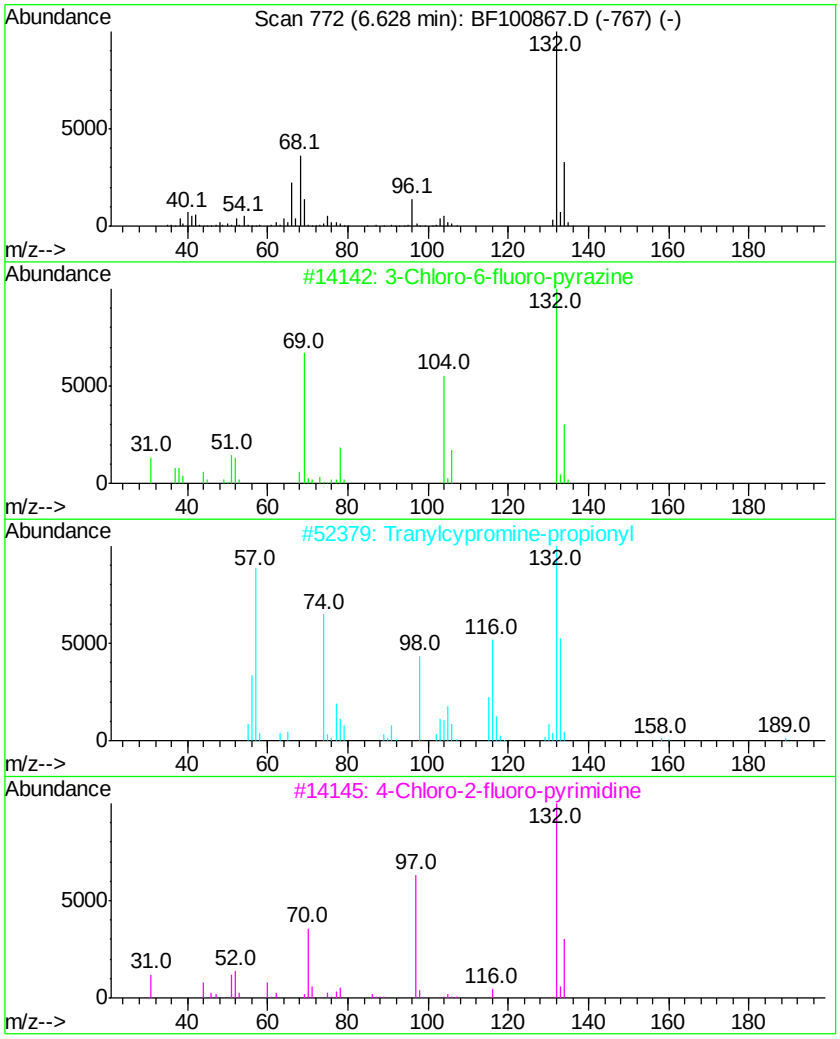
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

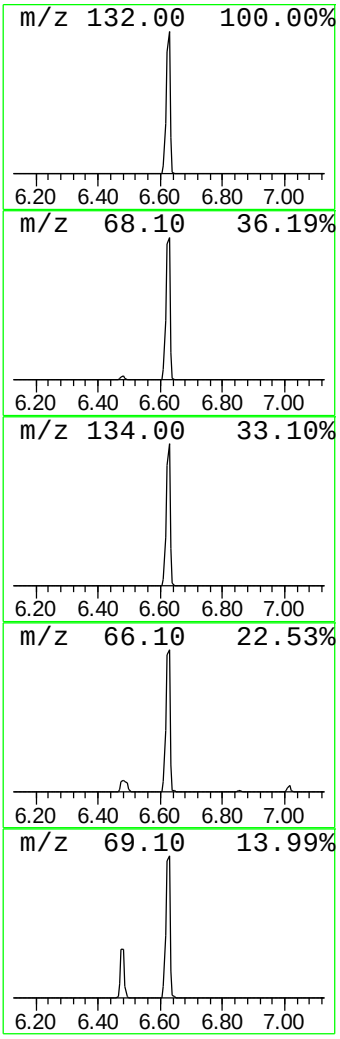
**********

Peak Number 3 unknown6.63 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 52.35 ng | 1042110 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 3 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

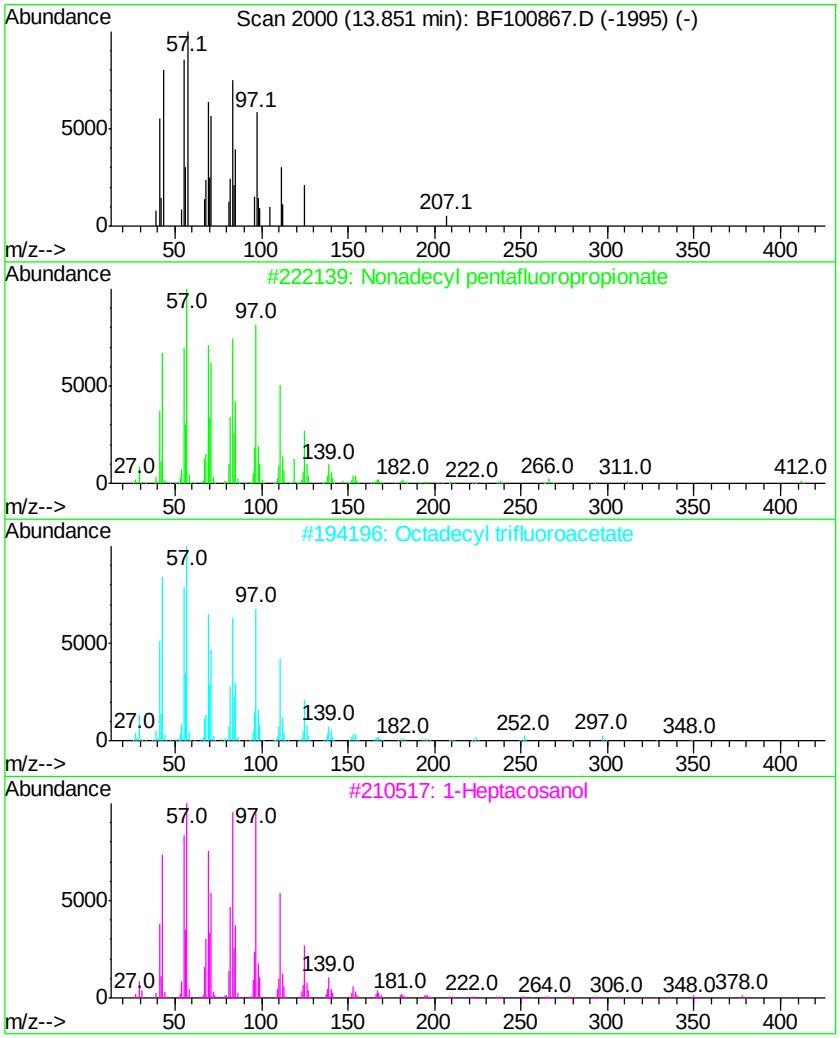
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

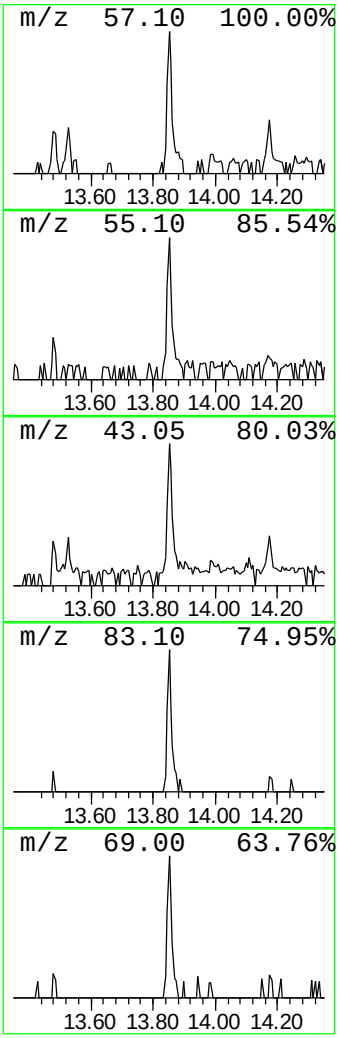
**********

Peak Number 5 Nonadecyl pentafluoropropio... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.85 | 2.31 ng | 40801 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91 |
| 2 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 87 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 87 |
| 4 | Docosyl pentafluoropropionate | 472 | C25H45F5O2 | 1000351-80-9 | 83 |
| 5 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
Data File : BF100867.D
Acq On : 23 Nov 2017 11:33
Operator : SJ/JU
Sample : I6541-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 111717-SIDI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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... | 2.13 | 8.8 | ng | 175602 | 1 | 6.86 | 398098 | 20.0 |
| 2-Pentanone, 4-hy... | 5.07 | 5.7 | ng | 113865 | 1 | 6.86 | 398098 | 20.0 |
| unknown6.63 | 6.63 | 52.4 | ng | 1042110 | 1 | 6.86 | 398098 | 20.0 |
| Nonadecyl pentafl... | 13.85 | 2.3 | ng | 40801 | 5 | 14.02 | 353029 | 20.0 |