LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080216\
Data File : BF089557.D
Acq On : 2 Aug 2016 20:10
Operator : UM/SJ
Sample : H4269-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

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-BF072716.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 | 1.644 | 4 | 5 | 47 | rVB | 770496 | 1652022 | 100.00% | 14.287% |
| 2 | 4.559 | 257 | 260 | 269 | rBV | 244239 | 415127 | 25.13% | 3.590% |
| 3 | 5.039 | 300 | 302 | 321 | rBV | 931054 | 1116106 | 67.56% | 9.652% |
| 4 | 5.450 | 337 | 338 | 345 | rVB | 17361 | 19524 | 1.18% | 0.169% |
| 5 | 6.136 | 395 | 398 | 400 | rBV | 1019638 | 1122975 | 67.98% | 9.711% |
| 6 | 6.239 | 405 | 407 | 409 | rBV | 1195748 | 1184743 | 71.71% | 10.246% |
| 7 | 6.467 | 426 | 427 | 438 | rBV4 | 165832 | 209050 | 12.65% | 1.808% |
| 8 | 6.627 | 438 | 441 | 443 | rBV | 764145 | 866314 | 52.44% | 7.492% |
| 9 | 7.050 | 476 | 478 | 488 | rBV | 405761 | 692607 | 41.92% | 5.990% |
| 10 | 7.187 | 488 | 490 | 496 | rVB | 20837 | 37321 | 2.26% | 0.323% |
| 11 | 7.759 | 538 | 540 | 552 | rBV | 240878 | 270773 | 16.39% | 2.342% |
| 12 | 8.833 | 632 | 634 | 637 | rBV | 1106749 | 1097405 | 66.43% | 9.490% |
| 13 | 9.233 | 667 | 669 | 672 | rBV | 248760 | 259369 | 15.70% | 2.243% |
| 14 | 9.496 | 690 | 692 | 695 | rBV | 321018 | 285044 | 17.25% | 2.465% |
| 15 | 10.285 | 759 | 761 | 771 | rBV | 625361 | 654934 | 39.64% | 5.664% |
| 16 | 10.422 | 771 | 773 | 780 | rVB | 26581 | 35116 | 2.13% | 0.304% |
| 17 | 10.868 | 810 | 812 | 813 | rBV | 19130 | 17383 | 1.05% | 0.150% |
| 18 | 10.971 | 818 | 821 | 826 | rBV | 235438 | 243336 | 14.73% | 2.104% |
| 19 | 11.234 | 842 | 844 | 848 | rBV | 22995 | 44178 | 2.67% | 0.382% |
| 20 | 12.548 | 957 | 959 | 962 | rBV | 845626 | 856148 | 51.82% | 7.404% |
| 21 | 13.474 | 1037 | 1040 | 1047 | rVB | 28574 | 48407 | 2.93% | 0.419% |
| 22 | 13.588 | 1048 | 1050 | 1058 | rBV | 196471 | 224020 | 13.56% | 1.937% |
| 23 | 14.914 | 1163 | 1166 | 1173 | rBV | 189112 | 211567 | 12.81% | 1.830% |

Sum of corrected areas: 11563469

LSC Report - Integrated Chromatogram

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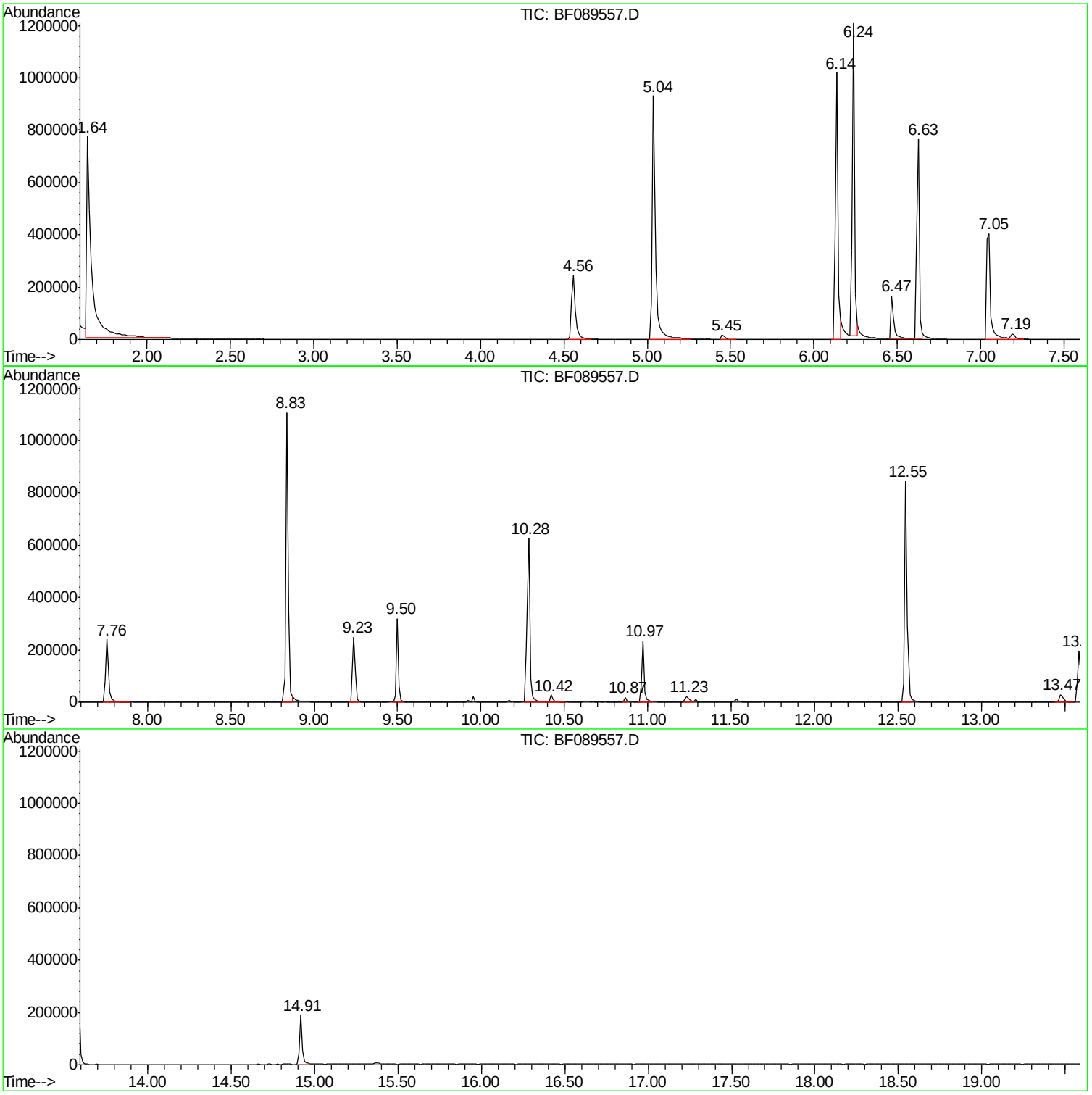
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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Data File : BF089557.D
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**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

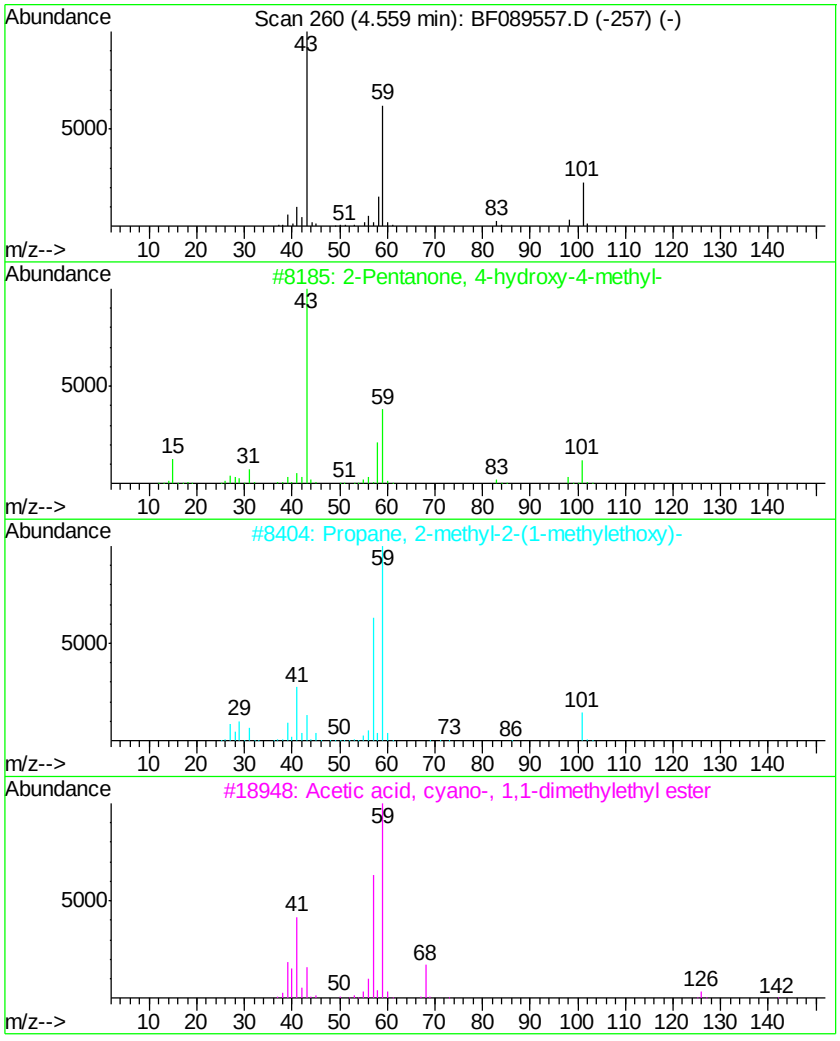
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

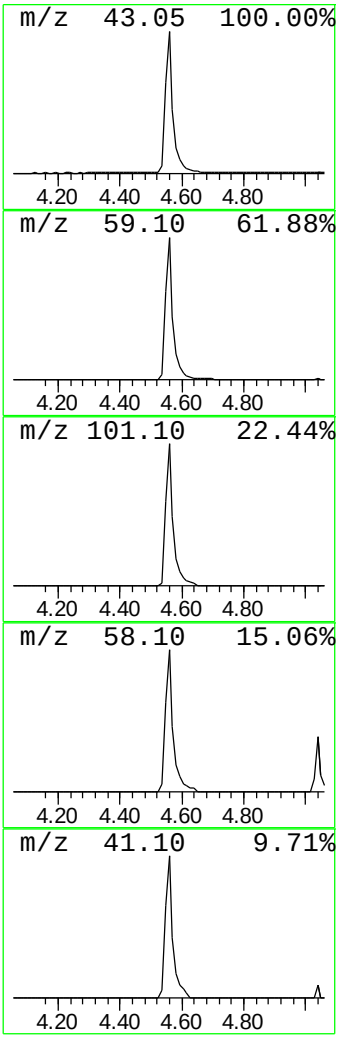
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.56 | 39.72 ng | 415127 | 1,4-Dichlorobenzene-d4 | 6.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 23 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080216\
Data File : BF089557.D
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Operator : UM/SJ
Sample : H4269-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

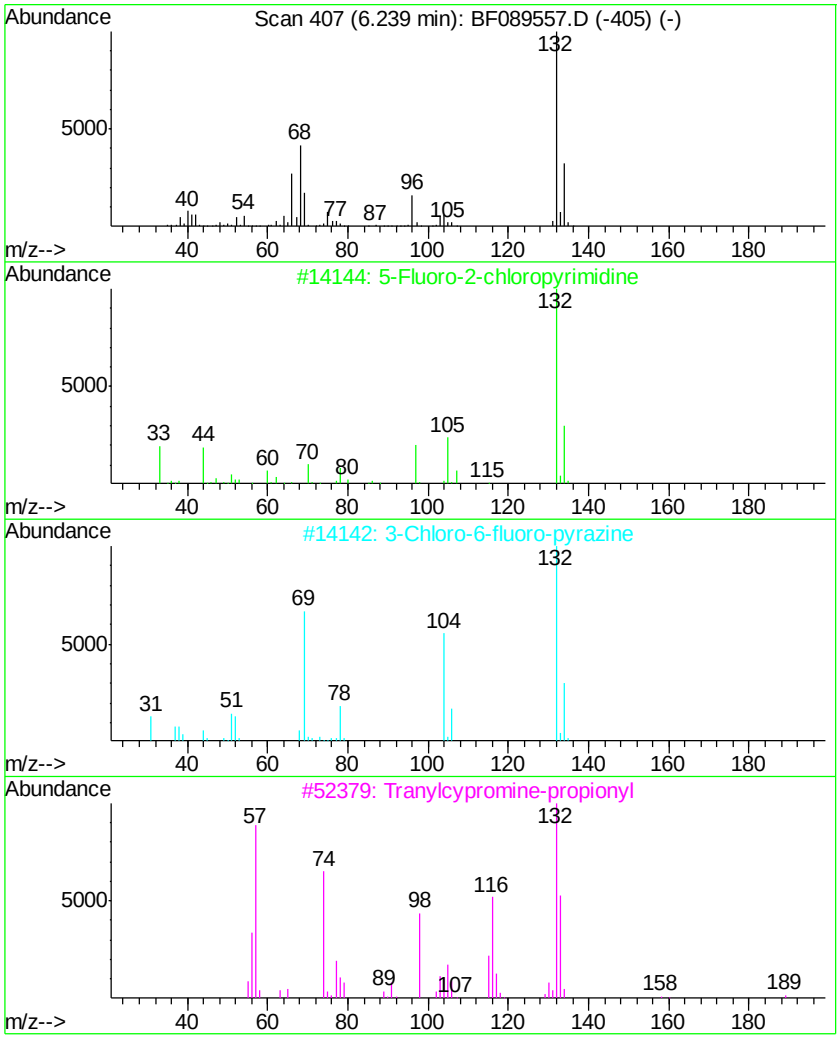
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

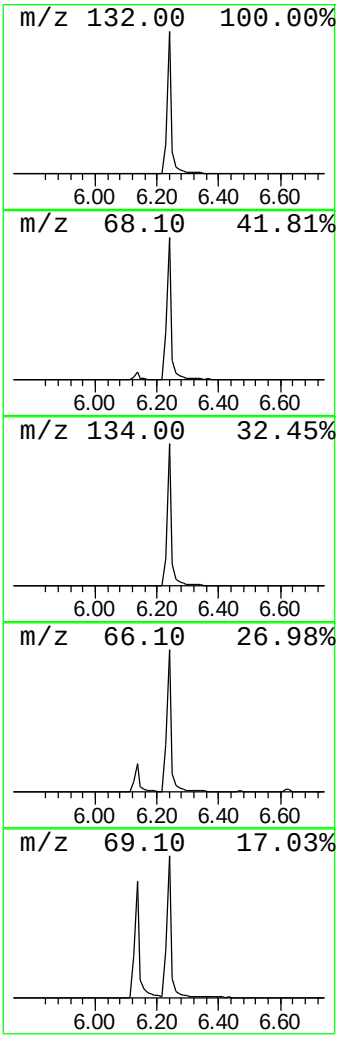
**********

Peak Number 3 unknown6.24 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.24 | 113.35 ng | 1184740 | 1,4-Dichlorobenzene-d4 | 6.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 27 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



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Data File : BF089557.D
Acq On : 2 Aug 2016 20:10
Operator : UM/SJ
Sample : H4269-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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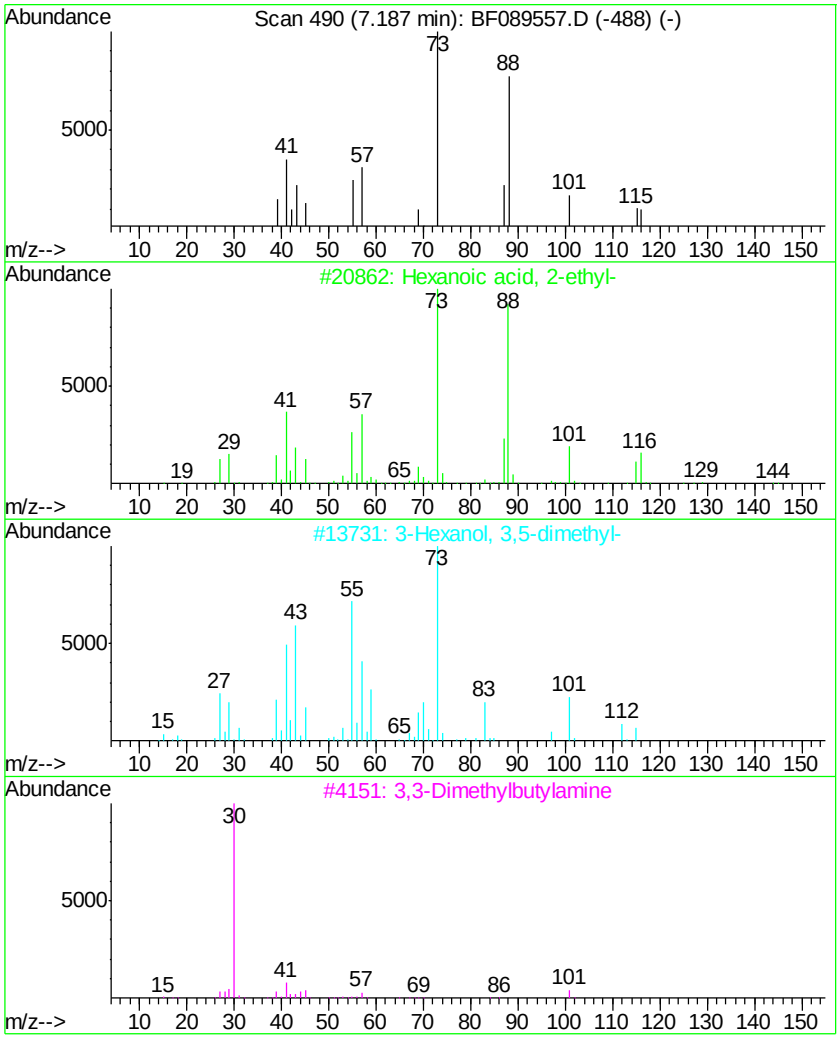
TIC Integration Parameters: LSCINT.P

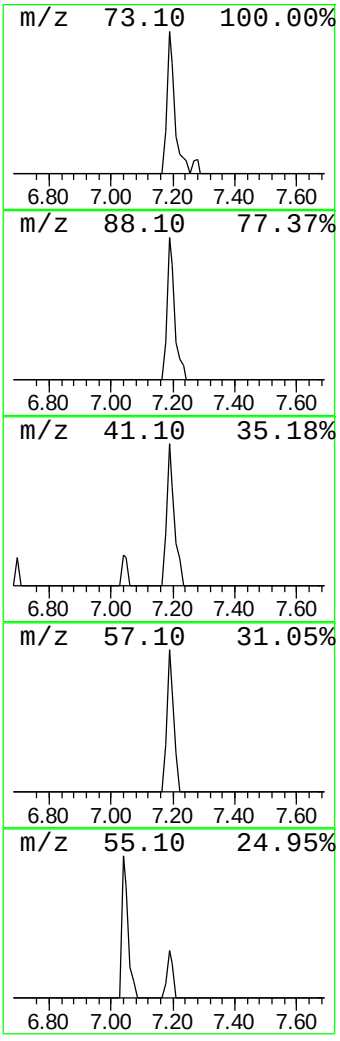
**********

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.19 | 2.76 ng | 37321 | Naphthalene-d8 | 7.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 72 |
| 2 | 3-Hexanol, 3,5-dimethyl- | 130 | C8H18O | 004209-91-0 | 16 |
| 3 | 3,3-Dimethylbutylamine | 101 | C6H15N | 015673-00-4 | 9 |
| 4 | Heptanoic acid, ethyl ester | 158 | C9H18O2 | 000106-30-9 | 9 |
| 5 | Pentanoic acid, 2-methyl-, methy... | 130 | C7H14O2 | 002177-77-7 | 9 |



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Operator : UM/SJ
Sample : H4269-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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TIC Library : C:\Database\NIST11.L
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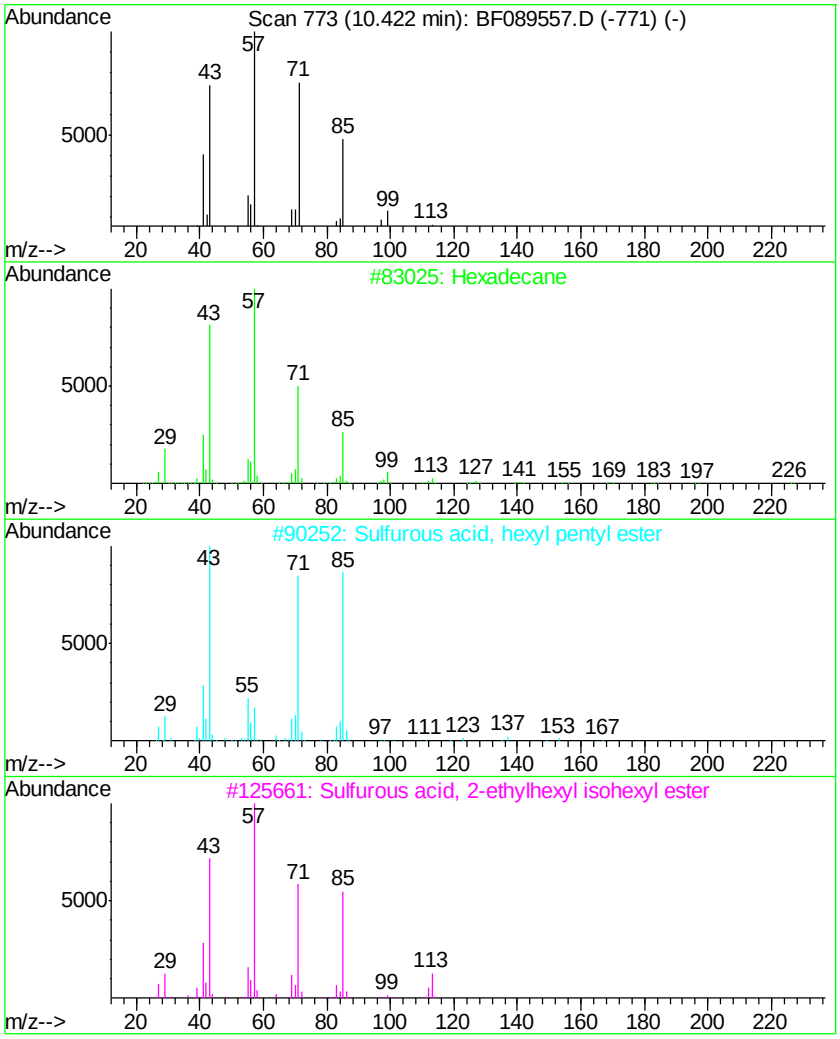
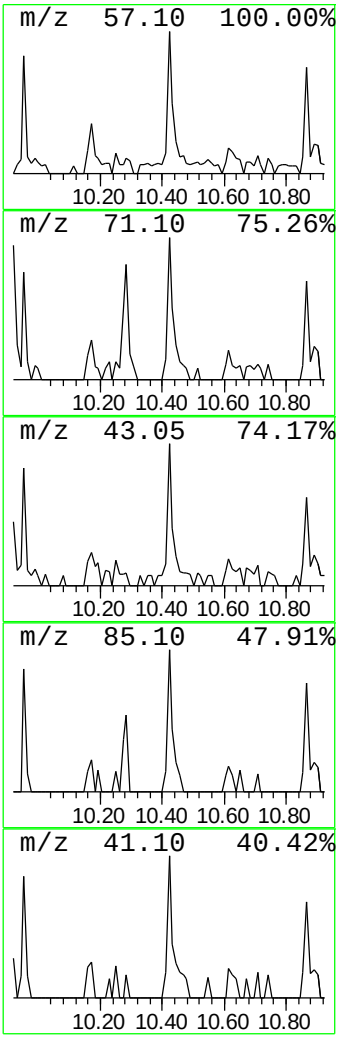
**********

Peak Number 6 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.42 | 2.89 ng | 35116 | Phenanthrene-d10 | 10.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 83 |
| 2 | Sulfurous acid, hexyl pentyl ester | 236 | C11H24O3S | 1000309-14-1 | 80 |
| 3 | Sulfurous acid, 2-ethylhexyl iso... | 278 | C14H30O3S | 1000309-19-0 | 78 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 78 |
| 5 | Oxalic acid, isohexyl neopentyl ... | 244 | C13H24O4 | 1000309-73-0 | 72 |



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Sample : H4269-16
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-55-18.0-19.0

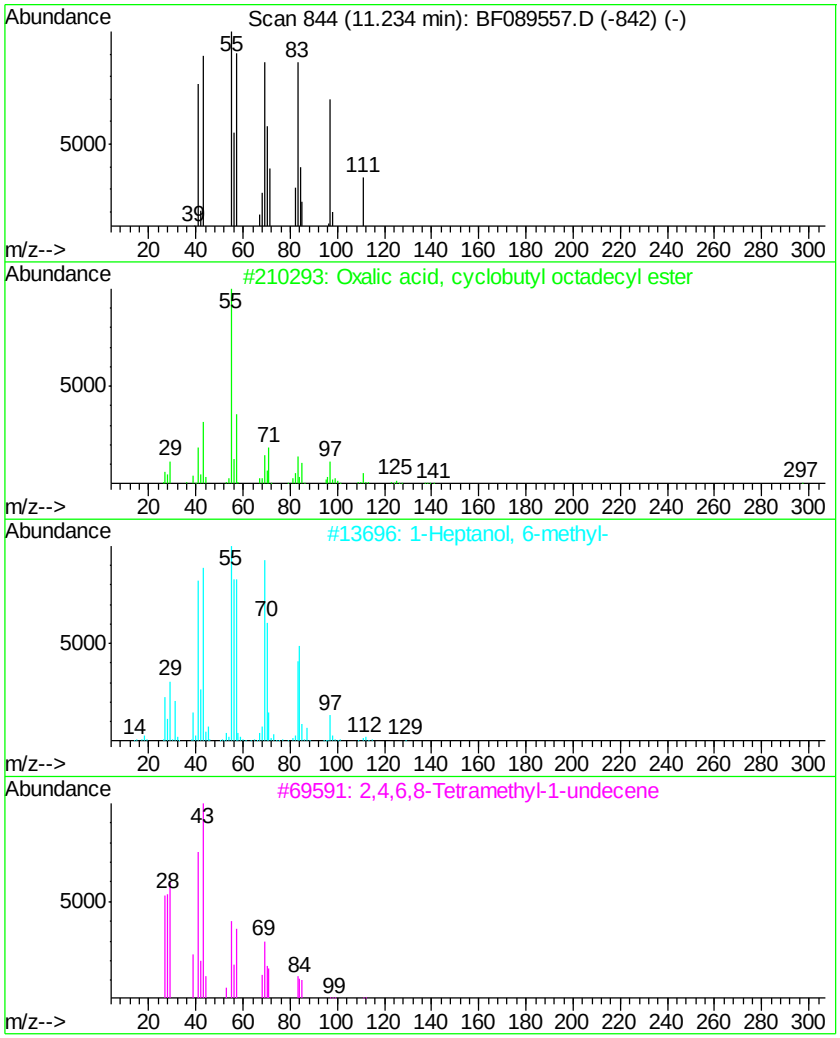
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

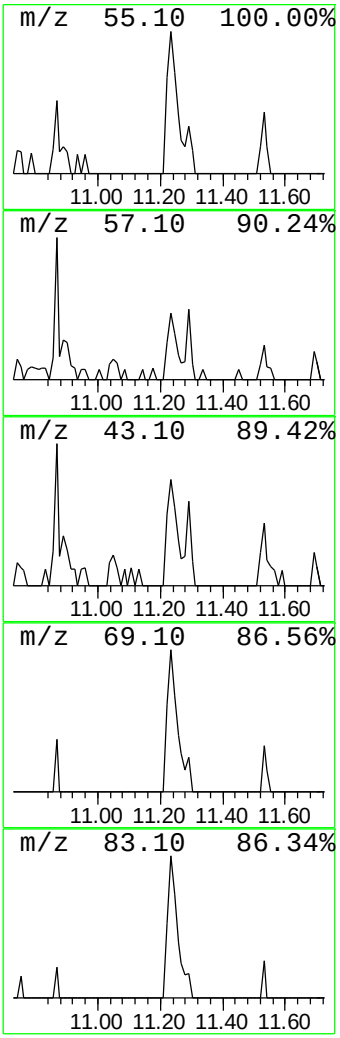
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 Oxalic acid, cyclobutyl oct... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.23 | 3.63 ng | 44178 | Phenanthrene-d10 | 10.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxalic acid, cyclobutyl octadecy... | 396 | C24H44O4 | 1000309-70-8 | 53 |
| 2 | 1-Heptanol, 6-methyl- | 130 | C8H18O | 001653-40-3 | 43 |
| 3 | 2,4,6,8-Tetramethyl-1-undecene | 210 | C15H30 | 059920-26-2 | 40 |
| 4 | 2-Hexenal, (E)- | 98 | C6H10O | 006728-26-3 | 38 |
| 5 | 1-Heptanol, 4-methyl- | 130 | C8H18O | 000817-91-4 | 38 |



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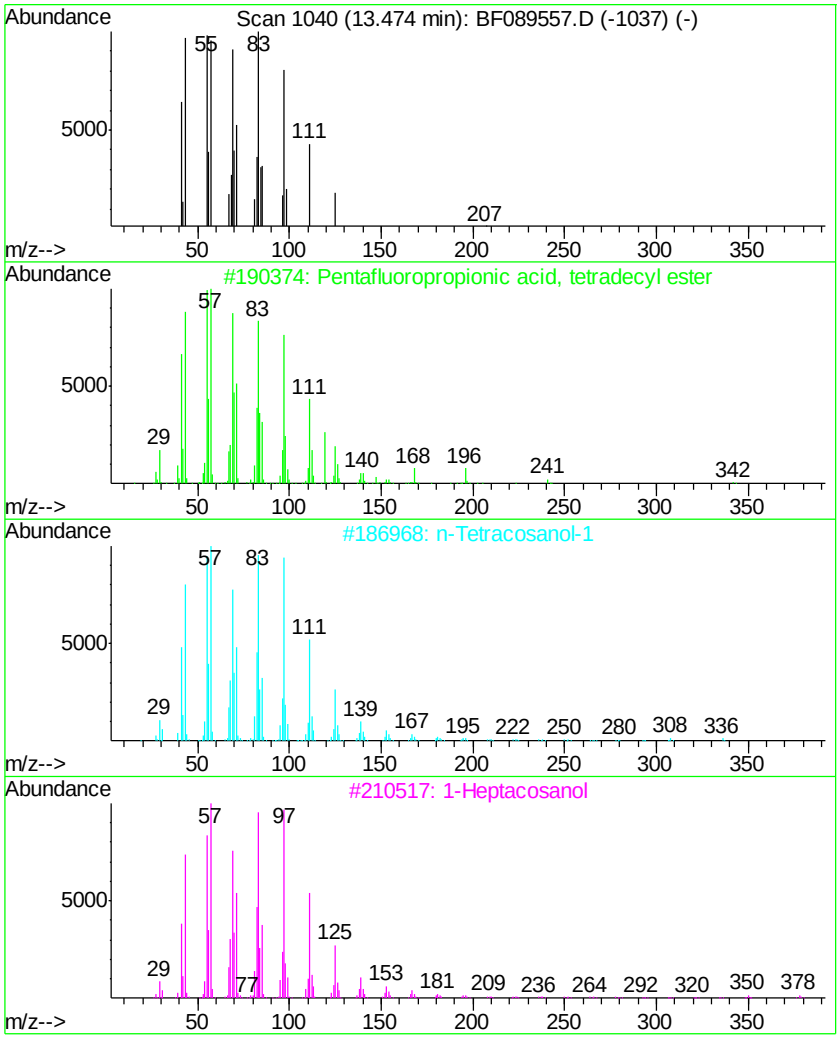
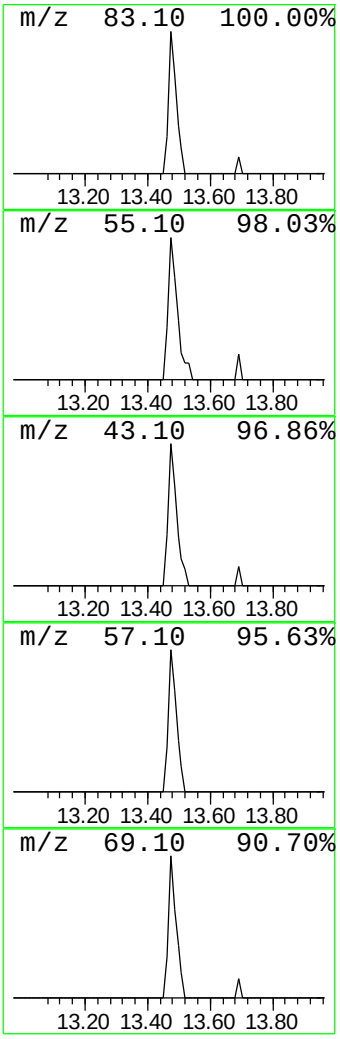
**********

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.47 | 4.32 ng | 48407 | Chrysene-d12 | 13.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 91 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |
| 5 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 91 |



# Tentatively Identified Compound (LSC) summary

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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... | 4.56 | 39.7 | ng | 415127 | 1 | 6.47 | 209050 | 20.0 |
| unknown6.24 | 6.24 | 113.3 | ng | 1184740 | 1 | 6.47 | 209050 | 20.0 |
| Hexanoic acid, 2-... | 7.19 | 2.8 | ng | 37321 | 2 | 7.76 | 270773 | 20.0 |
| Hexadecane | 10.42 | 2.9 | ng | 35116 | 4 | 10.97 | 243336 | 20.0 |
| Oxalic acid, cycl... | 11.23 | 3.6 | ng | 44178 | 4 | 10.97 | 243336 | 20.0 |
| Pentafluoropropio... | 13.47 | 4.3 | ng | 48407 | 5 | 13.59 | 224020 | 20.0 |