LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099059.D
Acq On : 4 Oct 2017 4:38
Operator : SJ/JU
Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

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-BF092317.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 | 2.140 | 5 | 9 | 19 | rVB | 111793 | 151965 | 5.38% | 0.629% |
| 2 | 5.092 | 508 | 511 | 523 | rVB | 485014 | 625493 | 22.16% | 2.590% |
| 3 | 5.492 | 574 | 579 | 582 | rBV | 2801866 | 2782261 | 98.58% | 11.521% |
| 4 | 6.504 | 745 | 751 | 754 | rBV | 2633963 | 2775602 | 98.34% | 11.493% |
| 5 | 6.645 | 770 | 775 | 778 | rBV | 2955242 | 2822437 | 100.00% | 11.687% |
| 6 | 6.875 | 808 | 814 | 817 | rBV | 840577 | 738963 | 26.18% | 3.060% |
| 7 | 6.998 | 832 | 835 | 837 | rBV | 49007 | 43860 | 1.55% | 0.182% |
| 8 | 7.028 | 837 | 840 | 844 | rVB | 2161979 | 2080920 | 73.73% | 8.617% |
| 9 | 7.439 | 904 | 910 | 913 | rBV | 1724916 | 1689726 | 59.87% | 6.997% |
| 10 | 7.516 | 919 | 923 | 932 | rVB | 24034 | 32390 | 1.15% | 0.134% |
| 11 | 8.157 | 1028 | 1032 | 1035 | rVB | 890392 | 804229 | 28.49% | 3.330% |
| 12 | 9.227 | 1209 | 1214 | 1217 | rBV | 2939630 | 2634643 | 93.35% | 10.910% |
| 13 | 9.616 | 1277 | 1280 | 1284 | rBV | 398006 | 334733 | 11.86% | 1.386% |
| 14 | 9.910 | 1326 | 1330 | 1334 | rVB | 831368 | 680279 | 24.10% | 2.817% |
| 15 | 10.698 | 1460 | 1464 | 1467 | rBV | 1304012 | 1139373 | 40.37% | 4.718% |
| 16 | 10.804 | 1479 | 1482 | 1489 | rBV | 41814 | 41122 | 1.46% | 0.170% |
| 17 | 11.392 | 1579 | 1582 | 1586 | rBV | 639316 | 560065 | 19.84% | 2.319% |
| 18 | 11.610 | 1613 | 1619 | 1627 | rBV2 | 47471 | 51246 | 1.82% | 0.212% |
| 19 | 12.427 | 1755 | 1758 | 1763 | rBV | 111658 | 105999 | 3.76% | 0.439% |
| 20 | 12.486 | 1764 | 1768 | 1775 | rVB3 | 38268 | 40942 | 1.45% | 0.170% |
| 21 | 12.780 | 1816 | 1818 | 1823 | rBV3 | 39012 | 40797 | 1.45% | 0.169% |
| 22 | 12.980 | 1847 | 1852 | 1855 | rBV | 2340738 | 2045085 | 72.46% | 8.468% |
| 23 | 13.451 | 1928 | 1932 | 1939 | rVB | 504335 | 431194 | 15.28% | 1.786% |
| 24 | 13.862 | 1999 | 2002 | 2006 | rBV | 74618 | 78427 | 2.78% | 0.325% |
| 25 | 14.004 | 2022 | 2026 | 2028 | rBV | 62683 | 54294 | 1.92% | 0.225% |
| 26 | 14.033 | 2028 | 2031 | 2035 | rVB | 781639 | 649541 | 23.01% | 2.690% |
| 27 | 14.651 | 2132 | 2136 | 2140 | rBV | 42230 | 39574 | 1.40% | 0.164% |
| 28 | 15.509 | 2277 | 2282 | 2292 | rVB | 558943 | 674287 | 23.89% | 2.792% |

Sum of corrected areas: 24149447

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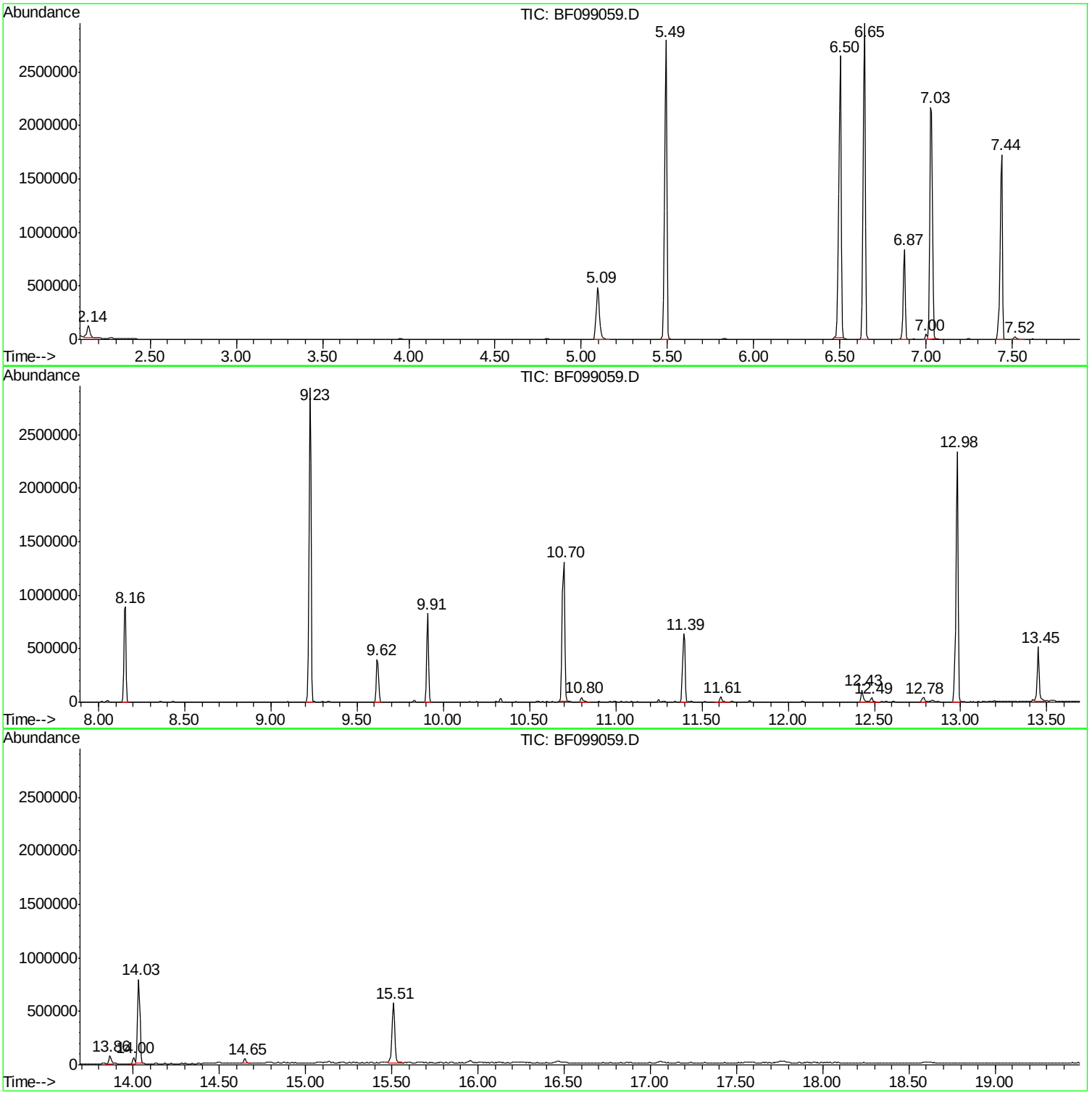
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

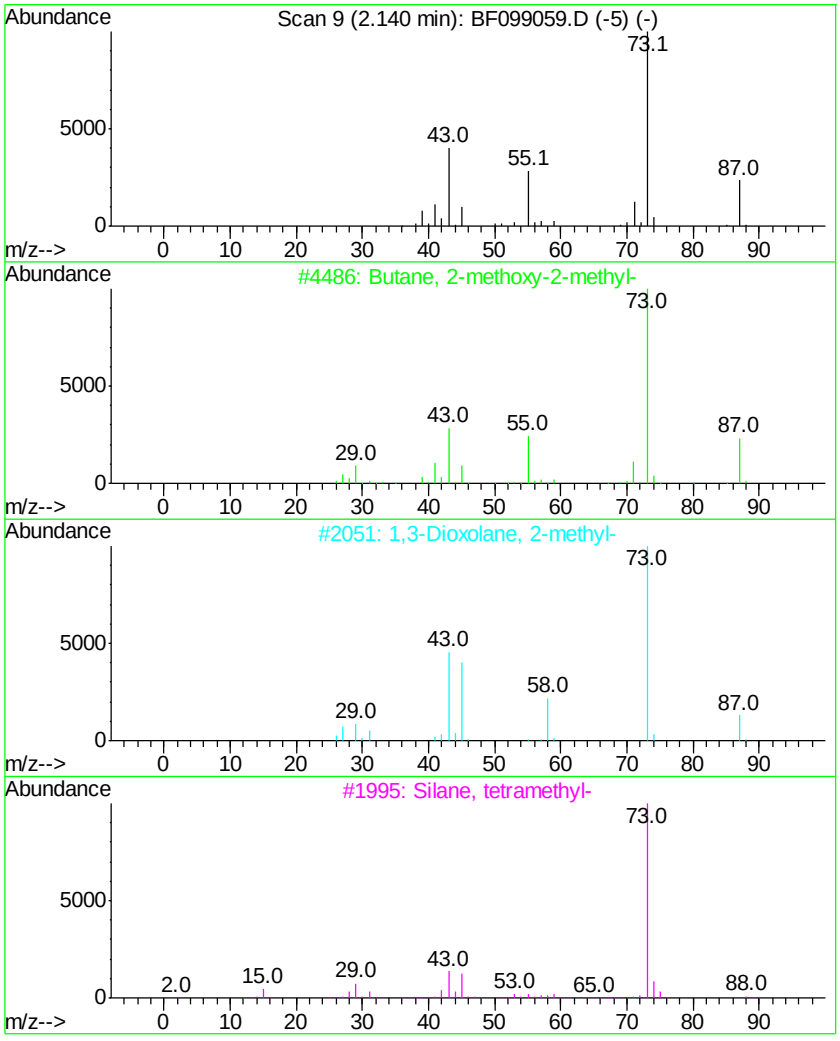
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

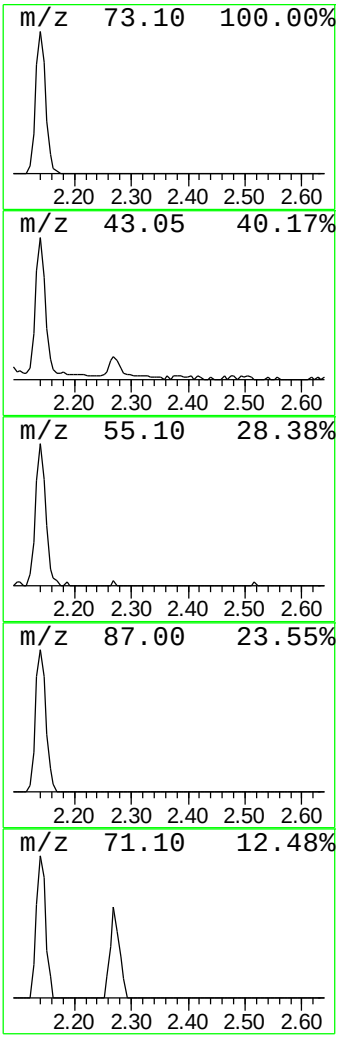
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.14 | 4.11 ng | 151965 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 25 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 1-(2-Methoxyethoxy)-2-methyl-2-p... | 162 | C8H18O3 | 1000364-24-4 | 9 |



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Data File : BF099059.D
Acq On : 4 Oct 2017 4:38
Operator : SJ/JU
Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

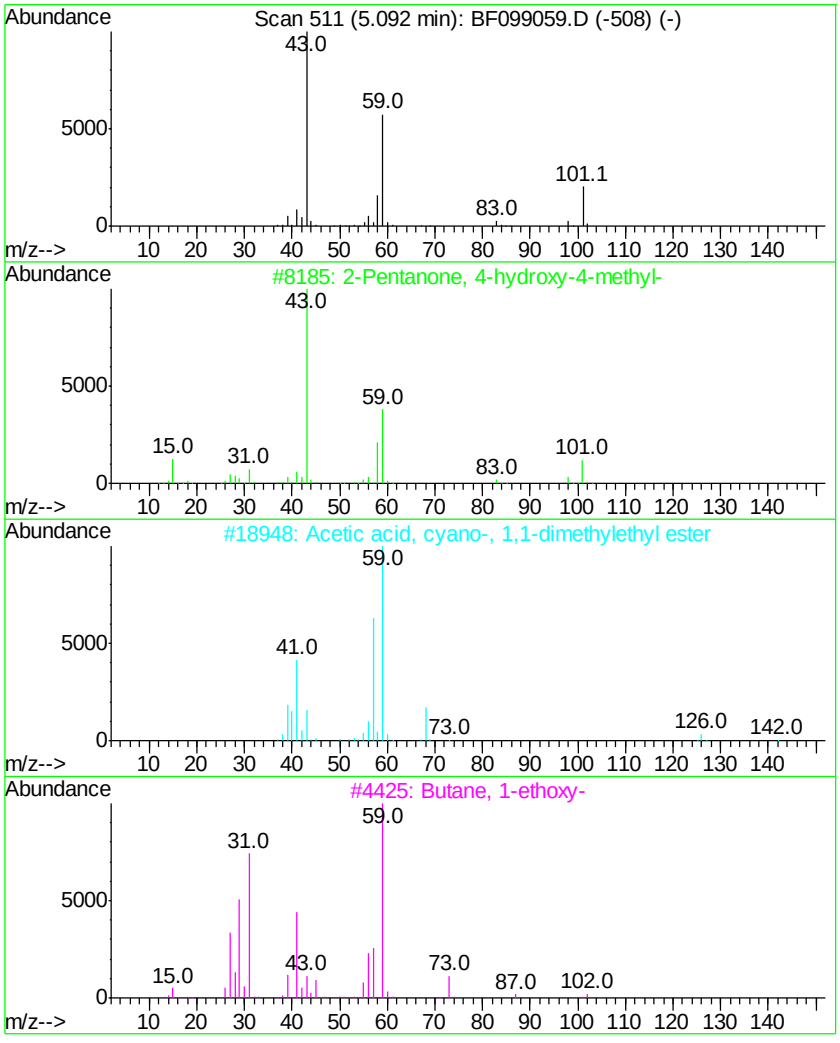
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

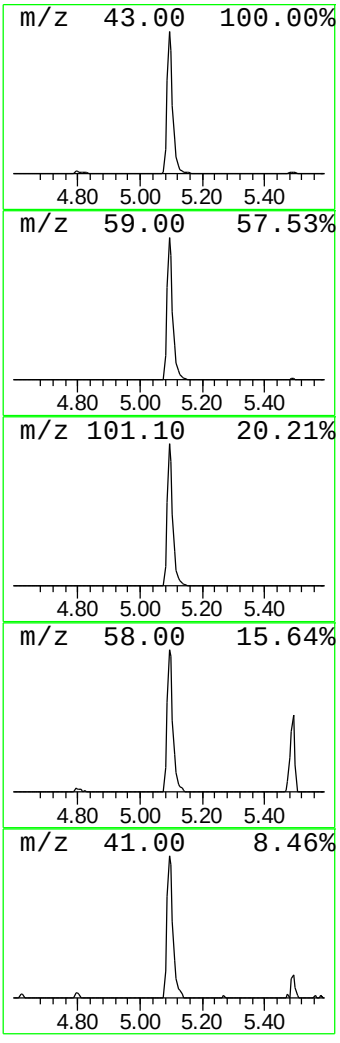
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 16.93 ng | 625493 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099059.D
Acq On : 4 Oct 2017 4:38
Operator : SJ/JU
Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

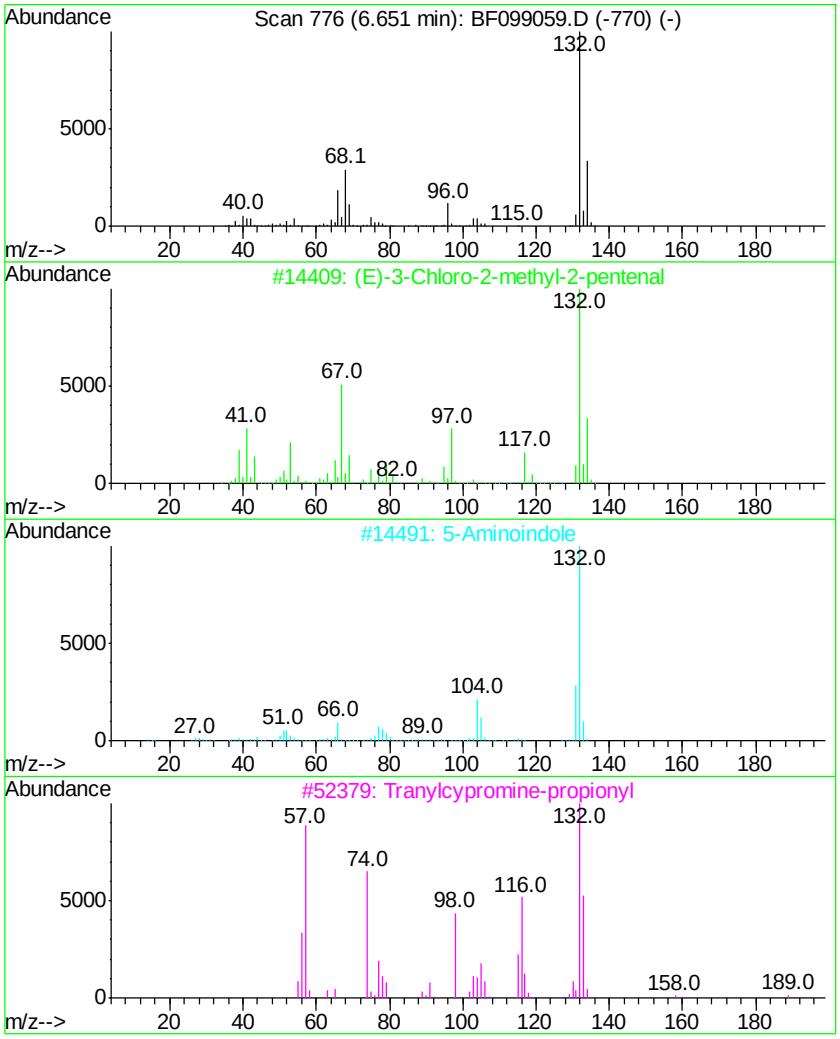
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

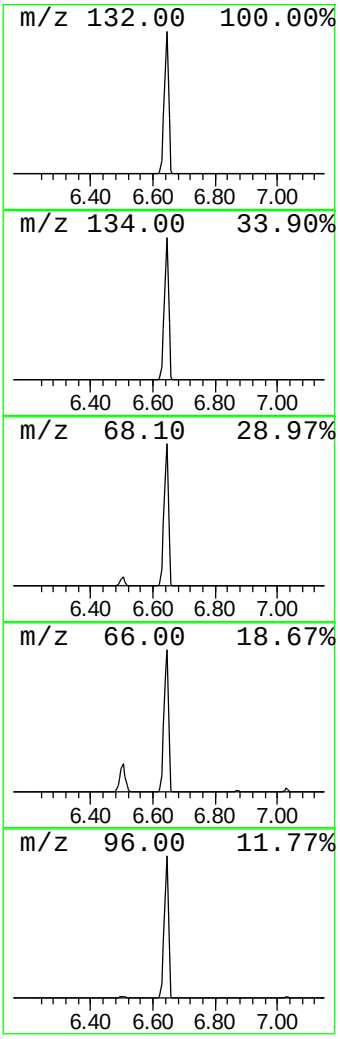
**********

Peak Number 3 unknown6.65 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.65 | 76.39 ng | 2822440 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



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Data File : BF099059.D
Acq On : 4 Oct 2017 4:38
Operator : SJ/JU
Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

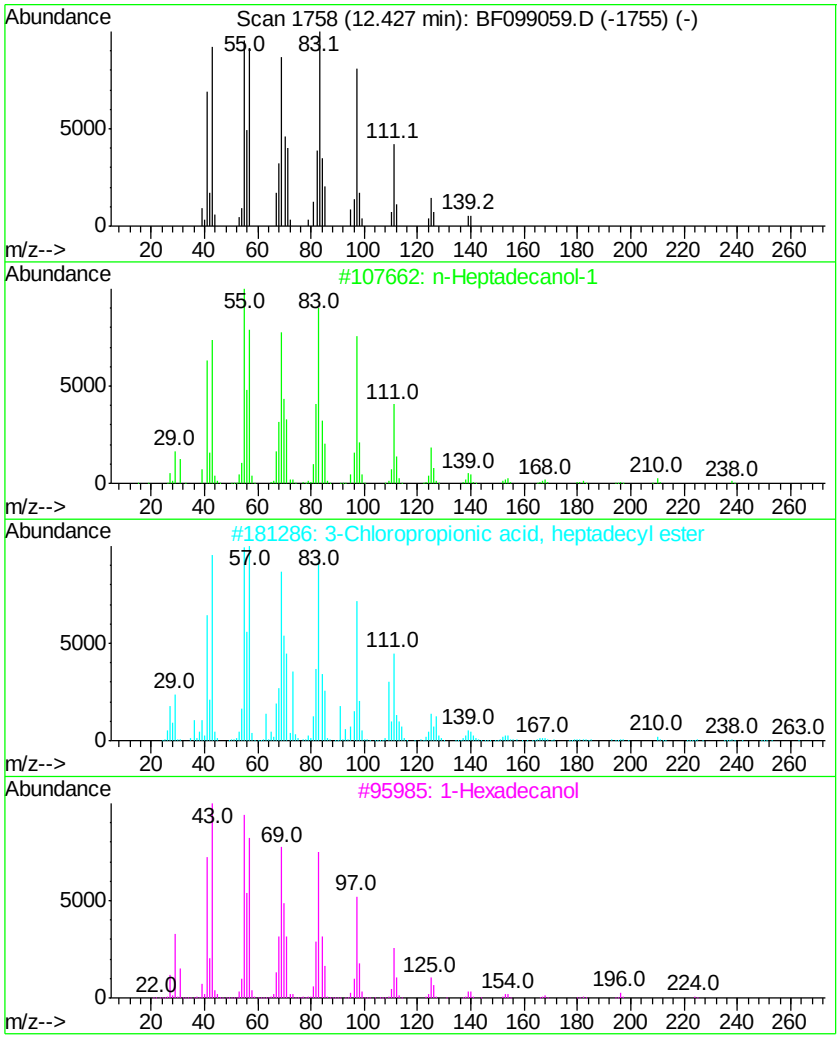
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

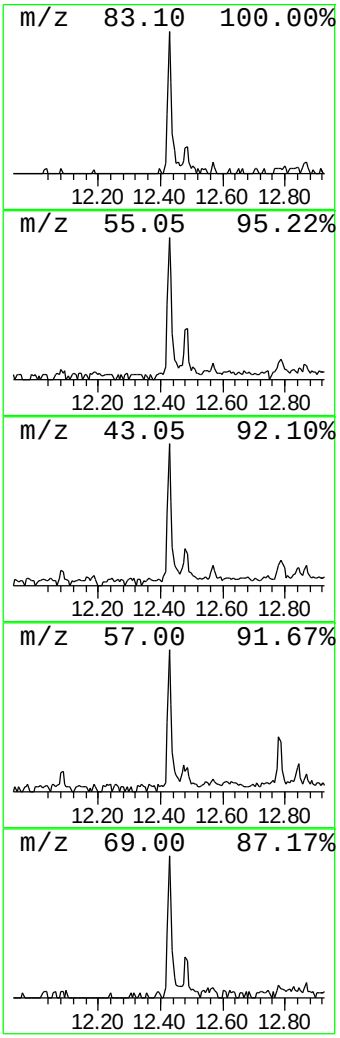
**********

Peak Number 5 n-Heptadecanol-1 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.43 | 3.79 ng | 105999 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 94 |
| 2 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 90 |
| 3 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 87 |
| 4 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 87 |
| 5 | 9-Octadecene, (E)- | 252 | C18H36 | 007206-25-9 | 83 |



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Data File : BF099059.D
Acq On : 4 Oct 2017 4:38
Operator : SJ/JU
Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

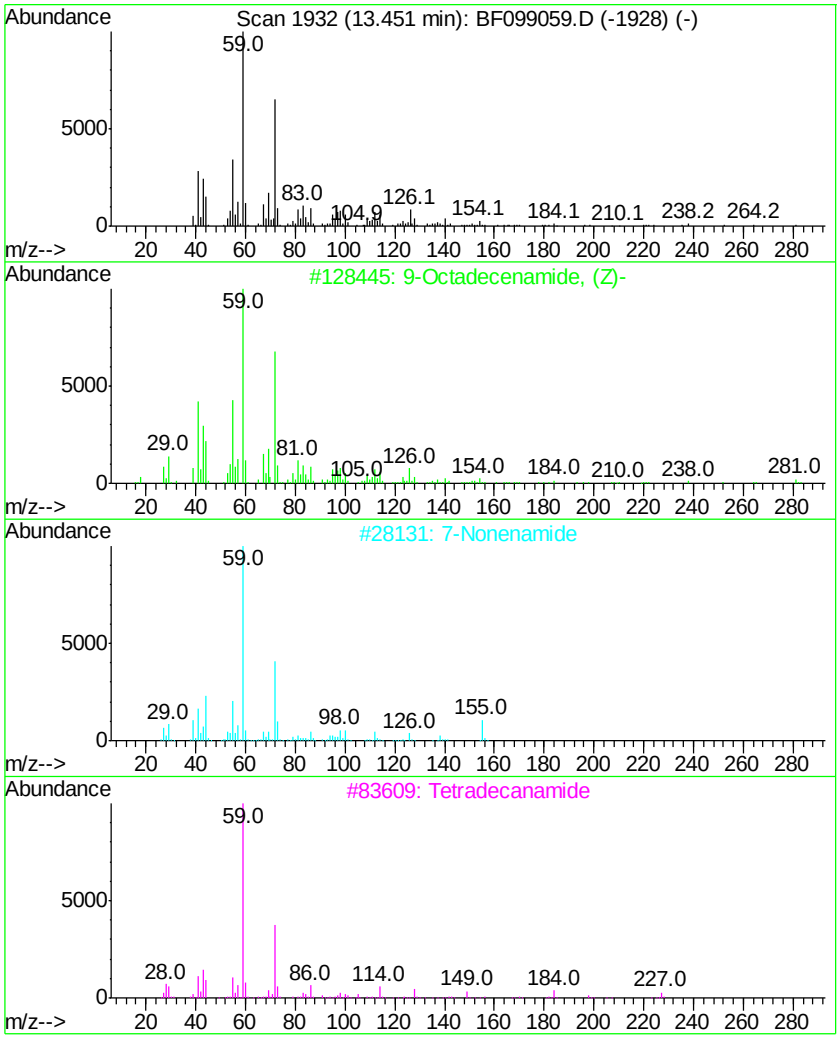
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

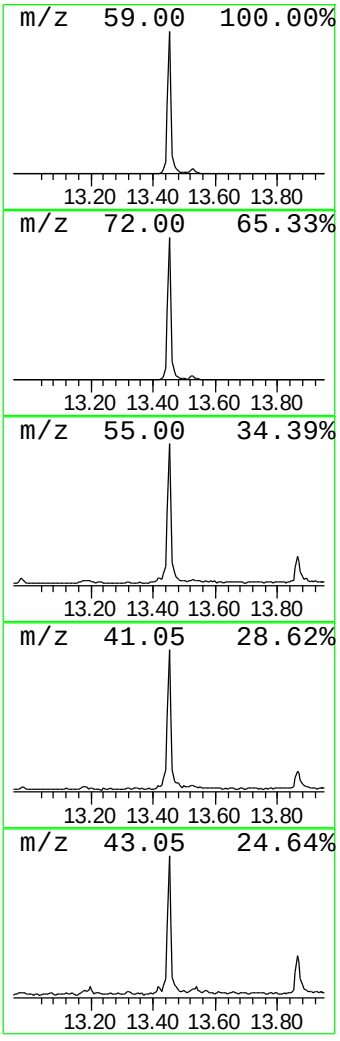
**********

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.45 | 13.28 ng | 431194 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 97 |
| 2 | 7-Nonenamide | 155 | C9H17NO | 090949-53-4 | 64 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 64 |
| 4 | Nonanamide | 157 | C9H19NO | 001120-07-6 | 64 |
| 5 | Octanamide | 143 | C8H17NO | 000629-01-6 | 56 |



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Sample : I5588-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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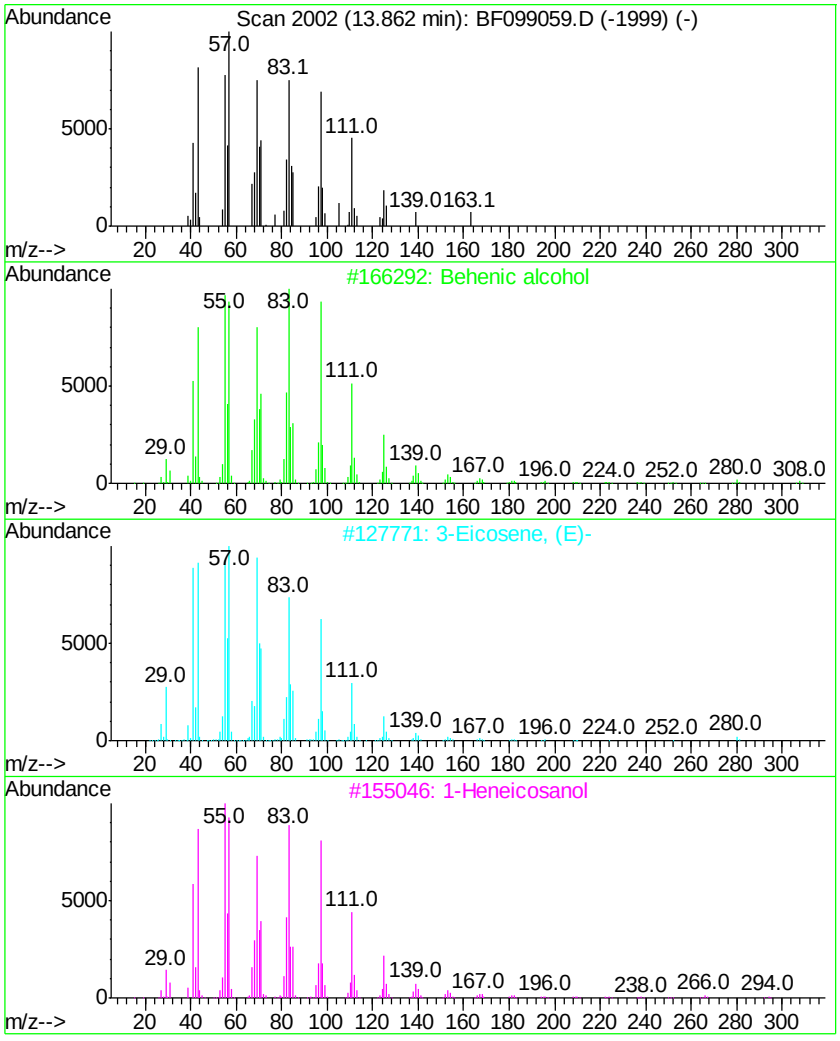
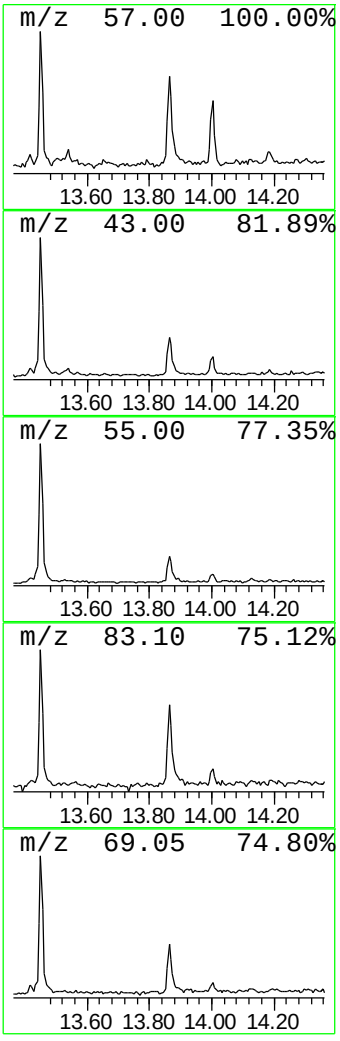
**********

Peak Number 7 Behenic alcohol Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.86 | 2.41 ng | 78427 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 91 |
| 2 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 91 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 90 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 90 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 90 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SASP2P-EPE-T8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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... | 2.14 | 4.1 | ng | 151965 | 1 | 6.87 | 738963 | 20.0 |
| 2-Pentanone, 4-hy... | 5.09 | 16.9 | ng | 625493 | 1 | 6.87 | 738963 | 20.0 |
| unknown6.65 | 6.65 | 76.4 | ng | 2822440 | 1 | 6.87 | 738963 | 20.0 |
| n-Heptadecanol-1 | 12.43 | 3.8 | ng | 105999 | 4 | 11.39 | 560065 | 20.0 |
| 9-Octadecenamide,... | 13.45 | 13.3 | ng | 431194 | 5 | 14.03 | 649541 | 20.0 |
| Behenic alcohol | 13.86 | 2.4 | ng | 78427 | 5 | 14.03 | 649541 | 20.0 |