LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020719\
Data File : BM018747.D
Acq On : 07 Feb 2019 20:53
Operator : JU/SJ
Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** DUPE-Y

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_M\METHODS\8270-BM010919.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 | 4.863 | 298 | 302 | 312 | rBV | 274264 | 395353 | 3.74% | 0.466% |
| 2 | 5.305 | 371 | 377 | 395 | rBV | 5897811 | 8524749 | 80.65% | 10.039% |
| 3 | 6.893 | 639 | 647 | 664 | rBV | 5636750 | 8956907 | 84.73% | 10.548% |
| 4 | 7.252 | 700 | 708 | 729 | rBV | 6235925 | 9681577 | 91.59% | 11.401% |
| 5 | 7.716 | 780 | 787 | 794 | rBV | 1066032 | 1698860 | 16.07% | 2.001% |
| 6 | 8.034 | 833 | 841 | 851 | rBV | 4529361 | 7294252 | 69.01% | 8.590% |
| 7 | 8.881 | 978 | 985 | 1002 | rBV | 3261166 | 5486407 | 51.90% | 6.461% |
| 8 | 10.504 | 1252 | 1261 | 1271 | rBV | 1240825 | 2091544 | 19.79% | 2.463% |
| 9 | 12.981 | 1674 | 1682 | 1699 | rBV | 7376249 | 10570593 | 100.00% | 12.448% |
| 10 | 13.828 | 1820 | 1826 | 1838 | rBV | 287090 | 460821 | 4.36% | 0.543% |
| 11 | 14.363 | 1909 | 1917 | 1933 | rBV2 | 1578151 | 2467249 | 23.34% | 2.905% |
| 12 | 15.857 | 2165 | 2171 | 2191 | rBV | 5397788 | 7793549 | 73.73% | 9.178% |
| 13 | 17.116 | 2379 | 2385 | 2396 | rBV | 1790269 | 2587303 | 24.48% | 3.047% |
| 14 | 18.004 | 2530 | 2536 | 2545 | rBV | 338050 | 508135 | 4.81% | 0.598% |
| 15 | 19.286 | 2750 | 2754 | 2759 | rBV2 | 83768 | 115307 | 1.09% | 0.136% |
| 16 | 19.745 | 2827 | 2832 | 2841 | rBV | 8422142 | 10163763 | 96.15% | 11.969% |
| 17 | 21.009 | 3043 | 3047 | 3057 | rBV | 528479 | 740059 | 7.00% | 0.871% |
| 18 | 21.309 | 3092 | 3098 | 3106 | rBV | 2015654 | 2696535 | 25.51% | 3.175% |
| 19 | 23.568 | 3475 | 3482 | 3492 | rVB | 1421460 | 2685706 | 25.41% | 3.163% |

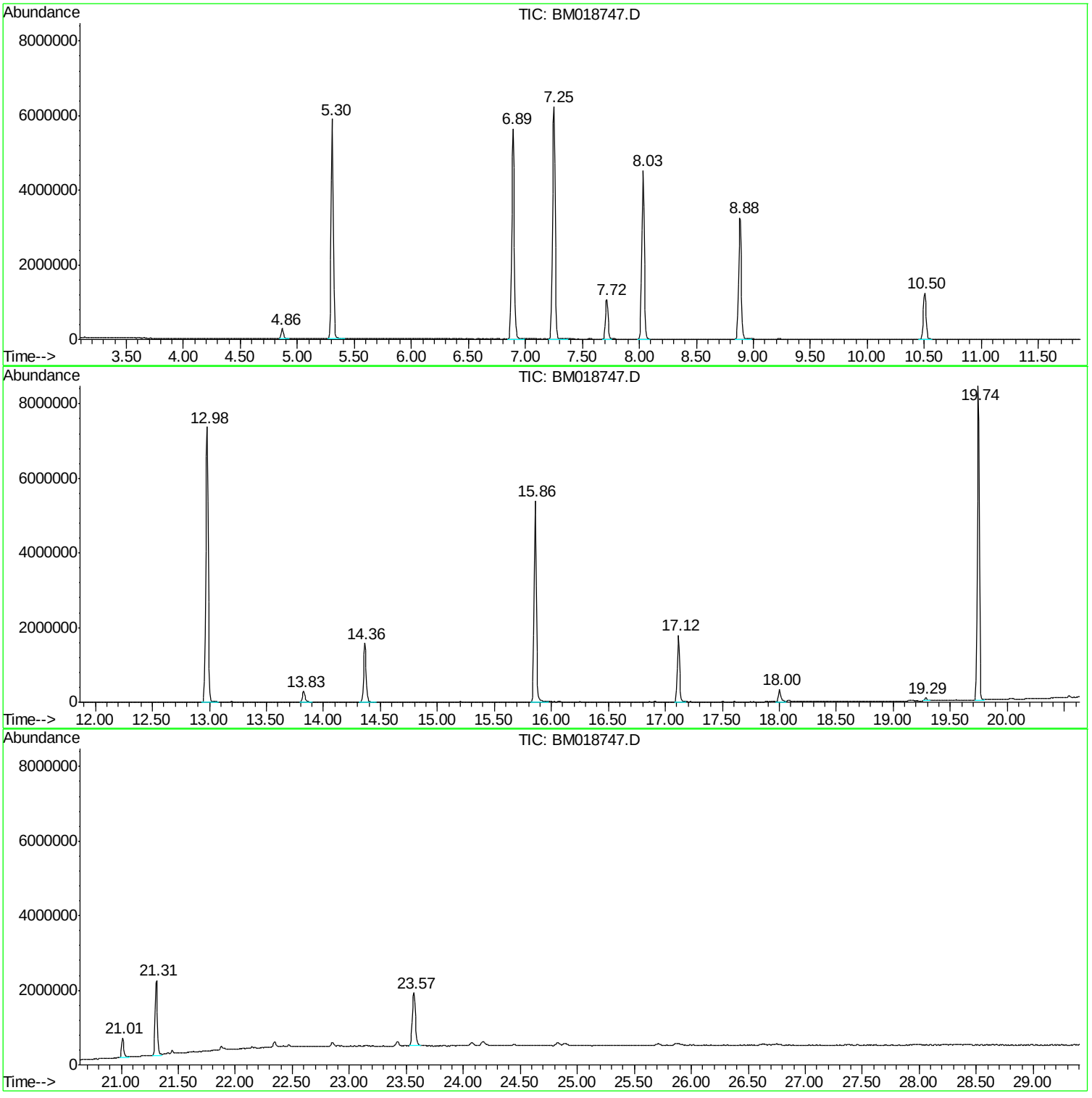
Sum of corrected areas: 84918669

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020719\
Data File : BM018747.D
Acq On : 07 Feb 2019 20:53
Operator : JU/SJ
Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
DUPE-Y

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020719\
Data File : BM018747.D
Acq On : 07 Feb 2019 20:53
Operator : JU/SJ
Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** DUPE-Y

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

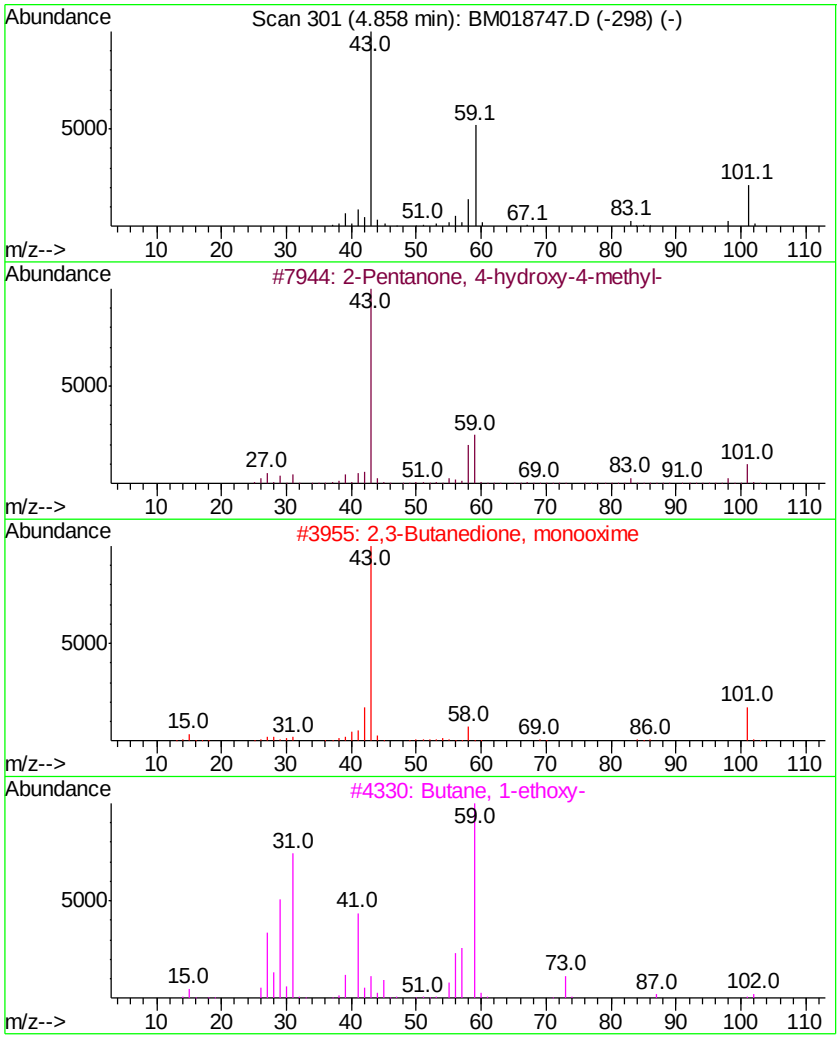
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

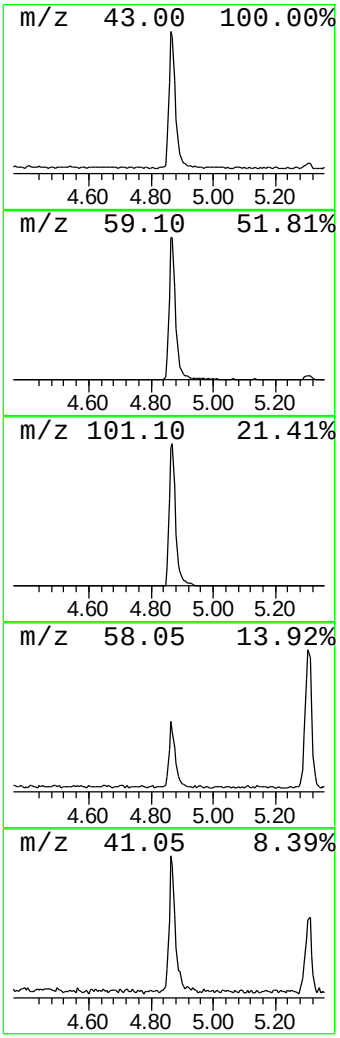
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.86 | 4.65 ng | 395353 | 1,4-Dichlorobenzene-d4 | 7.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 12 |
| 3 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 4 | Butane | 58 | C4H10 | 000106-97-8 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



Library Search Compound Report

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Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** DUPE-Y

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

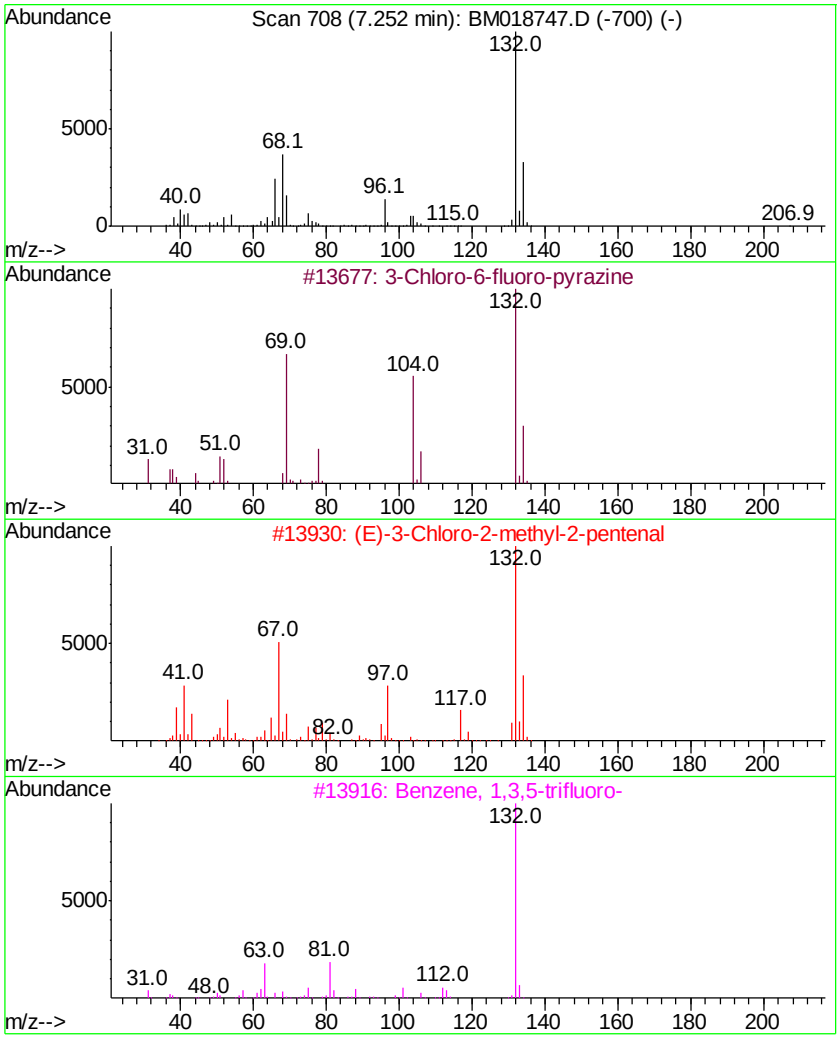
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

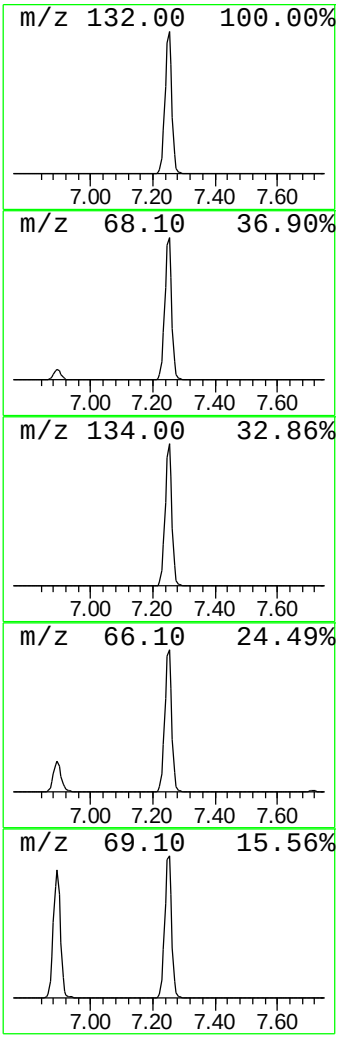
**********

Peak Number 2 unknown7.25 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.25 | 113.98 ng | 9681580 | 1,4-Dichlorobenzene-d4 | 7.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 9 |



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Operator : JU/SJ
Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** DUPE-Y

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

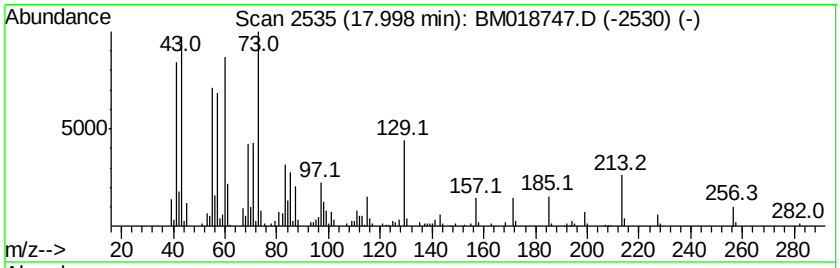
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

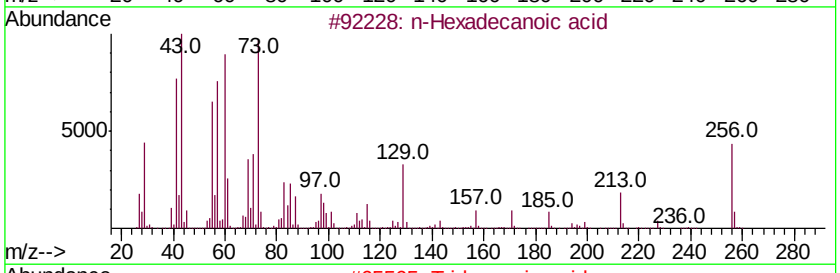
**********

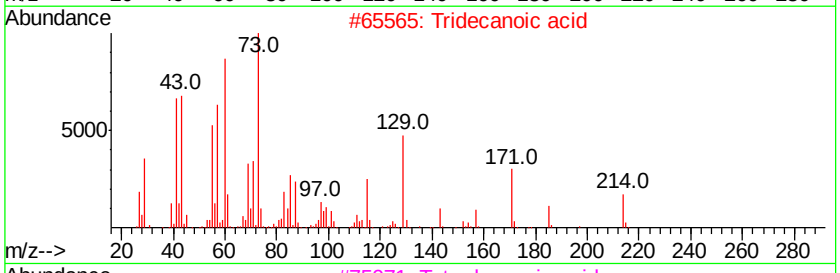
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

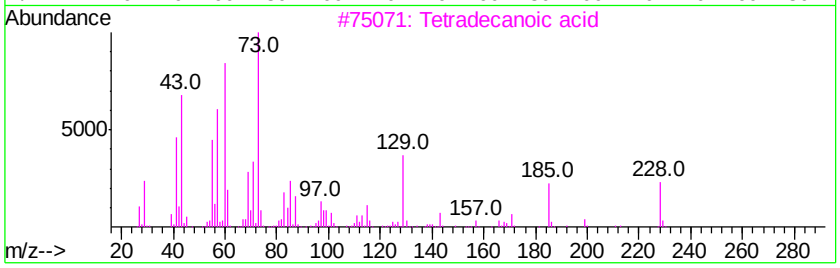
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.00 | 3.93 ng | 508135 | Phenanthrene-d10 | 17.12 |

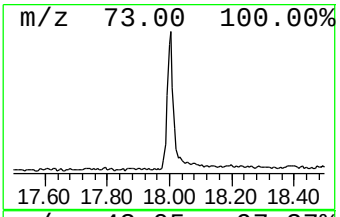
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 95 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 59 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |

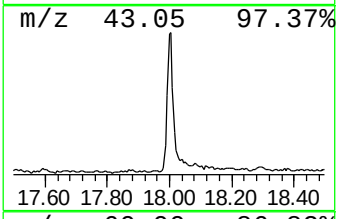


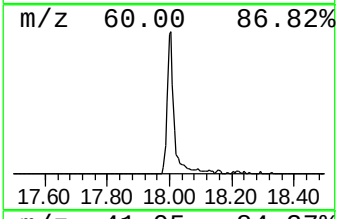



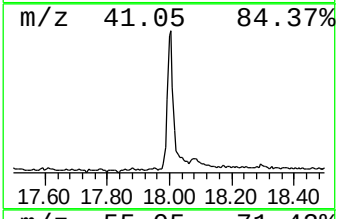



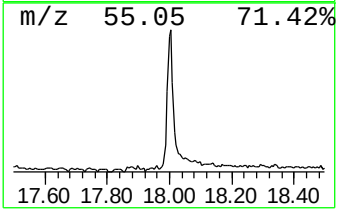



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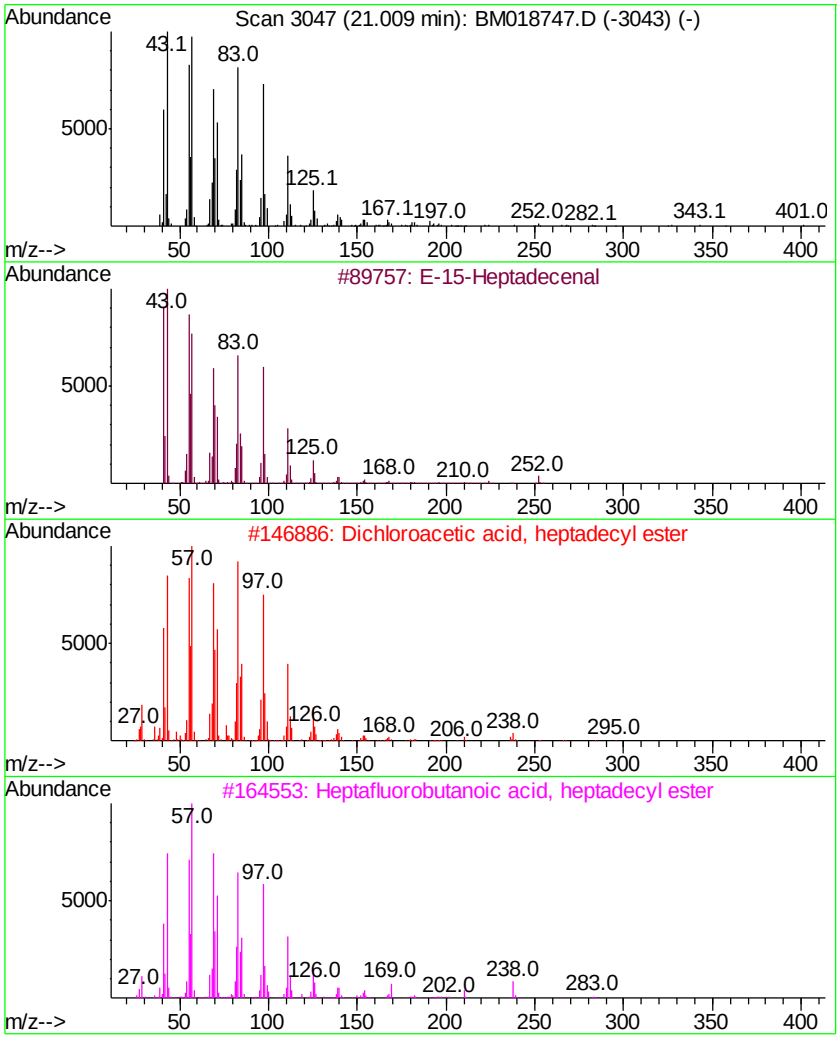
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

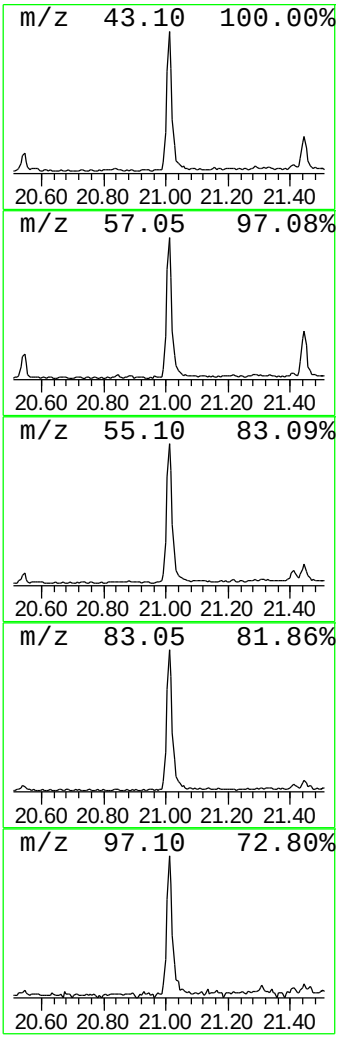
**********

Peak Number 5 E-15-Heptadecenal Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.01 | 5.49 ng | 740059 | Chrysene-d12 | 21.31 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 95 |
| 2 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 94 |
| 3 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 94 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 91 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM020719\
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Acq On : 07 Feb 2019 20:53
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Sample : K1390-15
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
DUPE-Y

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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... | 4.86 | 4.7 | ng | 395353 | 1 | 7.72 | 1698860 | 20.0 |
| unknown7.25 | 7.25 | 114.0 | ng | 9681580 | 1 | 7.72 | 1698860 | 20.0 |
| n-Hexadecanoic acid | 18.00 | 3.9 | ng | 508135 | 4 | 17.12 | 2587300 | 20.0 |
| E-15-Heptadecenal | 21.01 | 5.5 | ng | 740059 | 5 | 21.31 | 2696540 | 20.0 |