LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

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-BF100818.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 | 4.898 | 474 | 478 | 491 | rBV | 40579 | 62153 | 2.99% | 0.346% |
| 2 | 5.316 | 545 | 549 | 564 | rBV | 1174538 | 1532597 | 73.74% | 8.527% |
| 3 | 6.345 | 720 | 724 | 741 | rBV | 1252895 | 1832989 | 88.20% | 10.198% |
| 4 | 6.469 | 741 | 745 | 762 | rVB | 1555689 | 1870328 | 89.99% | 10.406% |
| 5 | 6.698 | 780 | 784 | 806 | rVB | 282194 | 470247 | 22.63% | 2.616% |
| 6 | 6.851 | 806 | 810 | 833 | rBV | 1230727 | 1359190 | 65.40% | 7.562% |
| 7 | 7.257 | 875 | 879 | 909 | rBV | 795803 | 1171232 | 56.36% | 6.517% |
| 8 | 7.975 | 997 | 1001 | 1028 | rBV | 442209 | 612903 | 29.49% | 3.410% |
| 9 | 9.051 | 1180 | 1184 | 1211 | rBV | 1735036 | 2049903 | 98.63% | 11.405% |
| 10 | 9.445 | 1248 | 1251 | 1264 | rBV | 70066 | 85823 | 4.13% | 0.478% |
| 11 | 9.722 | 1294 | 1298 | 1316 | rBV | 707409 | 724424 | 34.86% | 4.031% |
| 12 | 10.510 | 1428 | 1432 | 1452 | rBV | 1155990 | 1486501 | 71.53% | 8.271% |
| 13 | 11.198 | 1546 | 1549 | 1571 | rBV | 564172 | 791682 | 38.09% | 4.405% |
| 14 | 12.780 | 1814 | 1818 | 1834 | rBV | 2138490 | 2078273 | 100.00% | 11.563% |
| 15 | 13.686 | 1968 | 1972 | 1984 | rBV2 | 49802 | 88959 | 4.28% | 0.495% |
| 16 | 13.827 | 1992 | 1996 | 2010 | rBV | 570777 | 659214 | 31.72% | 3.668% |
| 17 | 13.998 | 2021 | 2025 | 2029 | rBV | 36045 | 32733 | 1.58% | 0.182% |
| 18 | 14.298 | 2070 | 2076 | 2080 | rBV | 38607 | 40376 | 1.94% | 0.225% |
| 19 | 14.592 | 2122 | 2126 | 2130 | rBV | 48863 | 48999 | 2.36% | 0.273% |
| 20 | 14.662 | 2134 | 2138 | 2142 | rBV | 257513 | 248468 | 11.96% | 1.382% |
| 21 | 14.904 | 2175 | 2179 | 2184 | rBV | 43876 | 49554 | 2.38% | 0.276% |
| 22 | 15.221 | 2229 | 2233 | 2247 | rBV | 316675 | 550412 | 26.48% | 3.062% |
| 23 | 15.645 | 2300 | 2305 | 2312 | rBV2 | 39457 | 58467 | 2.81% | 0.325% |
| 24 | 16.104 | 2377 | 2383 | 2392 | rVB2 | 25308 | 45249 | 2.18% | 0.252% |
| 25 | 16.633 | 2468 | 2473 | 2481 | rBV5 | 11151 | 22554 | 1.09% | 0.125% |

Sum of corrected areas: 17973230

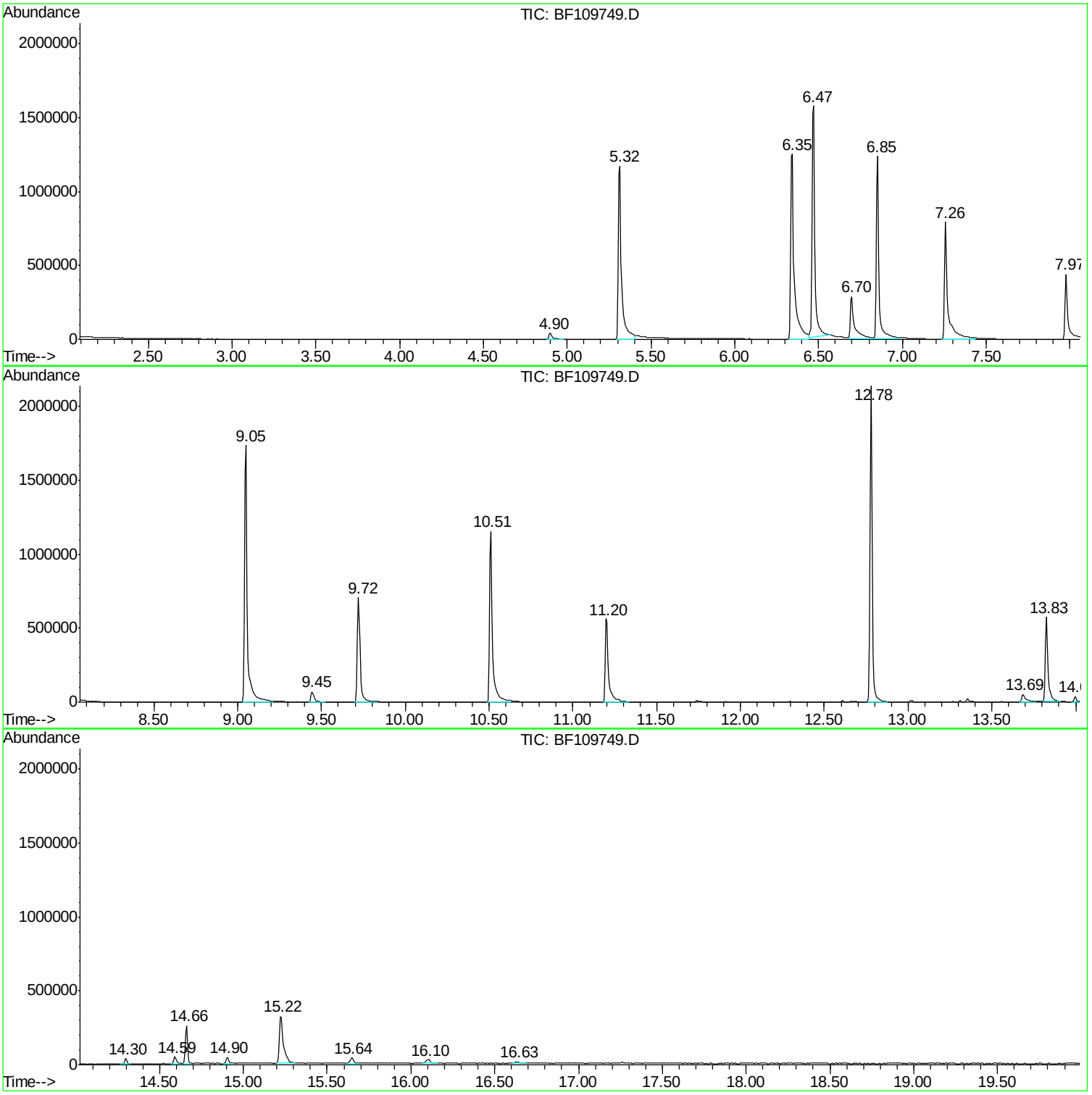
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

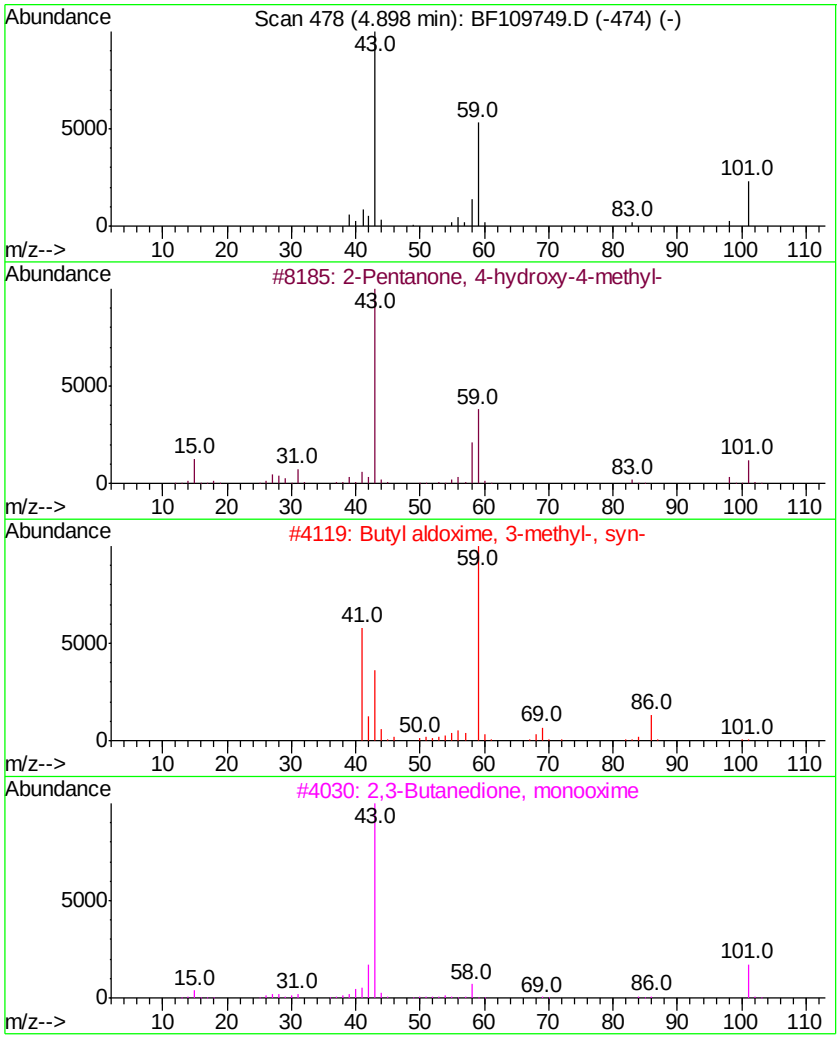
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

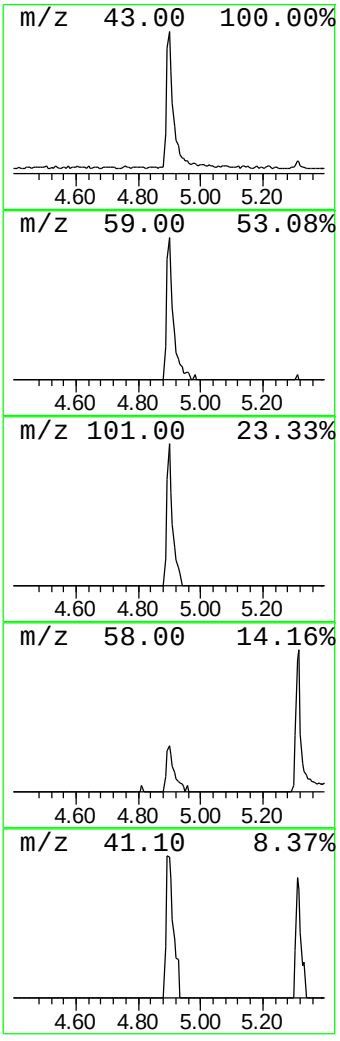
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.90 | 2.64 ng | 62153 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 17 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | Propylamine | 59 | C3H9N | 000107-10-8 | 9 |
| 5 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

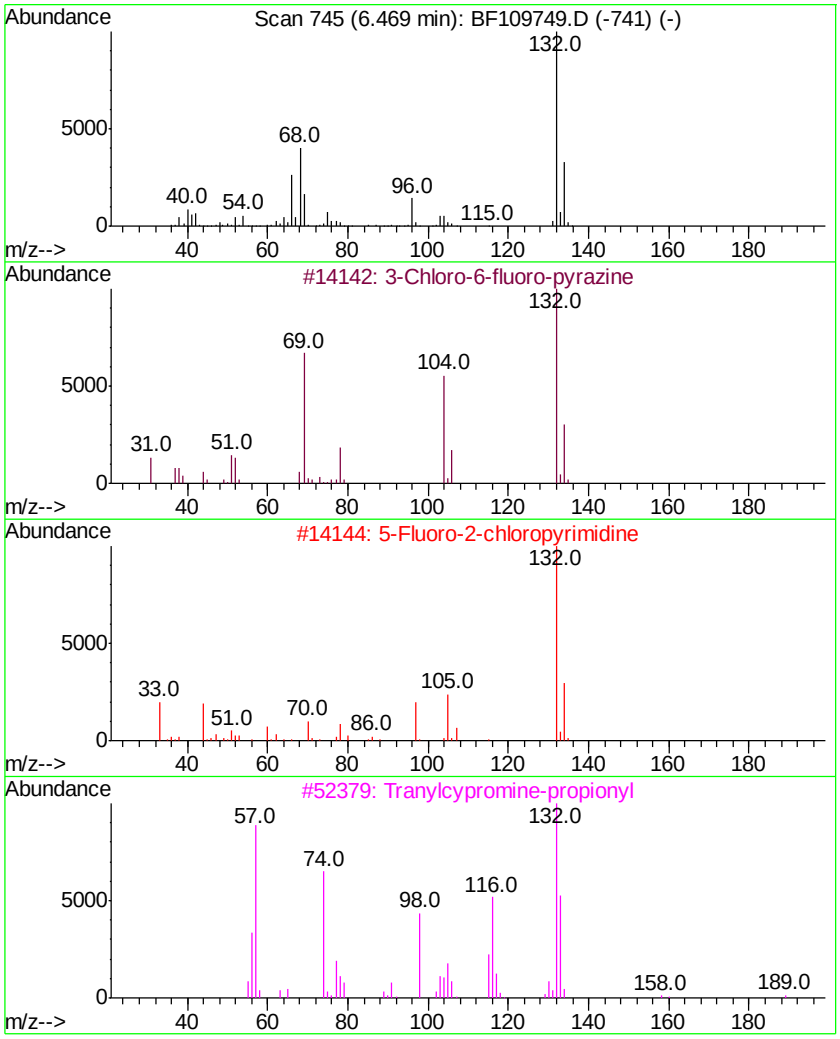
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

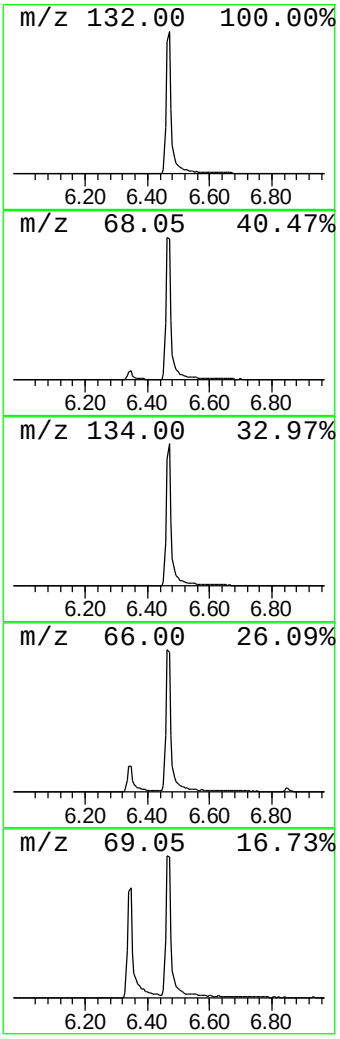
**********

Peak Number 2 unknown6.47 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.47 | 79.55 ng | 1870330 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

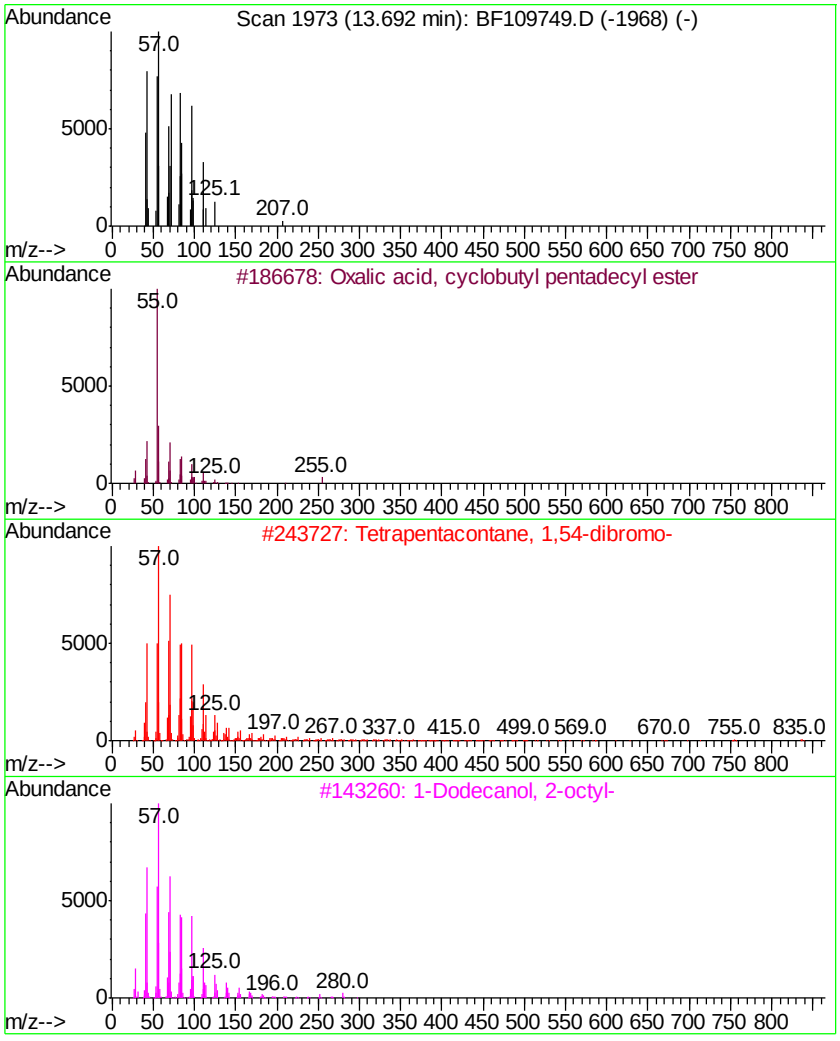
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

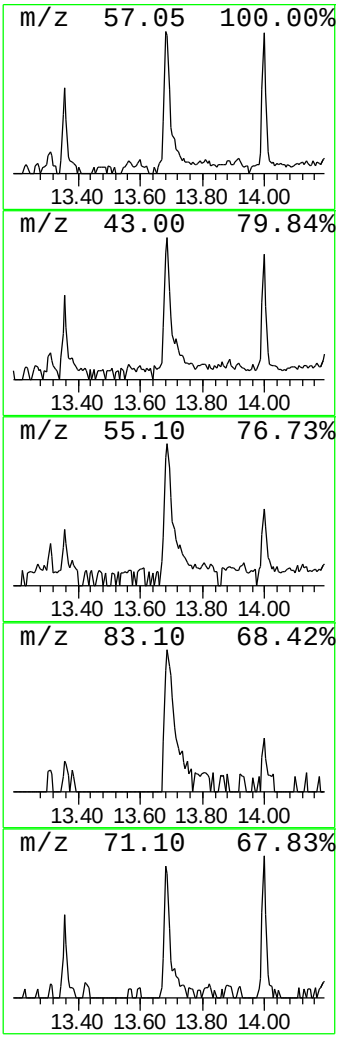
**********

Peak Number 4 Oxalic acid, cyclobutyl pen... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.69 | 2.70 ng | 88959 | Chrysene-d12 | 13.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxalic acid, cyclobutyl pentadec... | 354 | C21H38O4 | 1000309-70-5 | 90 |
| 2 | Tetrapentacontane, 1,54-dibromo- | 915 | C54H108Br2 | 1000156-09-4 | 90 |
| 3 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 87 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 58 |
| 5 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 58 |



# Library Search Compound Report

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Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

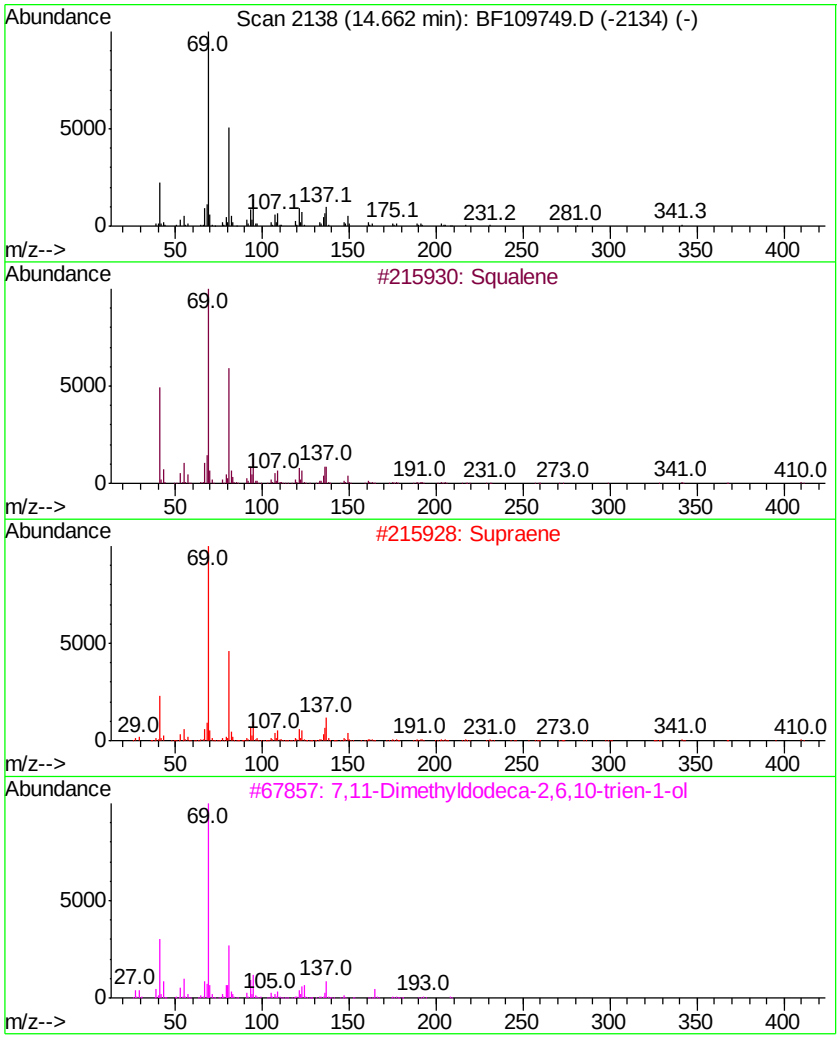
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

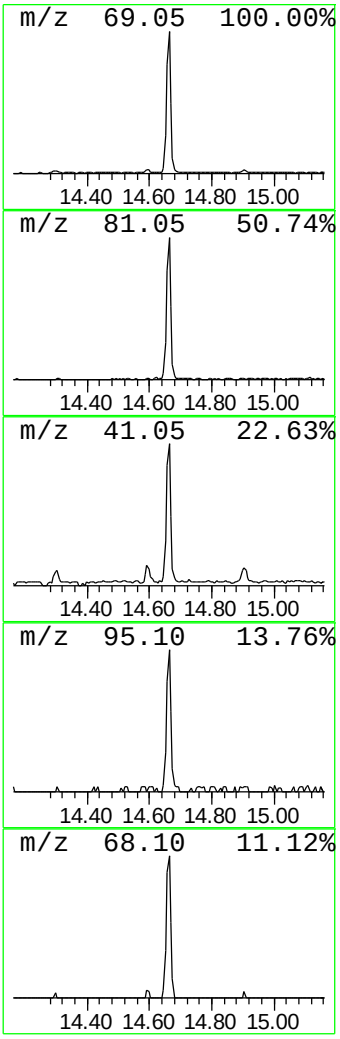
**********

Peak Number 5 Squalene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.66 | 9.03 ng | 248468 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 3 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72 |
| 4 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 264 | C17H28O2 | 004128-17-0 | 64 |
| 5 | 2,6-Octadiene, 4-methyl- | 124 | C9H16 | 074498-94-5 | 53 |



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Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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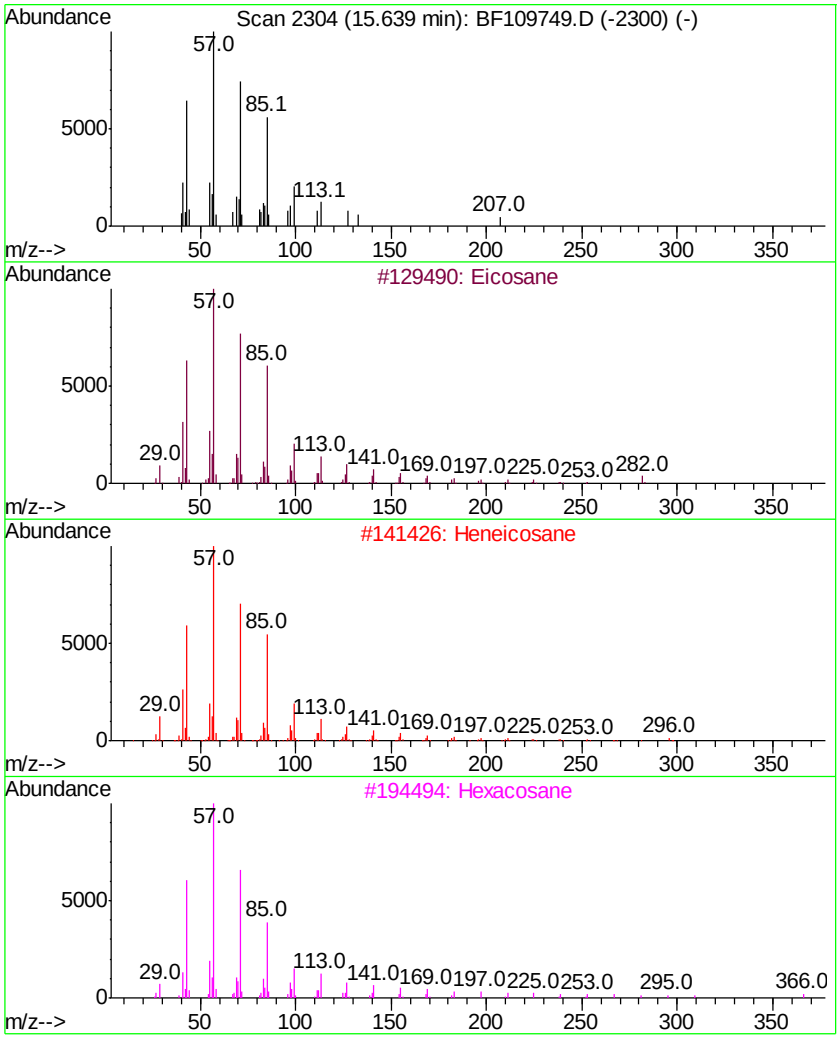
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

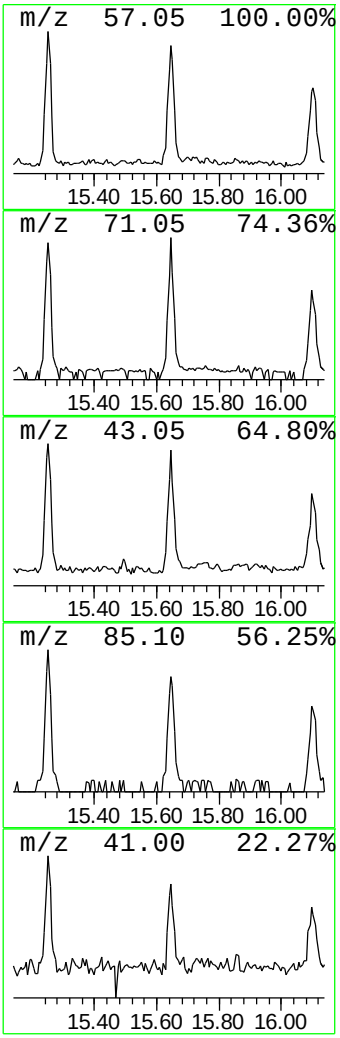
**********

Peak Number 6 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.64 | 2.12 ng | 58467 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 4 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101018\
Data File : BF109749.D
Acq On : 10 Oct 2018 18:23
Operator : JU/SJ
Sample : J5302-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-TW-4-(15.5-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.90 | 2.6 | ng | 62153 | 1 | 6.70 | 470247 | 20.0 |
| unknown6.47 | 6.47 | 79.5 | ng | 1870330 | 1 | 6.70 | 470247 | 20.0 |
| Oxalic acid, cycl... | 13.69 | 2.7 | ng | 88959 | 5 | 13.83 | 659214 | 20.0 |
| Squalene | 14.66 | 9.0 | ng | 248468 | 6 | 15.22 | 550412 | 20.0 |
| Eicosane | 15.64 | 2.1 | ng | 58467 | 6 | 15.22 | 550412 | 20.0 |