LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
Data File : BF081251.D
Acq On : 27 Aug 2015 17:35
Operator : UM/IZ
Sample : G3441-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VITALE FILL SOURCE 2A

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-BF081715.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 | 3.806 | 179 | 181 | 186 | rBB | 14301 | 23908 | 1.45% | 0.161% |
| 2 | 4.594 | 247 | 250 | 264 | rVB | 619522 | 1153044 | 70.08% | 7.749% |
| 3 | 5.063 | 289 | 291 | 294 | rBV | 1230728 | 1377041 | 83.69% | 9.254% |
| 4 | 5.486 | 327 | 328 | 331 | rBV | 22698 | 31406 | 1.91% | 0.211% |
| 5 | 6.160 | 384 | 387 | 389 | rBV | 1479909 | 1626739 | 98.86% | 10.932% |
| 6 | 6.274 | 394 | 397 | 399 | rBV | 1308054 | 1551793 | 94.31% | 10.429% |
| 7 | 6.503 | 415 | 417 | 419 | rBV | 346367 | 276622 | 16.81% | 1.859% |
| 8 | 6.663 | 428 | 431 | 433 | rBV | 1157840 | 1138883 | 69.22% | 7.654% |
| 9 | 7.074 | 465 | 467 | 470 | rBV | 917131 | 891810 | 54.20% | 5.993% |
| 10 | 7.200 | 473 | 478 | 480 | rVB | 14452 | 17079 | 1.04% | 0.115% |
| 11 | 7.795 | 528 | 530 | 532 | rVB | 273264 | 350984 | 21.33% | 2.359% |
| 12 | 8.743 | 611 | 613 | 618 | rBV | 13249 | 17595 | 1.07% | 0.118% |
| 13 | 8.869 | 621 | 624 | 627 | rBV | 1530918 | 1555881 | 94.56% | 10.456% |
| 14 | 9.269 | 657 | 659 | 661 | rBV | 283611 | 219978 | 13.37% | 1.478% |
| 15 | 9.532 | 680 | 682 | 684 | rBV | 501536 | 417731 | 25.39% | 2.807% |
| 16 | 9.955 | 717 | 719 | 721 | rBV | 14982 | 21222 | 1.29% | 0.143% |
| 17 | 10.321 | 748 | 751 | 753 | rBV | 765524 | 1060564 | 64.46% | 7.127% |
| 18 | 10.458 | 761 | 763 | 769 | rVB | 25501 | 29008 | 1.76% | 0.195% |
| 19 | 10.903 | 799 | 802 | 803 | rBV | 23787 | 20132 | 1.22% | 0.135% |
| 20 | 10.995 | 808 | 810 | 813 | rBV | 454793 | 428168 | 26.02% | 2.877% |
| 21 | 11.326 | 836 | 839 | 841 | rVB | 19340 | 18172 | 1.10% | 0.122% |
| 22 | 11.555 | 857 | 859 | 864 | rBV | 52735 | 76319 | 4.64% | 0.513% |
| 23 | 12.584 | 946 | 949 | 952 | rBV | 1646676 | 1645420 | 100.00% | 11.058% |
| 24 | 13.498 | 1026 | 1029 | 1037 | rBV | 108553 | 188203 | 11.44% | 1.265% |
| 25 | 13.612 | 1037 | 1039 | 1041 | rBV | 373511 | 411369 | 25.00% | 2.765% |
| 26 | 14.115 | 1081 | 1083 | 1089 | rBV4 | 7047 | 19478 | 1.18% | 0.131% |
| 27 | 14.938 | 1152 | 1155 | 1157 | rBV | 201294 | 293559 | 17.84% | 1.973% |
| 28 | 15.395 | 1192 | 1195 | 1197 | rBV2 | 8311 | 17878 | 1.09% | 0.120% |

Sum of corrected areas: 14879986

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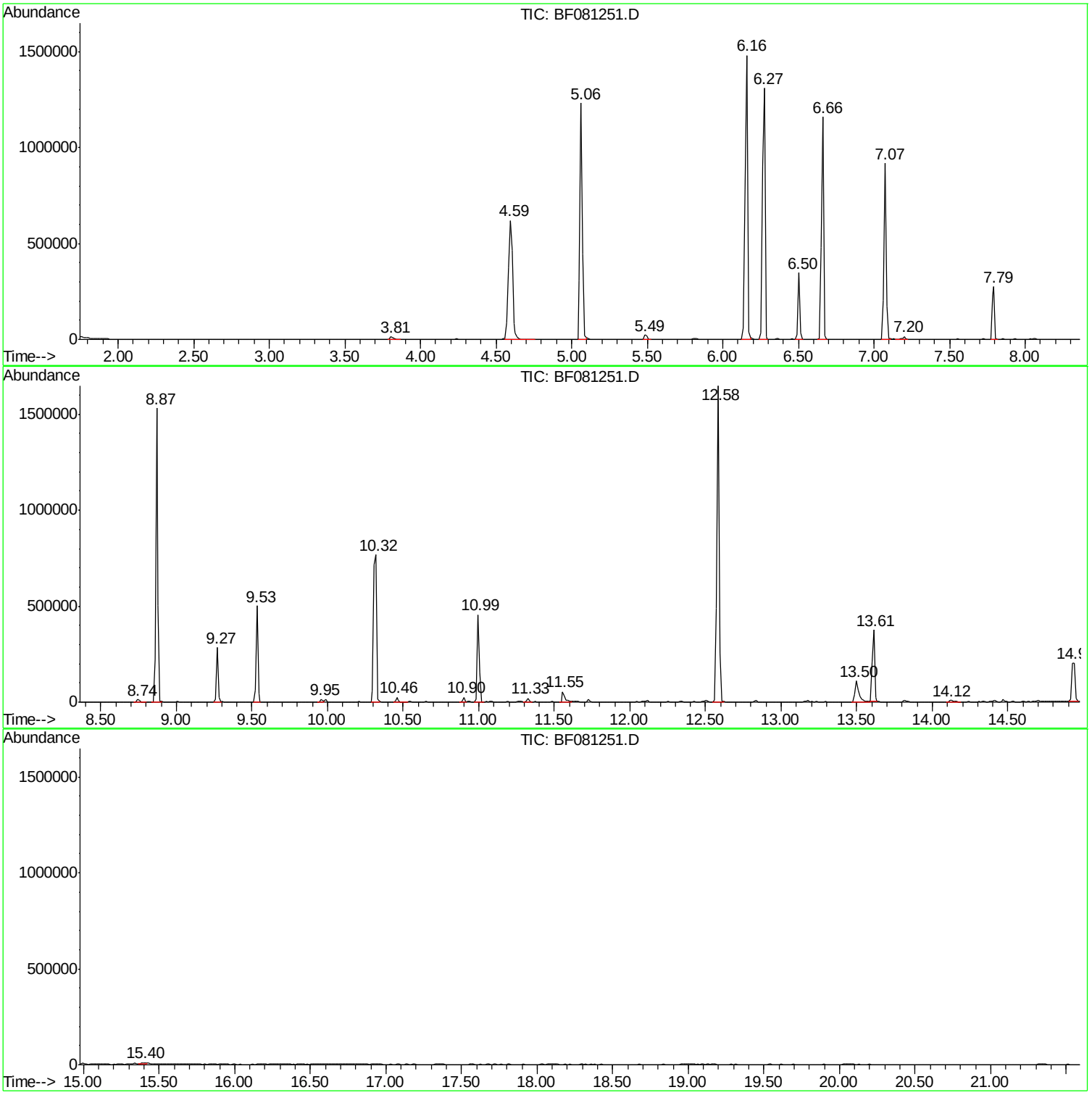
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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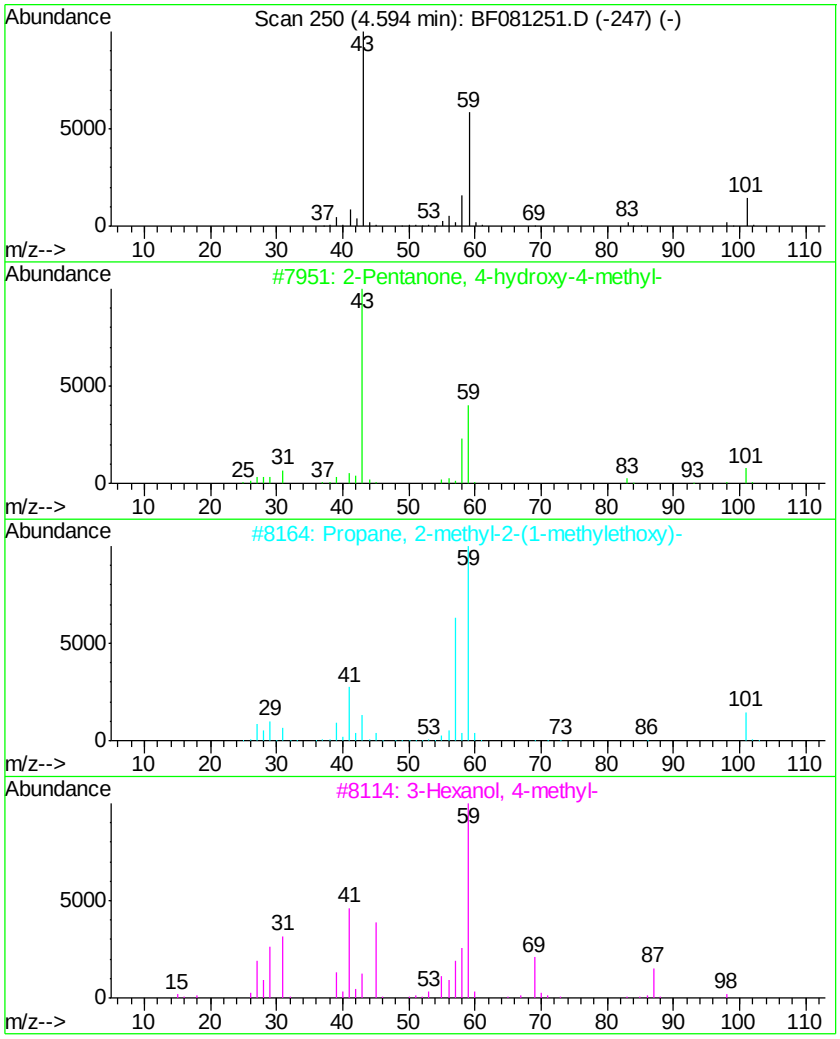
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

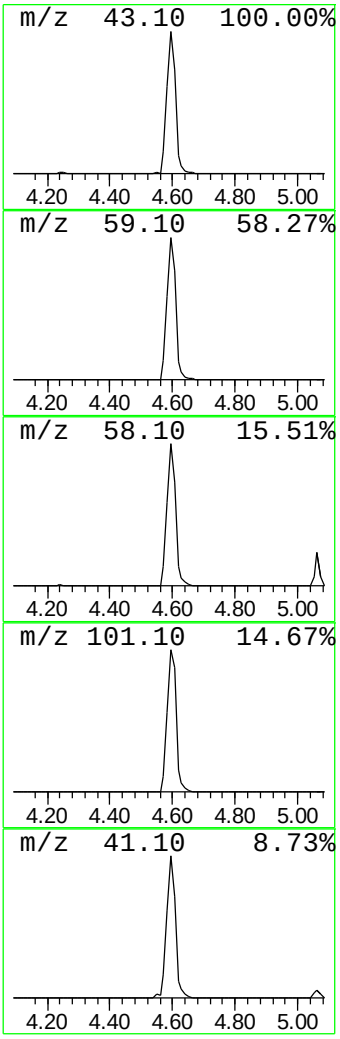
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.59 | 83.37 ng | 1153040 | 1,4-Dichlorobenzene-d4 | 6.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 36 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |



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Operator : UM/IZ
Sample : G3441-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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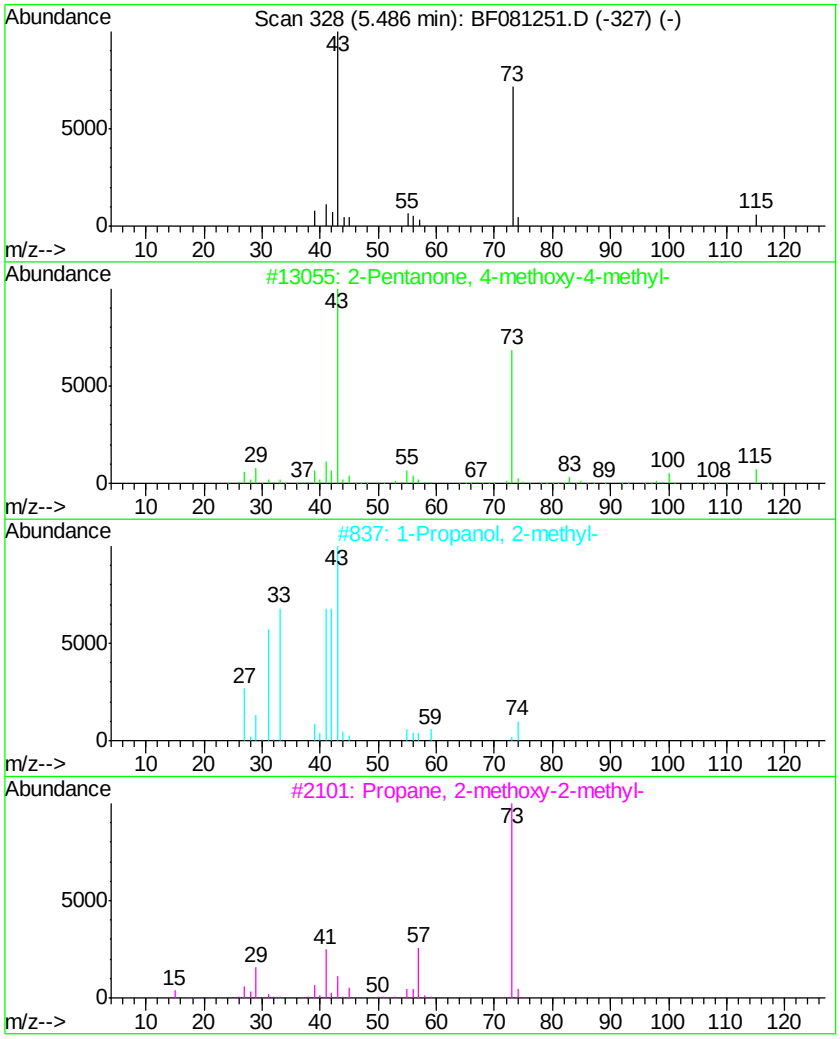
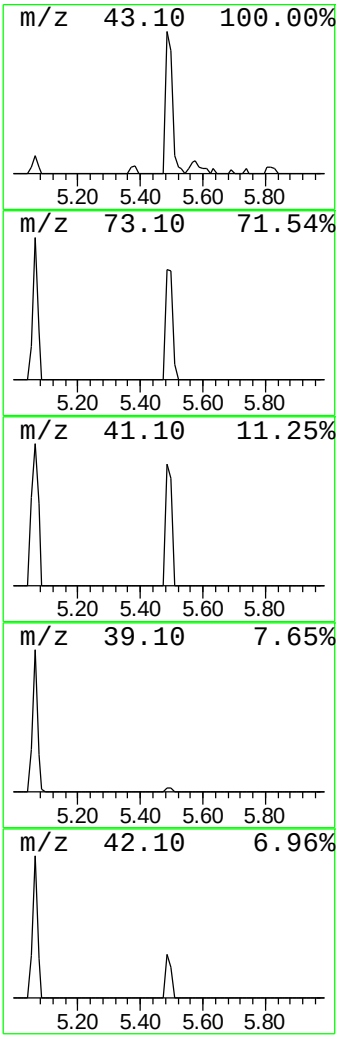
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.49 | 2.27 ng | 31406 | 1,4-Dichlorobenzene-d4 | 6.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 64 |
| 2 | 1-Propanol, 2-methyl- | 74 | C4H10O | 000078-83-1 | 9 |
| 3 | Propane, 2-methoxy-2-methyl- | 88 | C5H12O | 001634-04-4 | 9 |
| 4 | 2-Propanone, 1-(1,3-dioxolan-2-yl)- | 130 | C6H10O3 | 000767-04-4 | 9 |
| 5 | 5-Aminovaleric acid | 117 | C5H11NO2 | 000660-88-8 | 9 |



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Sample : G3441-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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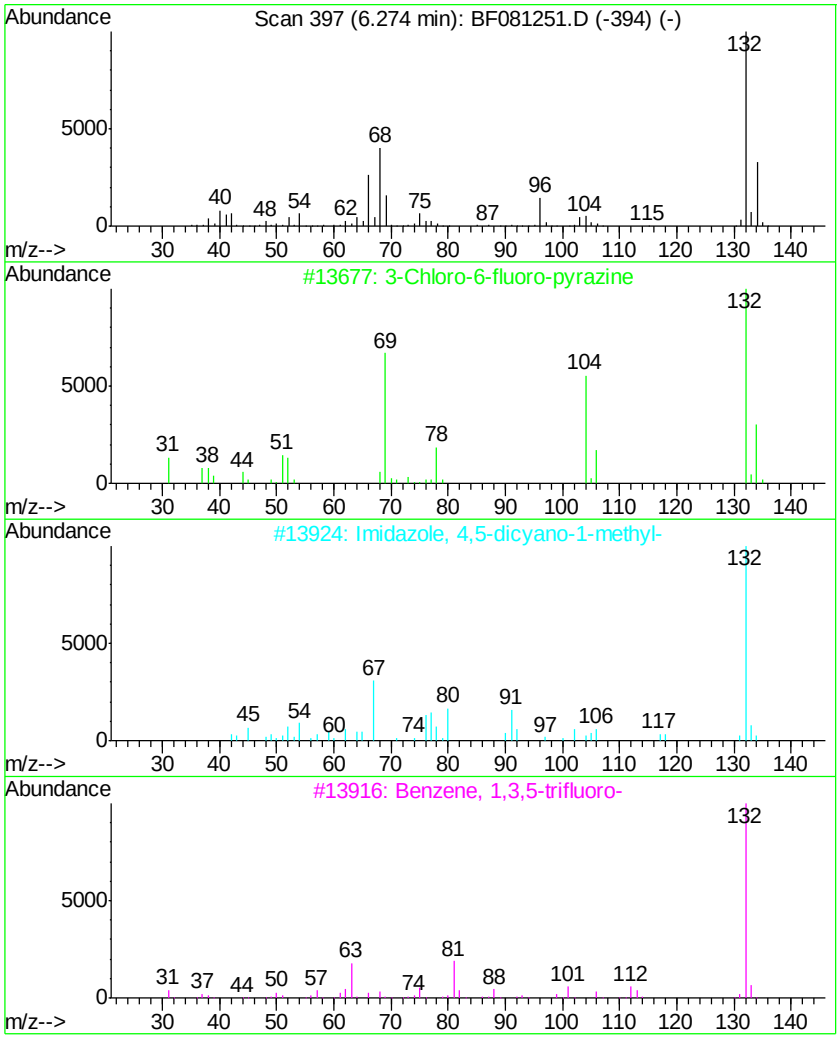
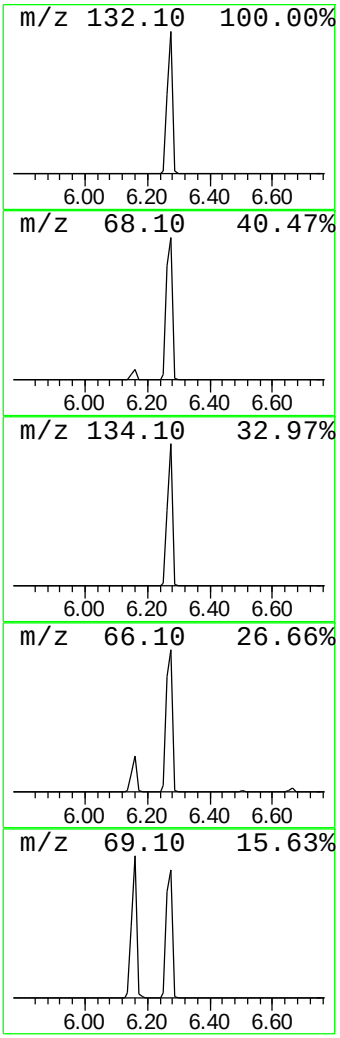
Peak Number 3 unknown6.27 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.27 | 112.20 ng | 1551790 | 1,4-Dichlorobenzene-d4 | 6.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 9 |
| 3 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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Sample : G3441-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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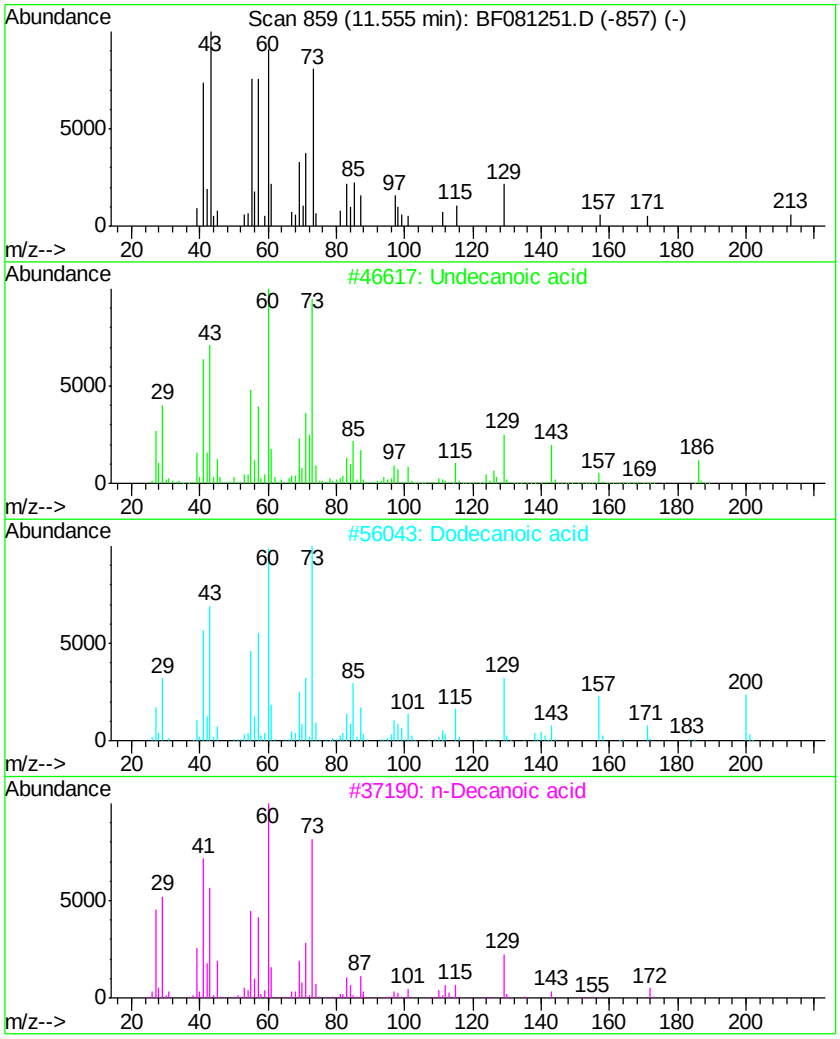
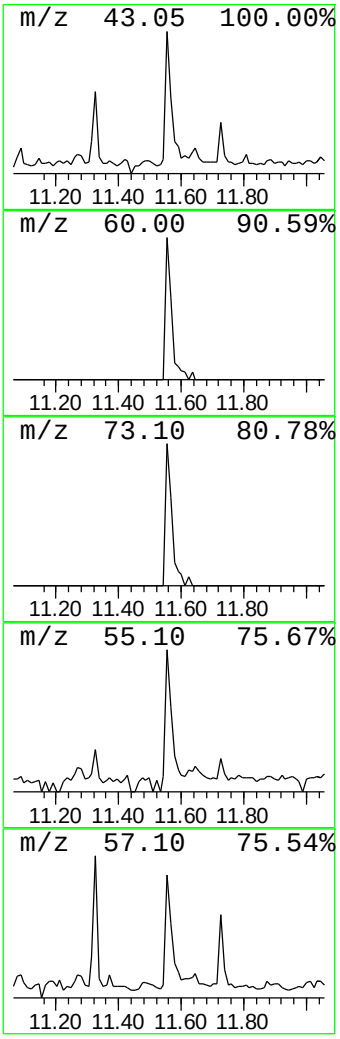
Peak Number 5 Undecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.56 | 3.56 ng | 76319 | Phenanthrene-d10 | 10.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 80 |
| 2 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 59 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | 11-Bromoundecanoic acid | 264 | C11H21BrO2 | 002834-05-1 | 53 |
| 5 | Heptanoic acid | 130 | C7H14O2 | 000111-14-8 | 43 |



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Operator : UM/IZ
Sample : G3441-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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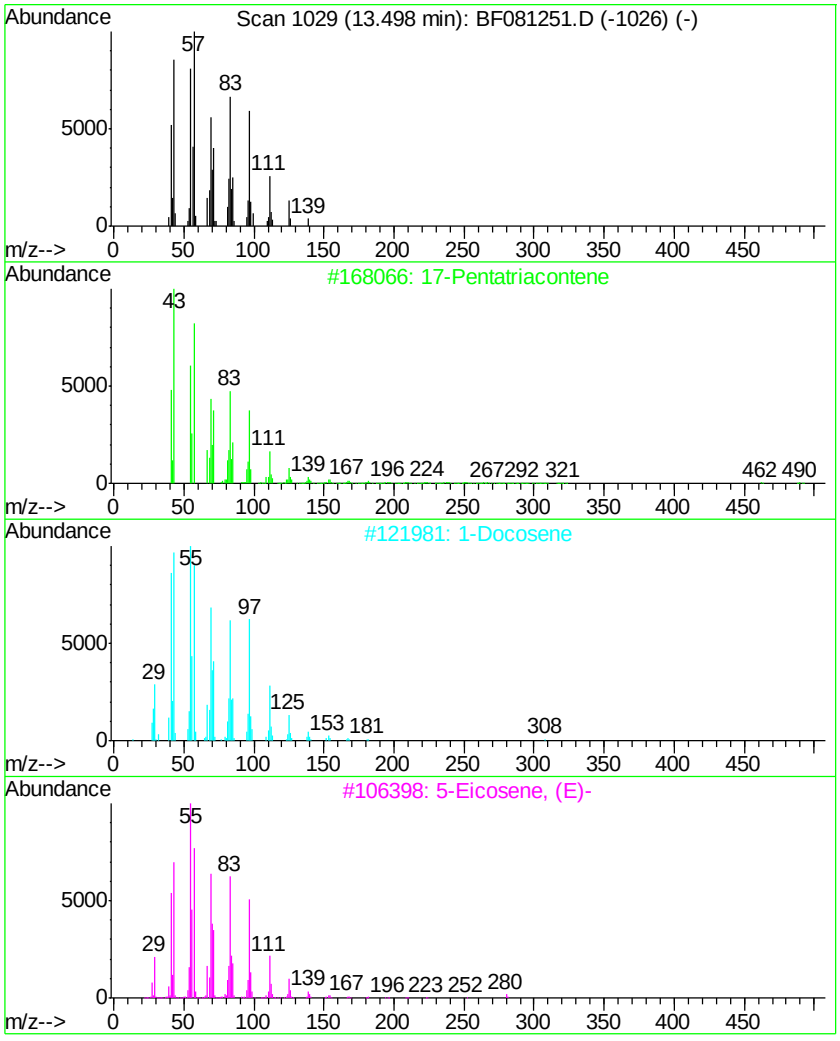
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

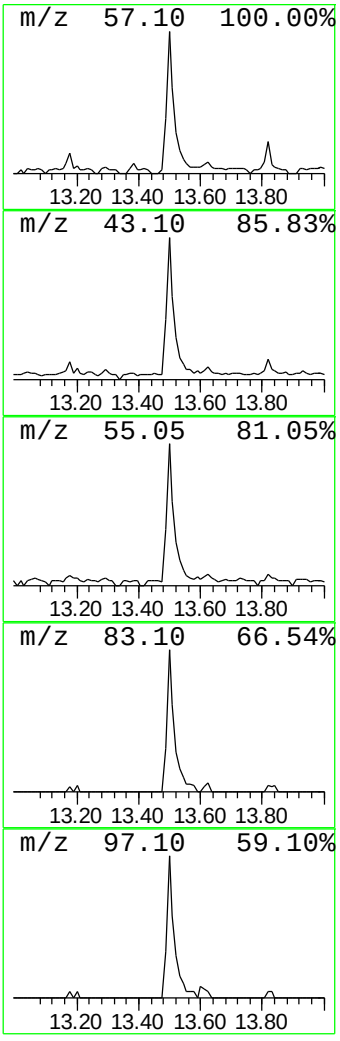
**********

Peak Number 6 17-Pentatriacontene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.50 | 9.15 ng | 188203 | Chrysene-d12 | 13.61 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 91 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 91 |
| 4 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 91 |
| 5 | 11-Tricosene | 322 | C23H46 | 052078-56-5 | 90 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VITALE FILL SOURCE 2A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.59 | 83.4 | ng | 1153040 | 1 | 6.50 | 276622 | 20.0 |
| 2-Pentanone, 4-me... | 5.49 | 2.3 | ng | 31406 | 1 | 6.50 | 276622 | 20.0 |
| unknown6.27 | 6.27 | 112.2 | ng | 1551790 | 1 | 6.50 | 276622 | 20.0 |
| Undecanoic acid | 11.56 | 3.6 | ng | 76319 | 4 | 10.99 | 428168 | 20.0 |
| 17-Pentatriacontene | 13.50 | 9.2 | ng | 188203 | 5 | 13.61 | 411369 | 20.0 |