LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

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-BF060517.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 | 4.604 | 510 | 513 | 539 | rBV | 57233 | 173273 | 7.68% | 0.975% |
| 2 | 5.281 | 623 | 628 | 663 | rBV | 1119729 | 1886458 | 83.64% | 10.618% |
| 3 | 6.939 | 905 | 910 | 922 | rBV | 1220522 | 1823842 | 80.87% | 10.266% |
| 4 | 7.039 | 922 | 927 | 938 | rVB | 1496296 | 2078107 | 92.14% | 11.697% |
| 5 | 7.380 | 981 | 985 | 996 | rBV | 364075 | 471203 | 20.89% | 2.652% |
| 6 | 7.622 | 1020 | 1026 | 1041 | rBV | 1145204 | 1575370 | 69.85% | 8.867% |
| 7 | 8.298 | 1136 | 1141 | 1163 | rBV | 835316 | 1157221 | 51.31% | 6.514% |
| 8 | 9.410 | 1326 | 1330 | 1353 | rBV | 487626 | 636605 | 28.23% | 3.583% |
| 9 | 11.198 | 1627 | 1634 | 1651 | rBV | 1735952 | 2255379 | 100.00% | 12.695% |
| 10 | 11.886 | 1747 | 1751 | 1763 | rBV | 176362 | 214081 | 9.49% | 1.205% |
| 11 | 12.233 | 1805 | 1810 | 1816 | rBV2 | 530262 | 654799 | 29.03% | 3.686% |
| 12 | 13.098 | 1952 | 1957 | 1962 | rVB | 21656 | 27081 | 1.20% | 0.152% |
| 13 | 13.527 | 2025 | 2030 | 2038 | rBV | 829570 | 1074416 | 47.64% | 6.048% |
| 14 | 13.862 | 2083 | 2087 | 2096 | rBV | 24774 | 34841 | 1.54% | 0.196% |
| 15 | 14.627 | 2212 | 2217 | 2229 | rVB | 445114 | 599959 | 26.60% | 3.377% |
| 16 | 15.156 | 2304 | 2307 | 2316 | rBB | 15377 | 22825 | 1.01% | 0.128% |
| 17 | 15.645 | 2385 | 2390 | 2400 | rBV2 | 121618 | 156235 | 6.93% | 0.879% |
| 18 | 16.450 | 2524 | 2527 | 2535 | rVB2 | 22760 | 29704 | 1.32% | 0.167% |
| 19 | 16.750 | 2573 | 2578 | 2586 | rBV2 | 55093 | 87734 | 3.89% | 0.494% |
| 20 | 17.003 | 2615 | 2621 | 2624 | rBV | 1330056 | 1622072 | 71.92% | 9.130% |
| 21 | 18.250 | 2827 | 2833 | 2844 | rBV | 107452 | 163586 | 7.25% | 0.921% |
| 22 | 18.339 | 2844 | 2848 | 2854 | rBV | 403875 | 462198 | 20.49% | 2.602% |
| 23 | 19.491 | 3039 | 3044 | 3049 | rVB | 47378 | 54704 | 2.43% | 0.308% |
| 24 | 19.615 | 3061 | 3065 | 3069 | rBV | 23642 | 36929 | 1.64% | 0.208% |
| 25 | 19.956 | 3120 | 3123 | 3127 | rBV | 21325 | 22925 | 1.02% | 0.129% |
| 26 | 20.003 | 3127 | 3131 | 3141 | rVV | 325108 | 415414 | 18.42% | 2.338% |
| 27 | 20.491 | 3211 | 3214 | 3220 | rBV6 | 19240 | 29251 | 1.30% | 0.165% |

Sum of corrected areas: 17766212

LSC Report - Integrated Chromatogram

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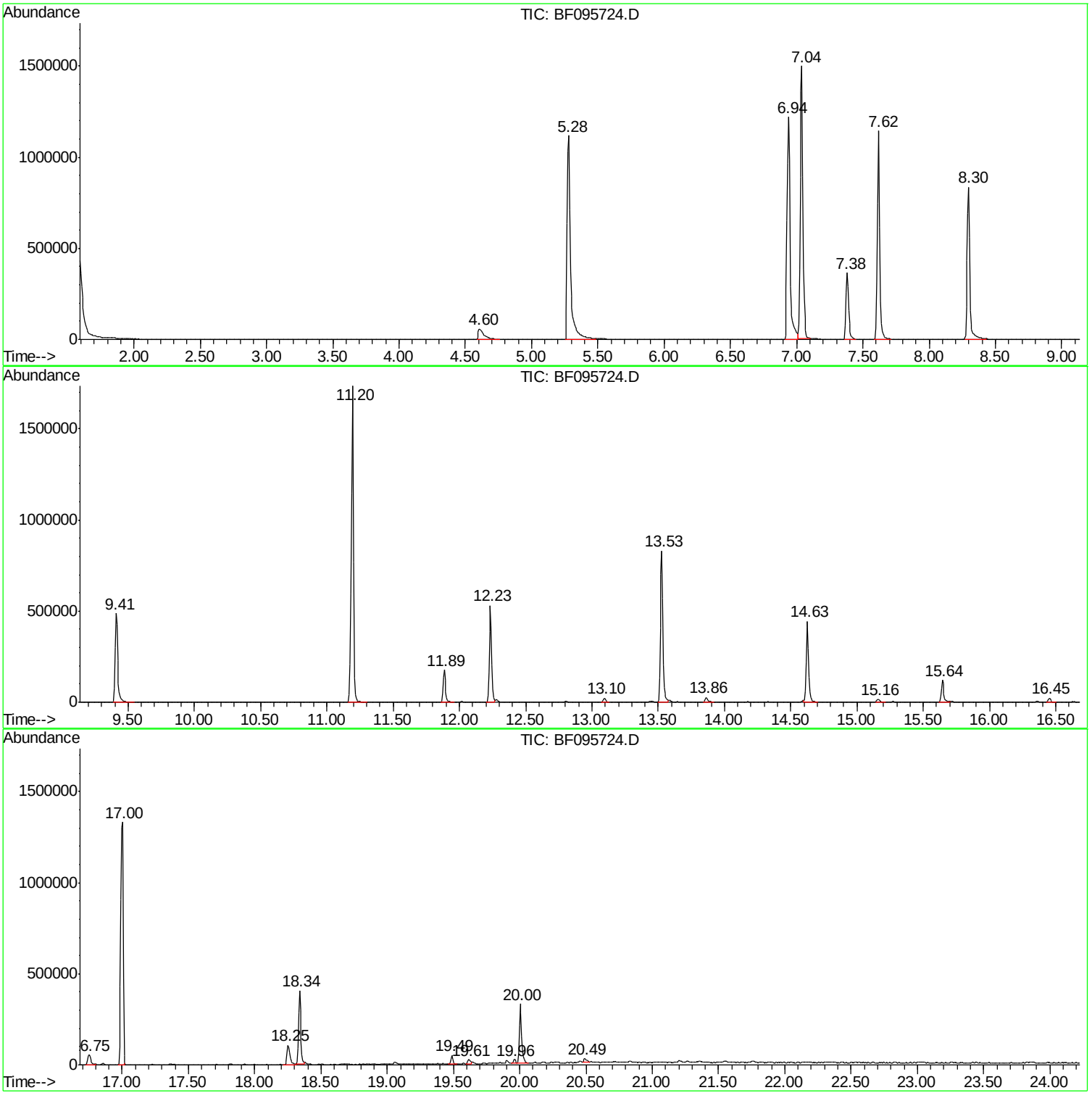
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

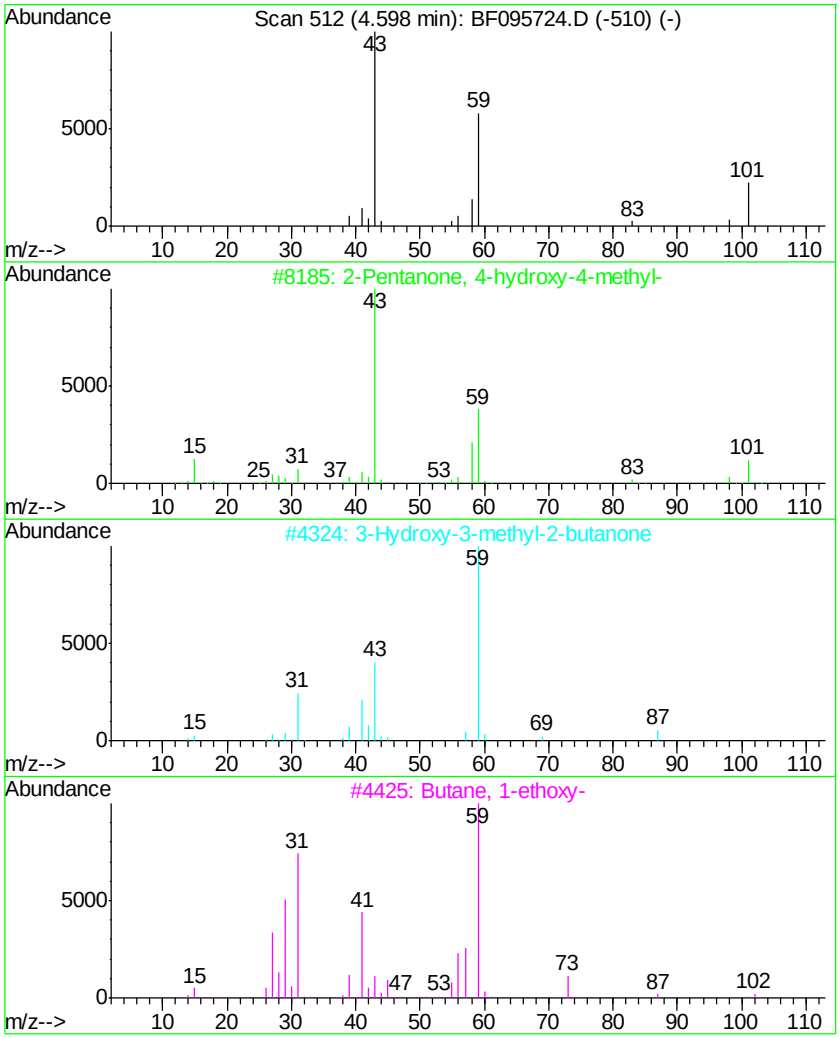
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

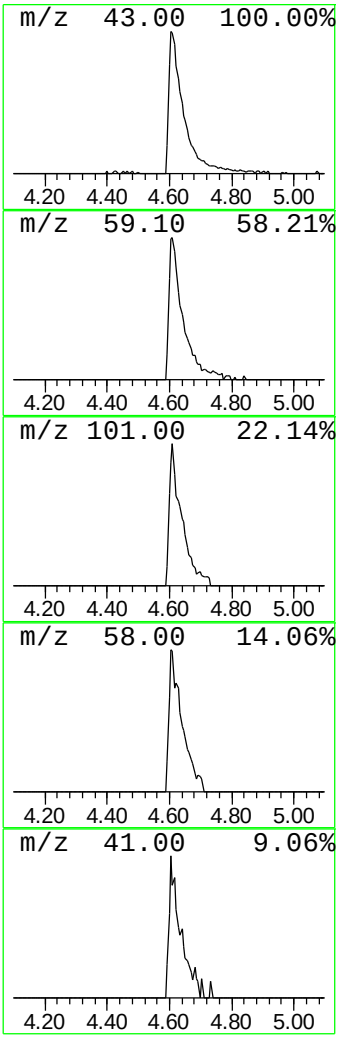
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.60 | 7.35 ng | 173273 | 1,4-Dichlorobenzene-d4 | 7.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 17 |
| 3 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

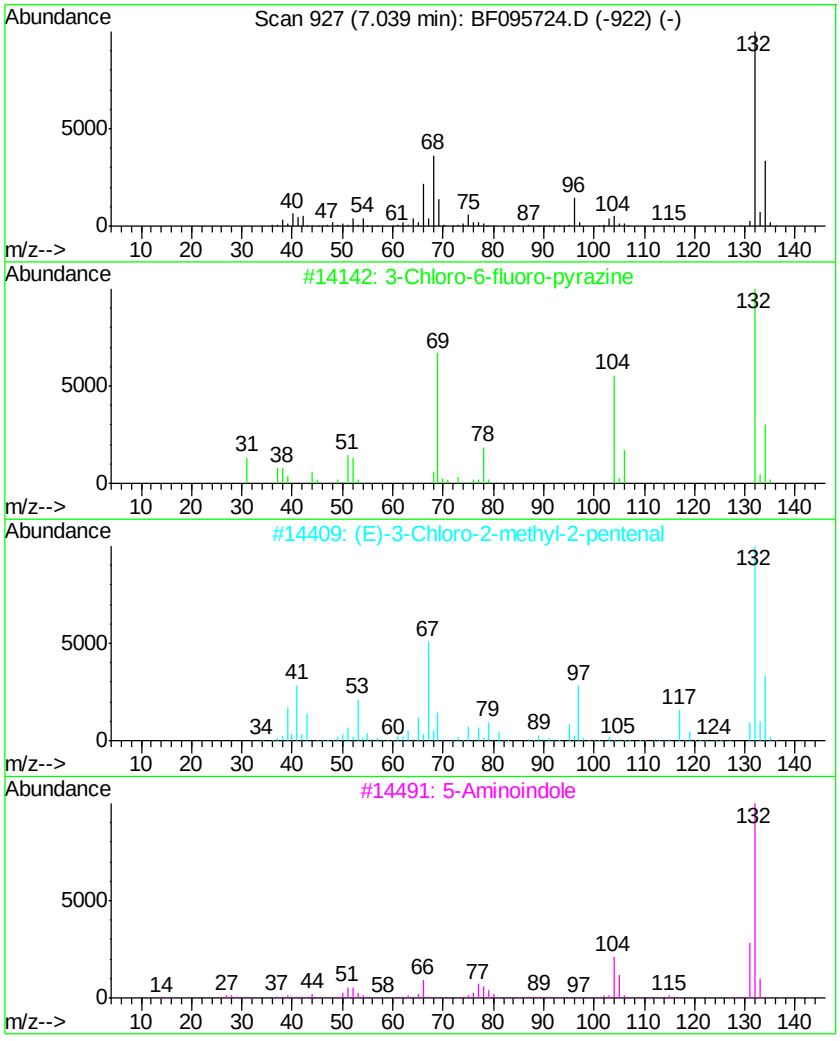
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

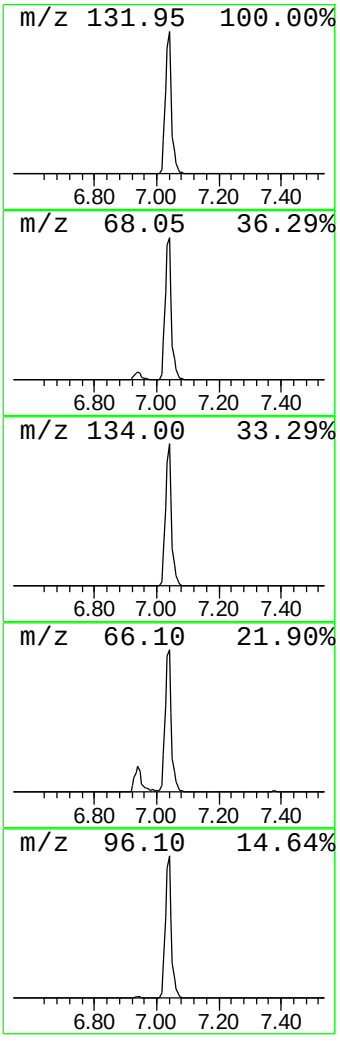
**********

Peak Number 2 unknown7.04 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.04 | 88.20 ng | 2078110 | 1,4-Dichlorobenzene-d4 | 7.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

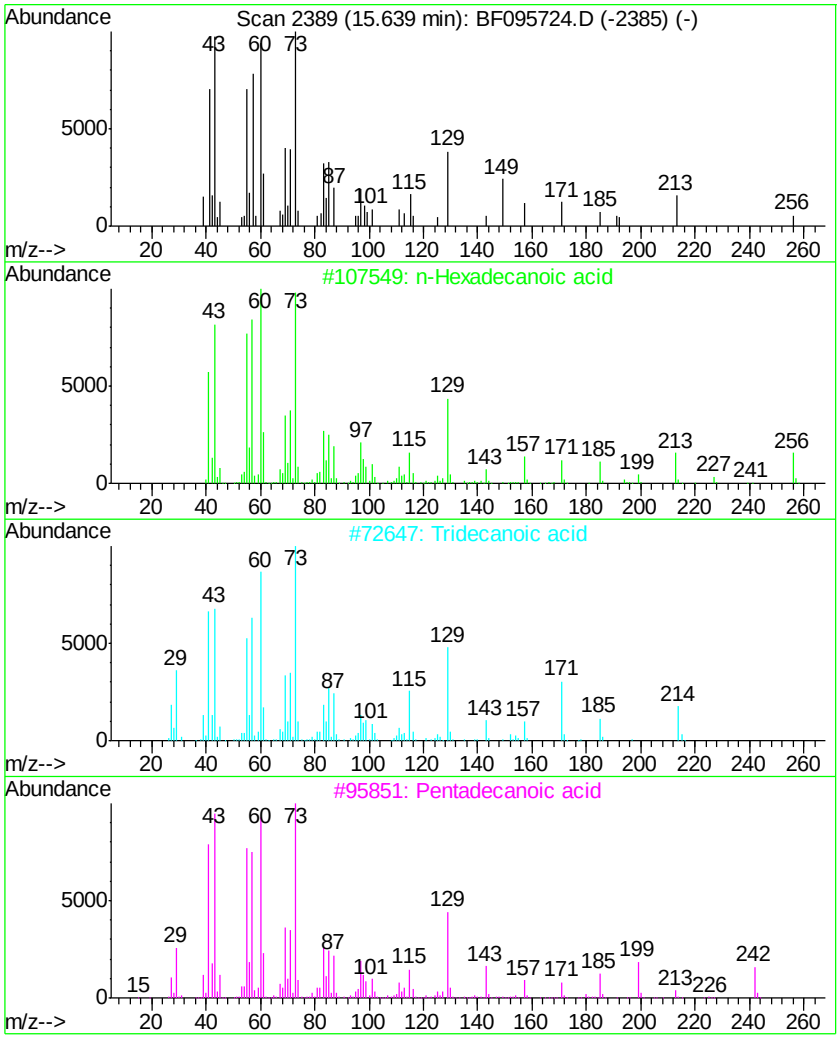
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

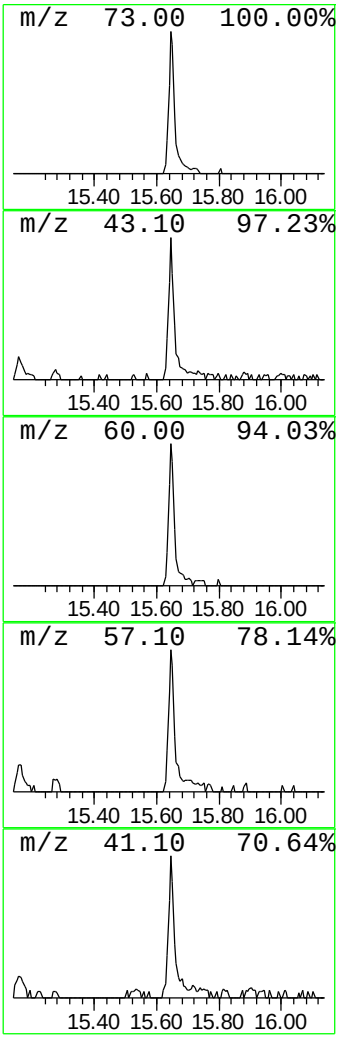
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.64 | 5.21 ng | 156235 | Phenanthrene-d10 | 14.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 94 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 58 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095724.D
Acq On : 6 Jun 2017 23:12
Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

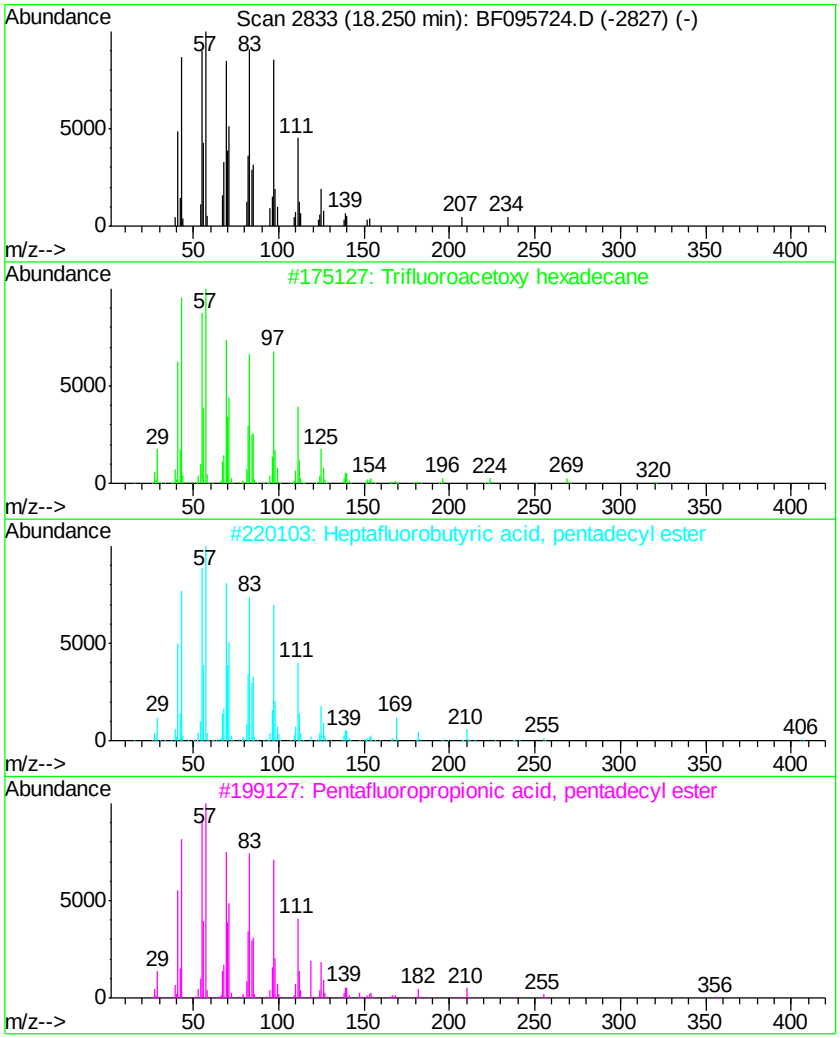
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

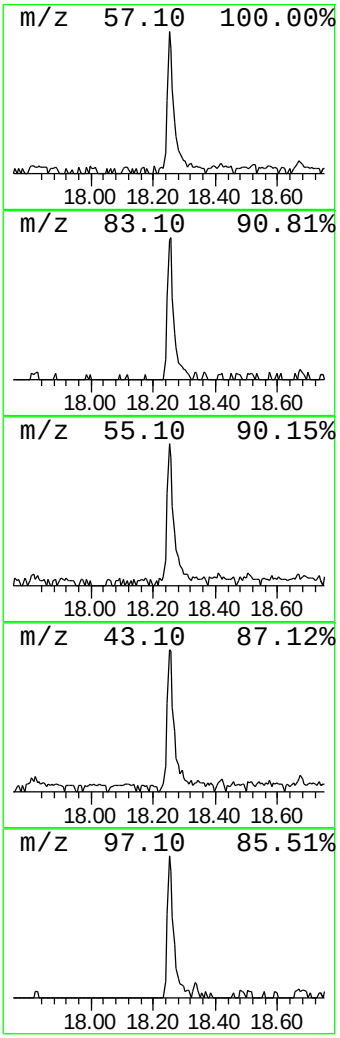
**********

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.25 | 7.08 ng | 163586 | Chrysene-d12 | 18.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 95 |
| 2 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 95 |
| 3 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 95 |
| 4 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 95 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |



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Operator : SJ/MA
Sample : I3478-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 146-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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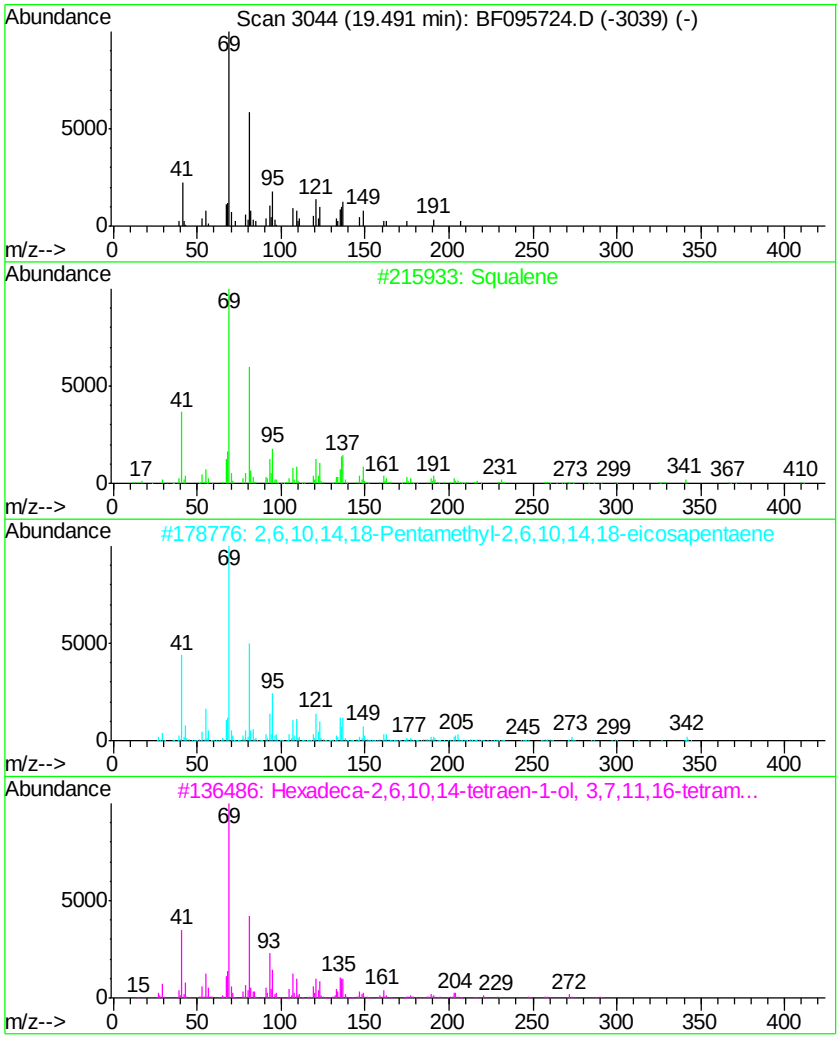
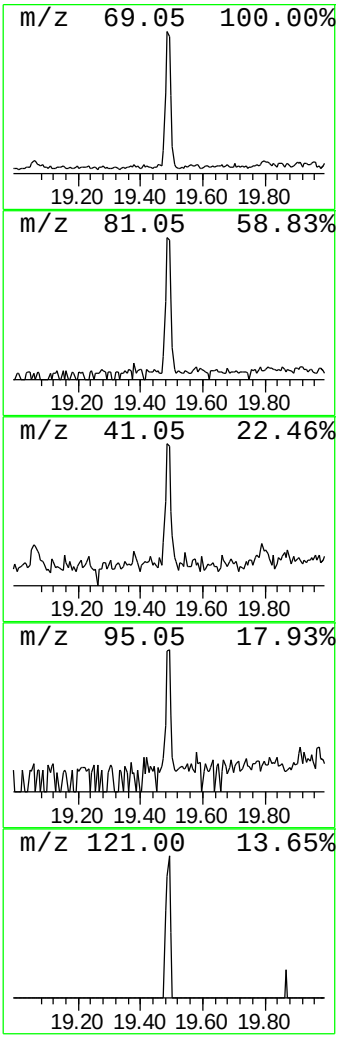
Peak Number 7 Squalene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.49 | 2.63 ng | 54704 | Perylene-d12 | 20.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42 | 075581-03-2 | 91 |
| 3 | Hexadeca-2,6,10,14-tetraen-1-ol,... | 290 | C20H34O | 007614-21-3 | 87 |
| 4 | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O | 1000163-04-7 | 86 |
| 5 | Supraene | 410 | C30H50 | 007683-64-9 | 78 |



Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 14 Sample Multiplier: 1

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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.60 | 7.3 | ng | 173273 | 1 | 7.38 | 471203 | 20.0 |
| unknown7.04 | 7.04 | 88.2 | ng | 2078110 | 1 | 7.38 | 471203 | 20.0 |
| n-Hexadecanoic acid | 15.64 | 5.2 | ng | 156235 | 4 | 14.63 | 599959 | 20.0 |
| Trifluoroacetoxy ... | 18.25 | 7.1 | ng | 163586 | 5 | 18.34 | 462198 | 20.0 |
| Squalene | 19.49 | 2.6 | ng | 54704 | 6 | 20.00 | 415414 | 20.0 |