LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

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-BF080818.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 | 2.366 | 3 | 5 | 12 | rVB | 614065 | 665639 | 10.64% | 1.342% |
| 2 | 5.254 | 490 | 496 | 499 | rBV | 2718927 | 2800154 | 44.74% | 5.643% |
| 3 | 5.637 | 556 | 561 | 564 | rBV | 2361329 | 2240342 | 35.80% | 4.515% |
| 4 | 6.631 | 724 | 730 | 733 | rBV | 5447159 | 5531025 | 88.37% | 11.147% |
| 5 | 6.784 | 752 | 756 | 759 | rBV | 4228882 | 3675525 | 58.73% | 7.408% |
| 6 | 7.019 | 792 | 796 | 799 | rBV | 2045330 | 1772570 | 28.32% | 3.572% |
| 7 | 7.172 | 818 | 822 | 826 | rVB | 5460313 | 4875366 | 77.90% | 9.826% |
| 8 | 7.578 | 886 | 891 | 894 | rBV | 4689169 | 4347024 | 69.46% | 8.761% |
| 9 | 8.301 | 1009 | 1014 | 1017 | rBV | 2521296 | 2206489 | 35.26% | 4.447% |
| 10 | 9.377 | 1191 | 1197 | 1200 | rBV | 6443712 | 6258621 | 100.00% | 12.613% |
| 11 | 9.766 | 1259 | 1263 | 1266 | rBV | 664828 | 521560 | 8.33% | 1.051% |
| 12 | 10.066 | 1309 | 1314 | 1317 | rBV | 2470228 | 2287932 | 36.56% | 4.611% |
| 13 | 10.854 | 1444 | 1448 | 1453 | rBV | 965752 | 921070 | 14.72% | 1.856% |
| 14 | 10.966 | 1462 | 1467 | 1470 | rBV2 | 105260 | 133932 | 2.14% | 0.270% |
| 15 | 11.430 | 1543 | 1546 | 1549 | rBV4 | 75122 | 89202 | 1.43% | 0.180% |
| 16 | 11.560 | 1564 | 1568 | 1571 | rBV | 2472655 | 2050151 | 32.76% | 4.132% |
| 17 | 13.148 | 1834 | 1838 | 1841 | rBV | 5380418 | 4577074 | 73.13% | 9.225% |
| 18 | 14.036 | 1986 | 1989 | 2001 | rBV2 | 164680 | 271356 | 4.34% | 0.547% |
| 19 | 14.212 | 2015 | 2019 | 2023 | rBV | 1938124 | 1857605 | 29.68% | 3.744% |
| 20 | 14.354 | 2041 | 2043 | 2048 | rVB | 101934 | 82886 | 1.32% | 0.167% |
| 21 | 14.665 | 2093 | 2096 | 2099 | rVB | 119548 | 111035 | 1.77% | 0.224% |
| 22 | 14.989 | 2147 | 2151 | 2155 | rBV3 | 128955 | 217787 | 3.48% | 0.439% |
| 23 | 15.077 | 2163 | 2166 | 2174 | rVB | 352129 | 388817 | 6.21% | 0.784% |
| 24 | 15.359 | 2212 | 2214 | 2221 | rVB | 104500 | 135403 | 2.16% | 0.273% |
| 25 | 15.777 | 2280 | 2285 | 2293 | rVB2 | 1174738 | 1599980 | 25.56% | 3.225% |

Sum of corrected areas: 49618545

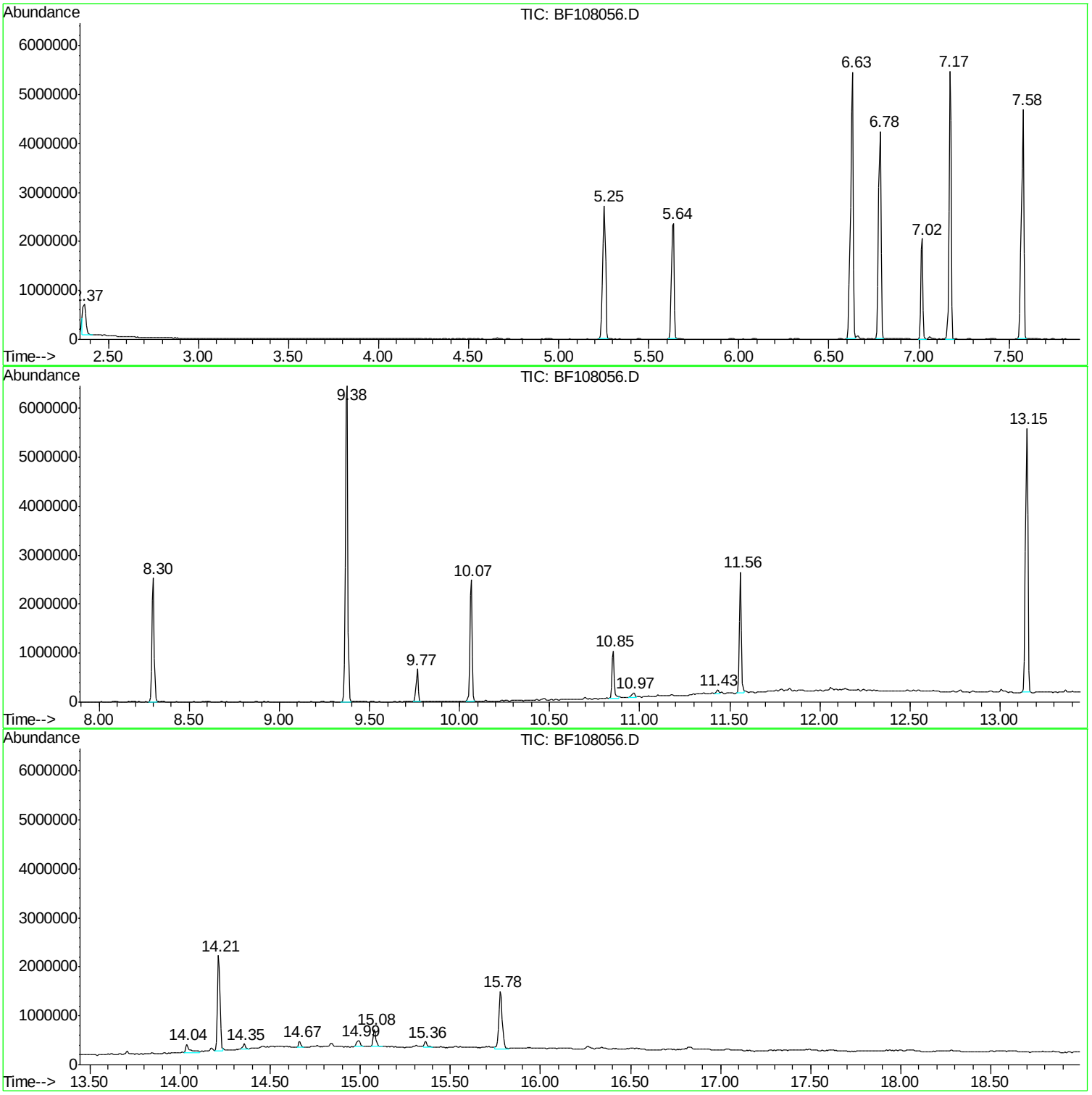
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

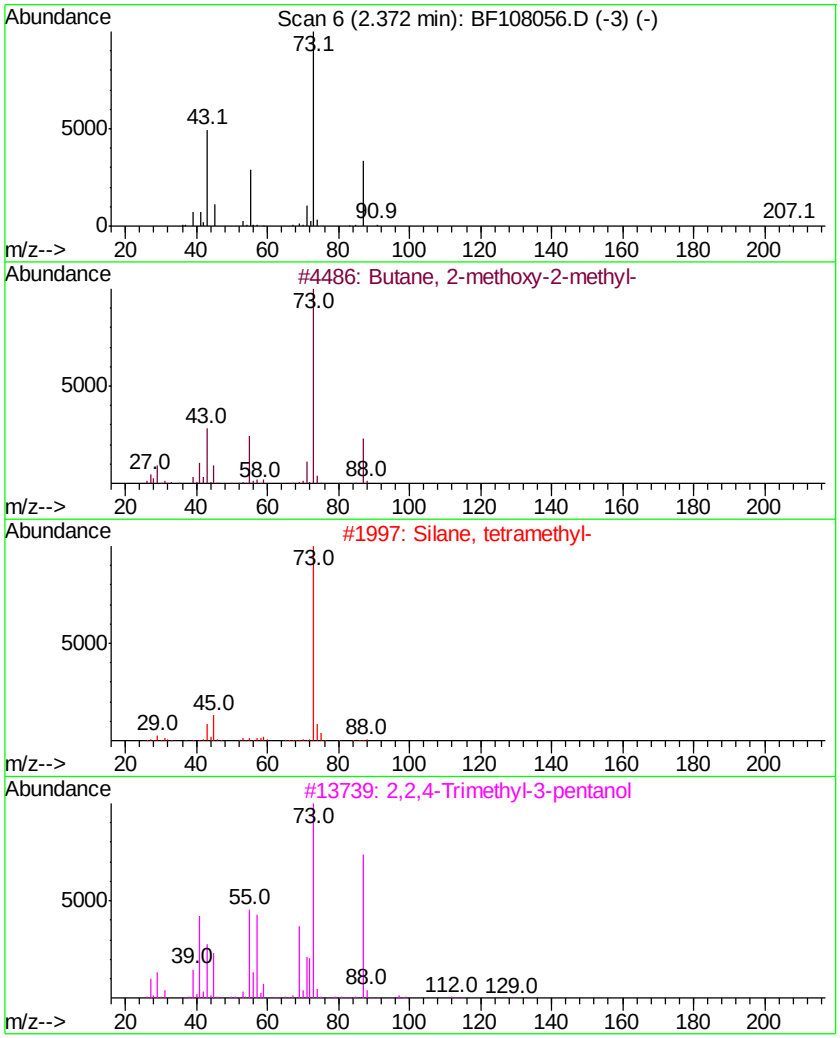
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

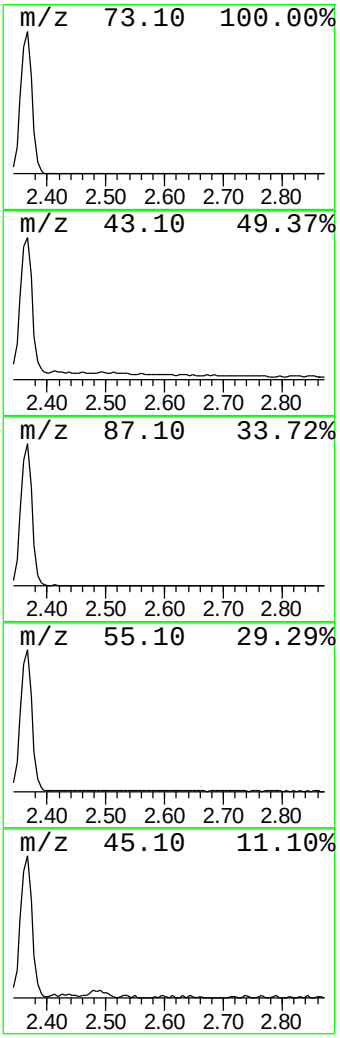
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.37 | 7.51 ng | 665639 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 38 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 33 |
| 4 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 25 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

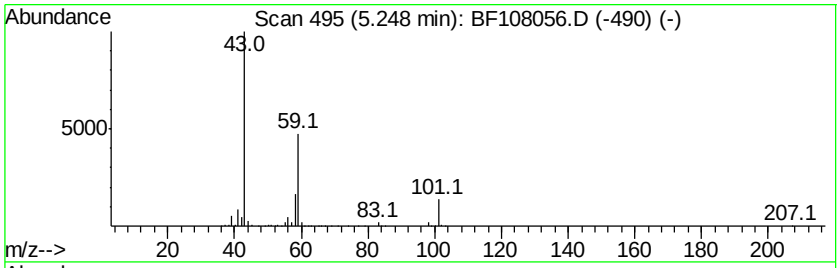
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

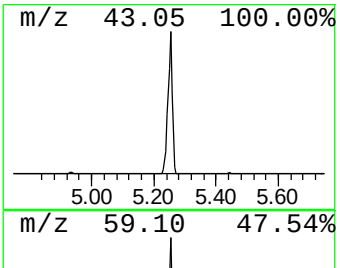
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.25 | 31.59 ng | 2800150 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 5 | Formamide, N,N-diethyl- | 101 | C5H11NO | 000617-84-5 | 7 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

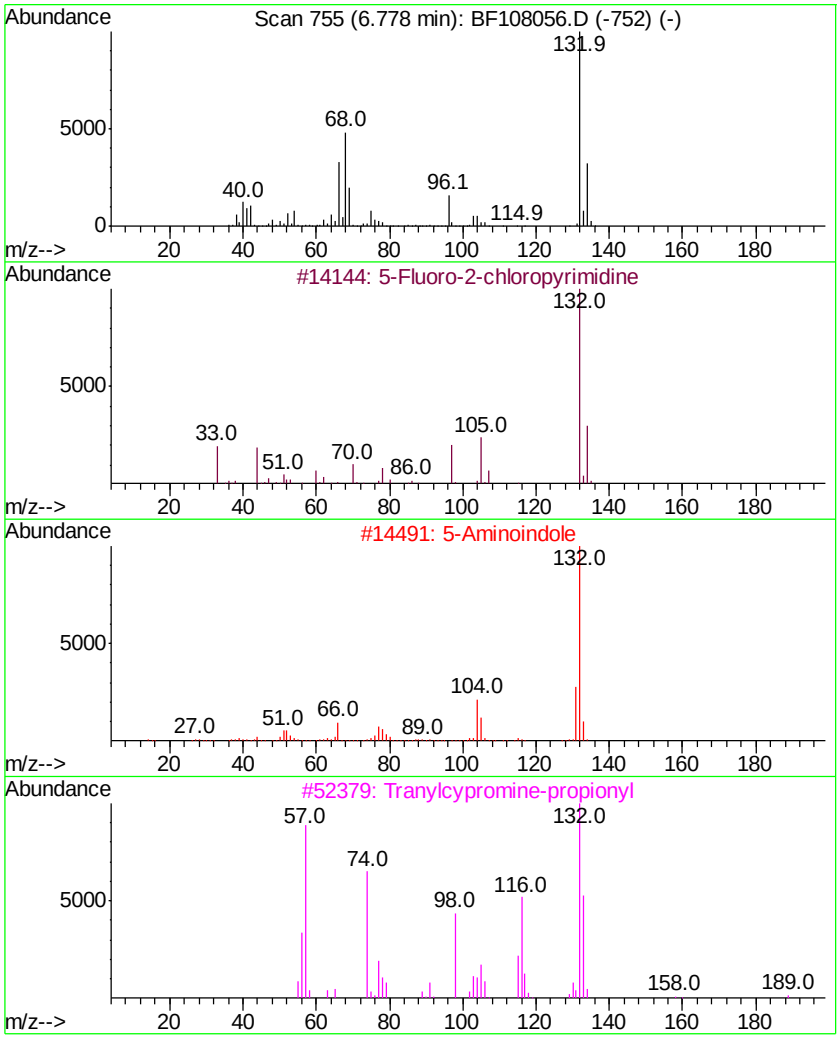
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

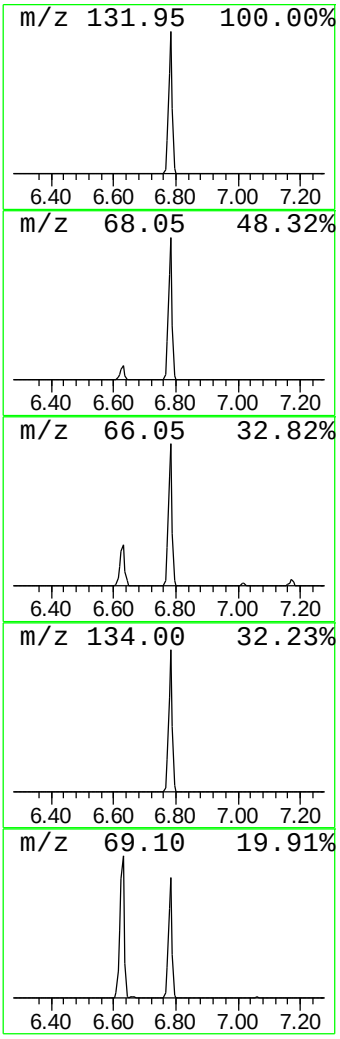
**********

Peak Number 3 unknown6.78 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.78 | 41.47 ng | 3675530 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

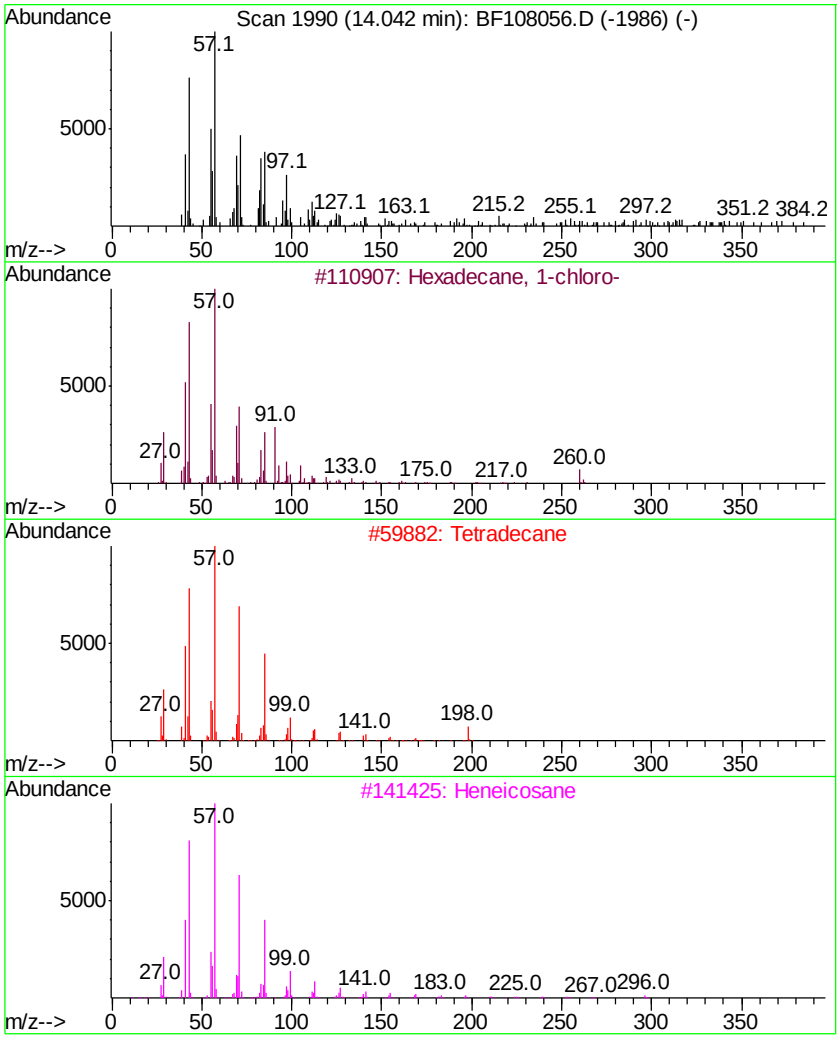
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

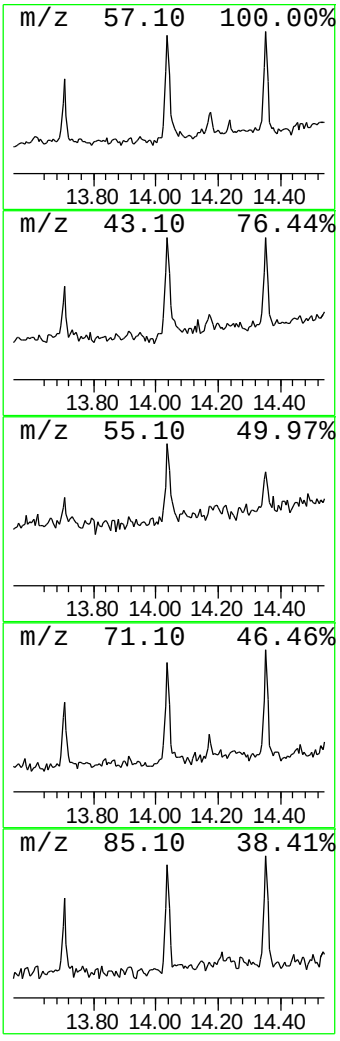
**********

Peak Number 5 Hexadecane, 1-chloro- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.04 | 2.92 ng | 271356 | Chrysene-d12 | 14.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane, 1-chloro- | 260 | C16H33Cl | 004860-03-1 | 94 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 92 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 89 |
| 5 | 1-Chloroeicosane | 316 | C20H41Cl | 042217-02-7 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

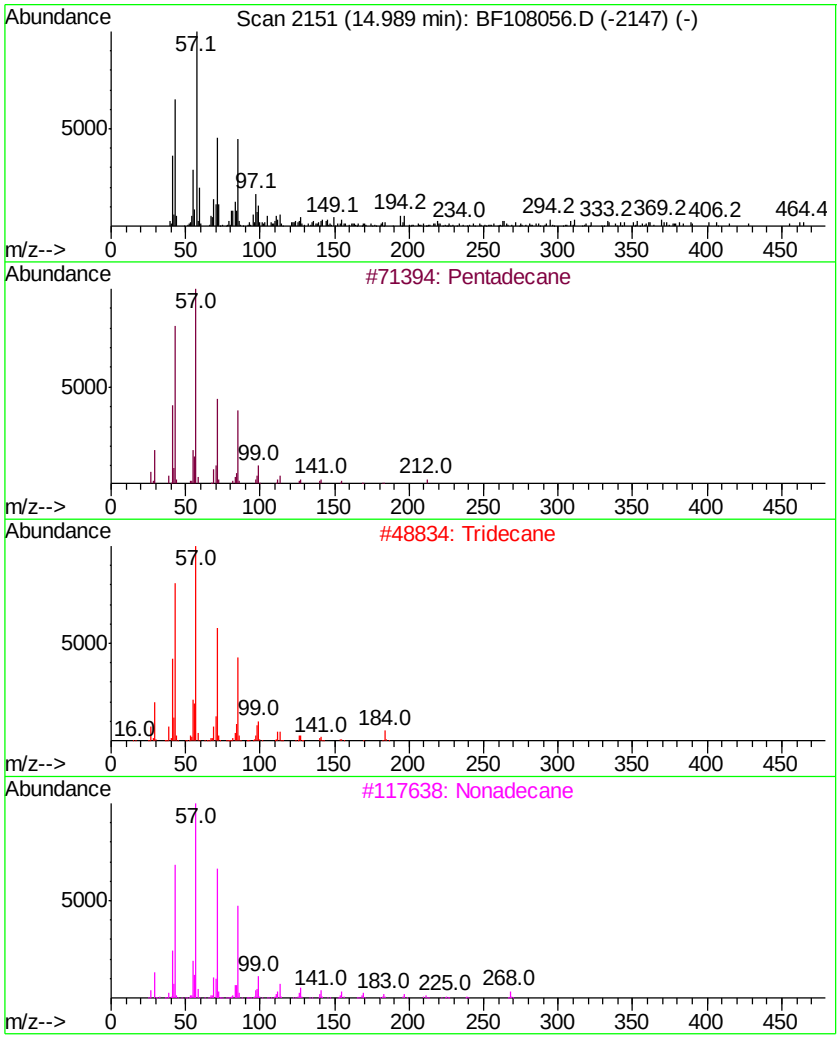
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

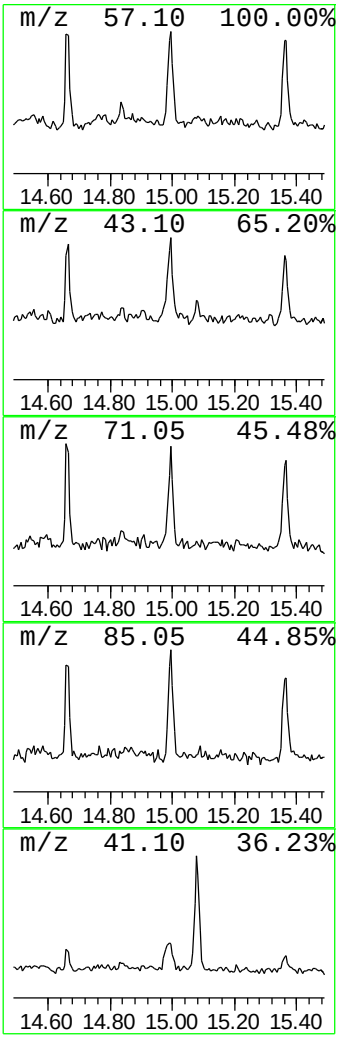
**********

Peak Number 6 Pentadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.99 | 2.34 ng | 217787 | Chrysene-d12 | 14.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 83 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 58 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 52 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 52 |
| 5 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 51 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

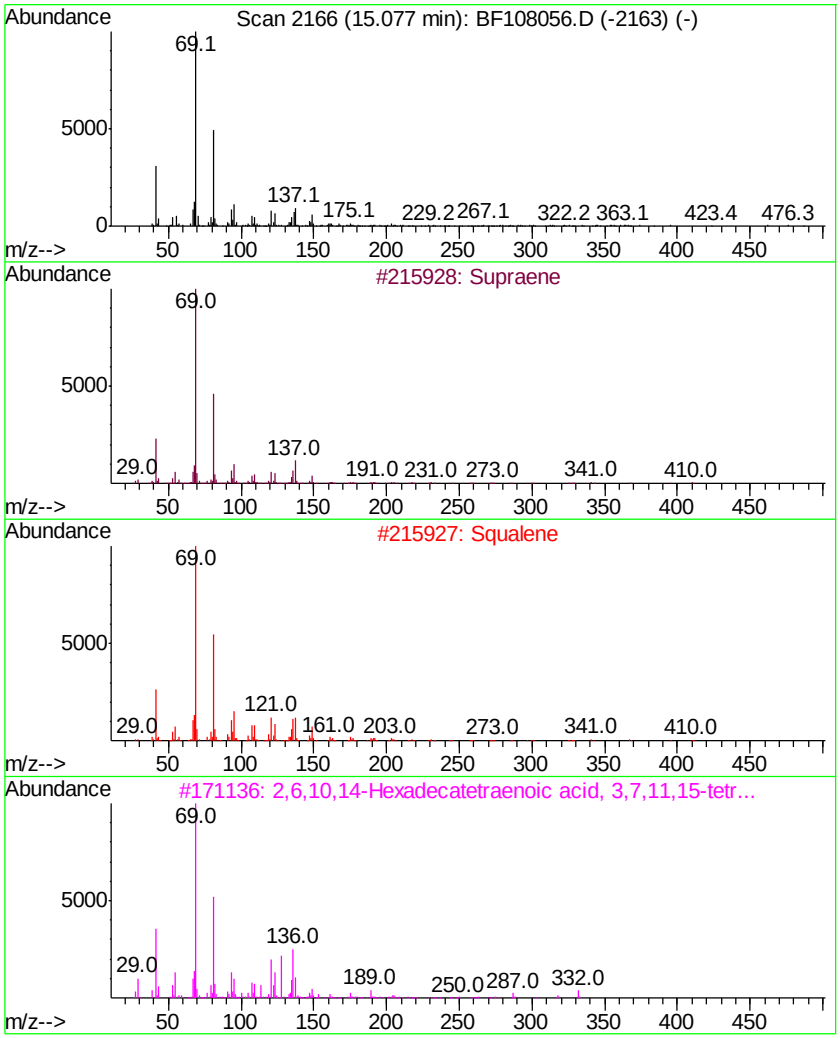
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

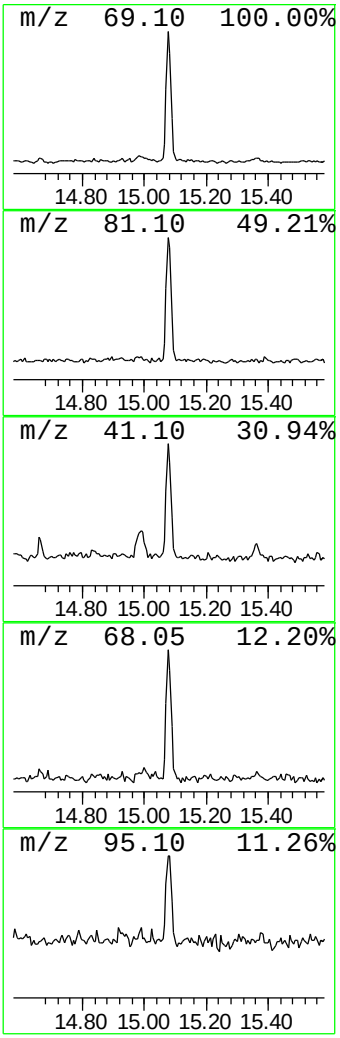
**********

Peak Number 7 Supraene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.08 | 4.86 ng | 388817 | Perylene-d12 | 15.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 2 | Squalene | 410 | C30H50 | 000111-02-4 | 86 |
| 3 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 64 |
| 4 | 4-Oxo-.beta.-damascone | 206 | C13H18O2 | 053398-08-6 | 59 |
| 5 | 1,6-Octadiene, 3,5-dimethyl-, tr... | 138 | C10H18 | 074630-87-8 | 53 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080918\
Data File : BF108056.D
Acq On : 9 Aug 2018 16:55
Operator : JU/SJ
Sample : J4393-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JTY-BALLARDS-1-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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... | 2.37 | 7.5 | ng | 665639 | 1 | 7.02 | 1772570 | 20.0 |
| 2-Pentanone, 4-hy... | 5.25 | 31.6 | ng | 2800150 | 1 | 7.02 | 1772570 | 20.0 |
| unknown6.78 | 6.78 | 41.5 | ng | 3675530 | 1 | 7.02 | 1772570 | 20.0 |
| Hexadecane, 1-chl... | 14.04 | 2.9 | ng | 271356 | 5 | 14.21 | 1857610 | 20.0 |
| Pentadecane | 14.99 | 2.3 | ng | 217787 | 5 | 14.21 | 1857610 | 20.0 |
| Supraene | 15.08 | 4.9 | ng | 388817 | 6 | 15.78 | 1599980 | 20.0 |