LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

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-BF072517.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 | 4.540 | 464 | 468 | 485 | rBV | 132958 | 244707 | 10.59% | 1.206% |
| 2 | 5.004 | 544 | 547 | 574 | rBV | 1882715 | 2309749 | 100.00% | 11.379% |
| 3 | 6.081 | 726 | 730 | 744 | rBV | 1959586 | 2238383 | 96.91% | 11.028% |
| 4 | 6.187 | 744 | 748 | 759 | rVB | 2041865 | 2085078 | 90.27% | 10.272% |
| 5 | 6.410 | 783 | 786 | 797 | rVB | 661845 | 610428 | 26.43% | 3.007% |
| 6 | 6.563 | 809 | 812 | 822 | rBV | 1576487 | 1591627 | 68.91% | 7.841% |
| 7 | 6.981 | 879 | 883 | 900 | rBV | 1387981 | 1396244 | 60.45% | 6.879% |
| 8 | 7.692 | 1000 | 1004 | 1009 | rBV | 995848 | 853411 | 36.95% | 4.204% |
| 9 | 7.734 | 1009 | 1011 | 1017 | rVB2 | 24465 | 25132 | 1.09% | 0.124% |
| 10 | 8.769 | 1183 | 1187 | 1191 | rBV | 2002849 | 1995788 | 86.41% | 9.833% |
| 11 | 9.175 | 1252 | 1256 | 1265 | rBV | 287799 | 261179 | 11.31% | 1.287% |
| 12 | 9.433 | 1296 | 1300 | 1309 | rBV | 858994 | 822397 | 35.61% | 4.052% |
| 13 | 9.892 | 1375 | 1378 | 1381 | rVB | 41379 | 33001 | 1.43% | 0.163% |
| 14 | 10.222 | 1431 | 1434 | 1451 | rBV | 1207289 | 1288796 | 55.80% | 6.349% |
| 15 | 10.363 | 1454 | 1458 | 1465 | rVV | 66223 | 84002 | 3.64% | 0.414% |
| 16 | 10.810 | 1530 | 1534 | 1536 | rBV2 | 28720 | 30329 | 1.31% | 0.149% |
| 17 | 10.910 | 1547 | 1551 | 1559 | rVB | 856960 | 761308 | 32.96% | 3.751% |
| 18 | 11.469 | 1642 | 1646 | 1652 | rBV | 158580 | 143841 | 6.23% | 0.709% |
| 19 | 12.245 | 1775 | 1778 | 1788 | rBV | 118940 | 133561 | 5.78% | 0.658% |
| 20 | 12.333 | 1790 | 1793 | 1799 | rVB2 | 20096 | 25388 | 1.10% | 0.125% |
| 21 | 12.492 | 1815 | 1820 | 1823 | rBV | 1685403 | 1633353 | 70.72% | 8.047% |
| 22 | 13.421 | 1973 | 1978 | 1990 | rBV2 | 89847 | 197880 | 8.57% | 0.975% |
| 23 | 13.533 | 1993 | 1997 | 2005 | rVB | 606881 | 595031 | 25.76% | 2.932% |
| 24 | 14.027 | 2077 | 2081 | 2083 | rBV | 37083 | 37583 | 1.63% | 0.185% |
| 25 | 14.057 | 2083 | 2086 | 2095 | rVB4 | 46317 | 91012 | 3.94% | 0.448% |
| 26 | 14.604 | 2176 | 2179 | 2183 | rBV | 42897 | 41960 | 1.82% | 0.207% |
| 27 | 14.657 | 2183 | 2188 | 2194 | rVV6 | 20257 | 46069 | 1.99% | 0.227% |
| 28 | 14.868 | 2220 | 2224 | 2229 | rBV | 461380 | 517043 | 22.39% | 2.547% |
| 29 | 15.062 | 2251 | 2257 | 2262 | rBV8 | 17447 | 44914 | 1.94% | 0.221% |
| 30 | 15.245 | 2284 | 2288 | 2294 | rVB | 30910 | 43255 | 1.87% | 0.213% |
| 31 | 15.862 | 2390 | 2393 | 2399 | rVB7 | 20160 | 30965 | 1.34% | 0.153% |
| 32 | 16.239 | 2450 | 2457 | 2462 | rBV5 | 29389 | 60154 | 2.60% | 0.296% |
| 33 | 17.262 | 2627 | 2631 | 2635 | rBV7 | 12273 | 24231 | 1.05% | 0.119% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 20297799

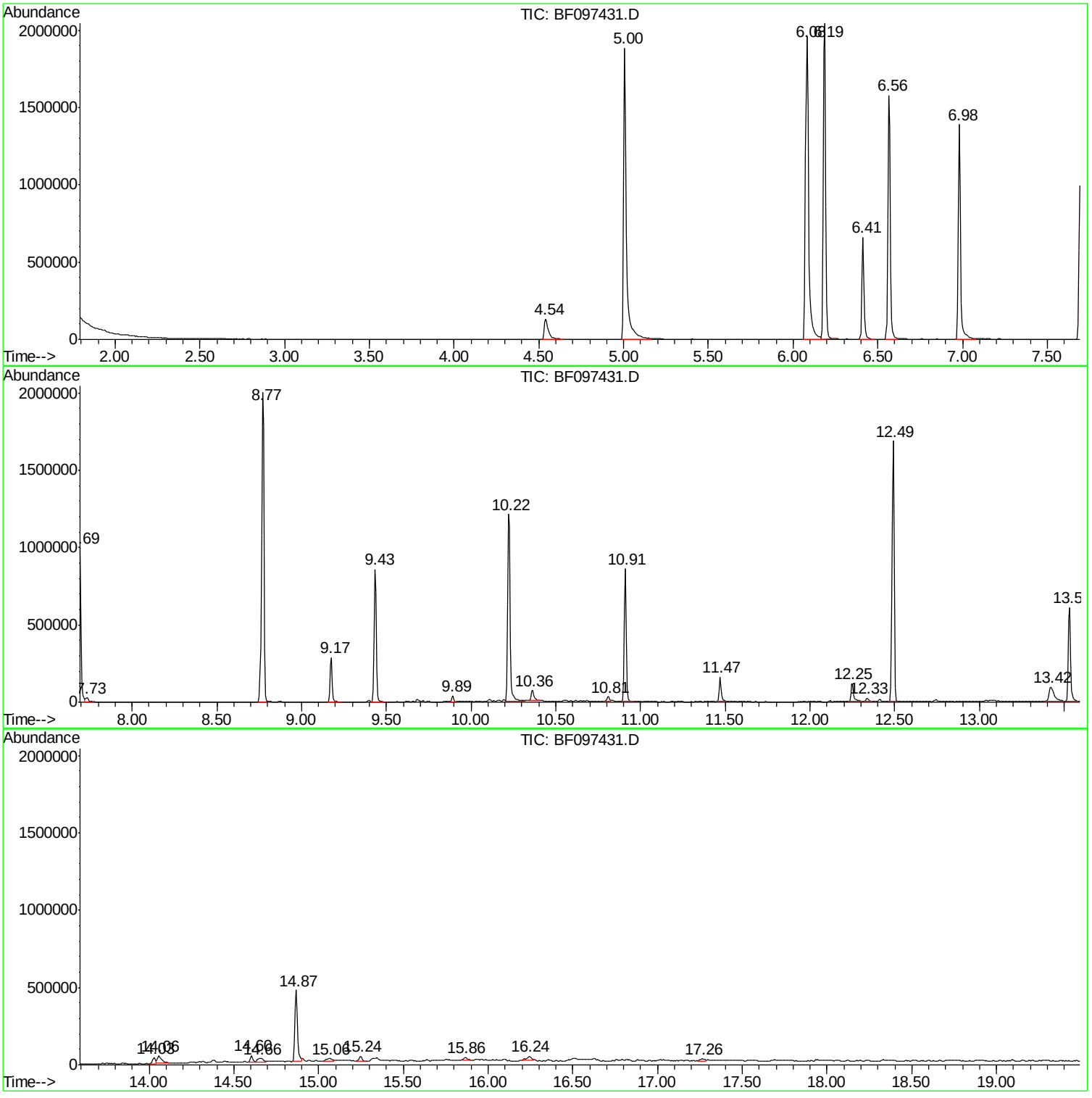
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

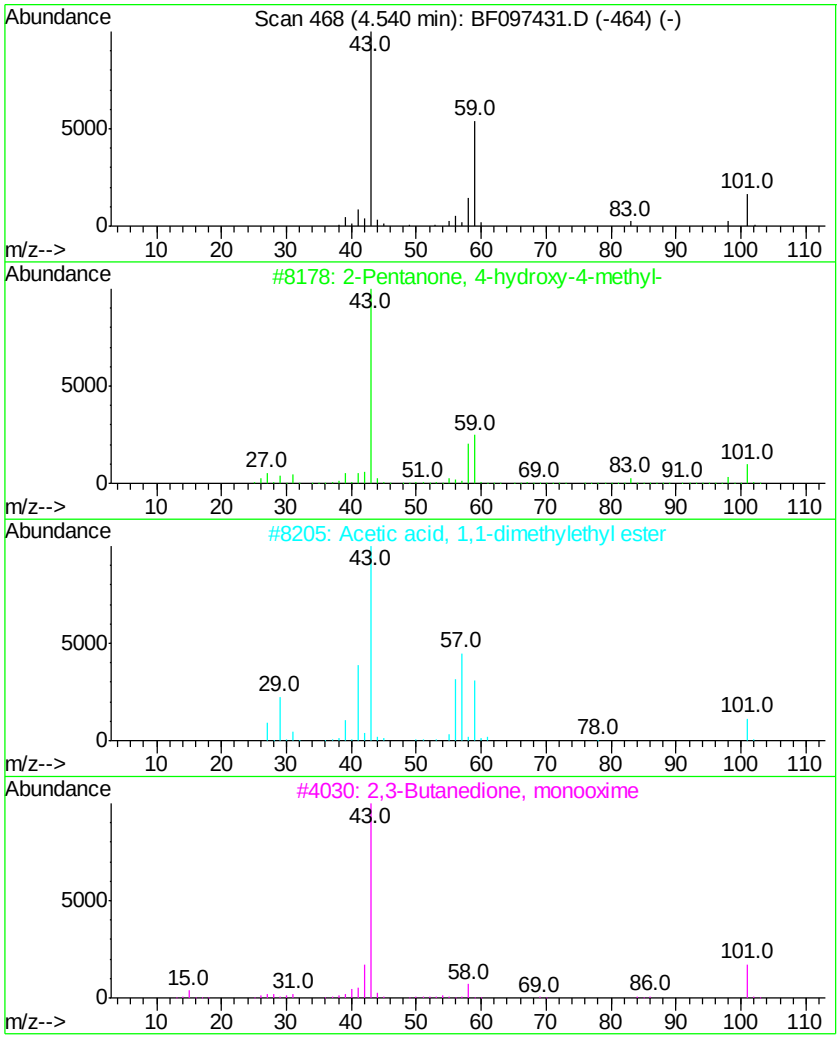
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

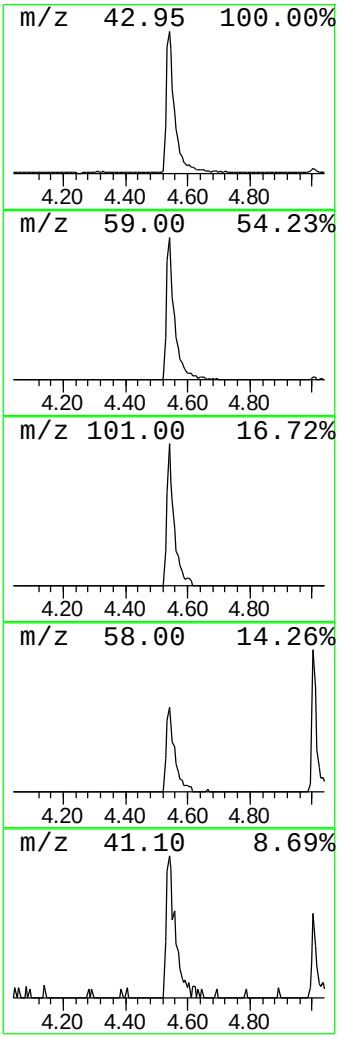
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.54 | 8.02 ng | 244707 | 1,4-Dichlorobenzene-d4 | 6.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 28 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 9 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

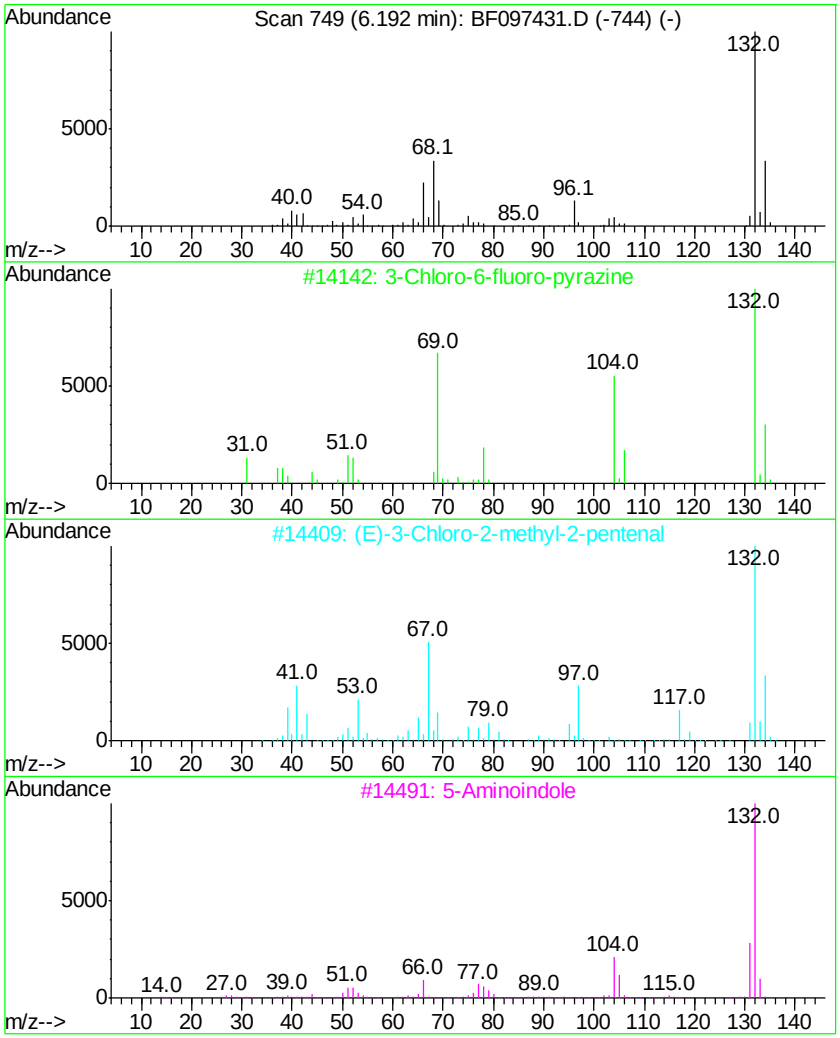
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

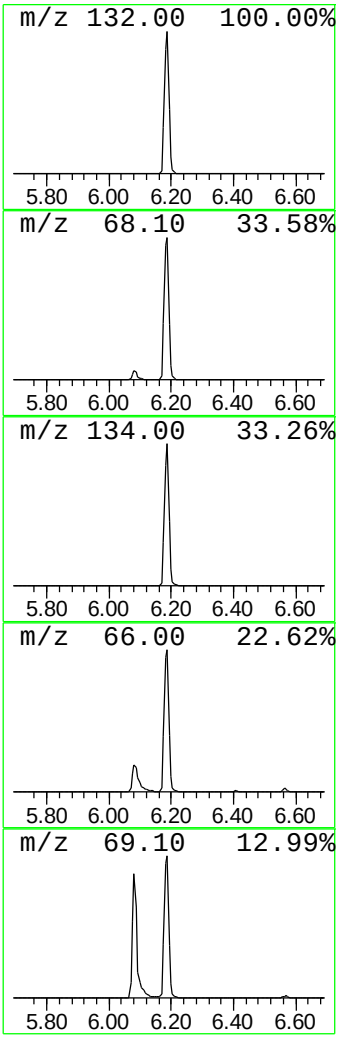
**********

Peak Number 2 unknown6.19 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.19 | 68.32 ng | 2085080 | 1,4-Dichlorobenzene-d4 | 6.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

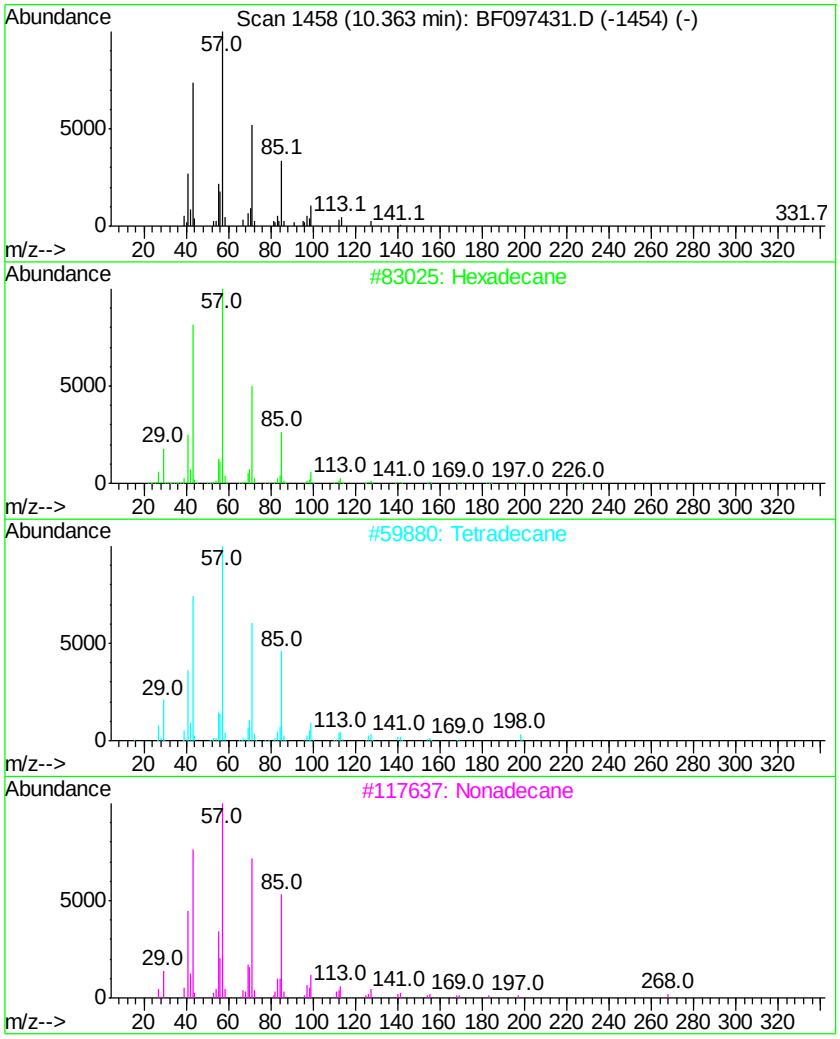
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

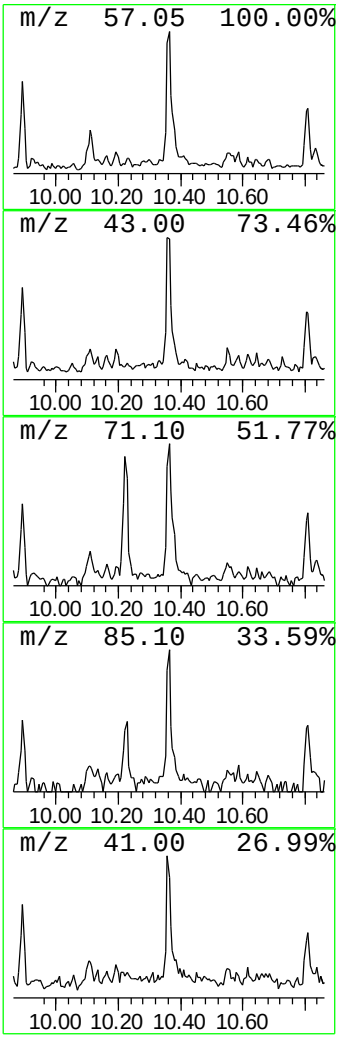
**********

Peak Number 4 Hexadecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.36 | 2.21 ng | 84002 | Phenanthrene-d10 | 10.91 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 83 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 72 |
| 4 | Decane, 2,9-dimethyl- | 170 | C12H26 | 001002-17-1 | 59 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 59 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

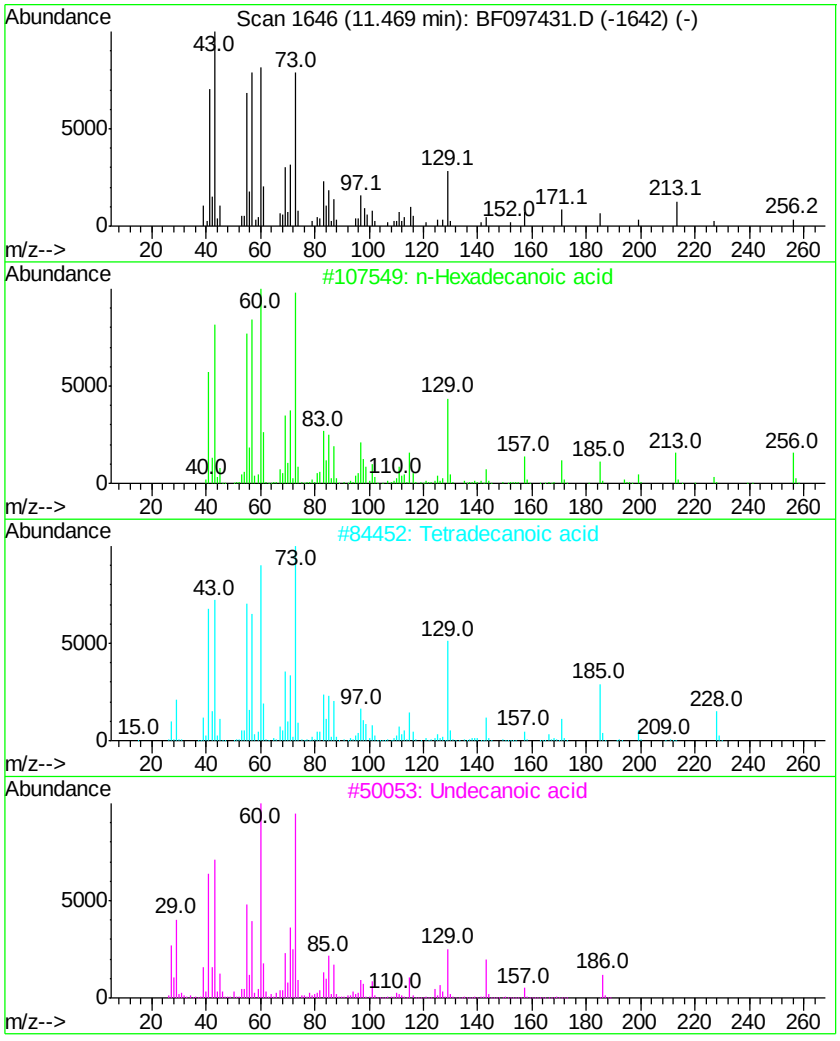
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

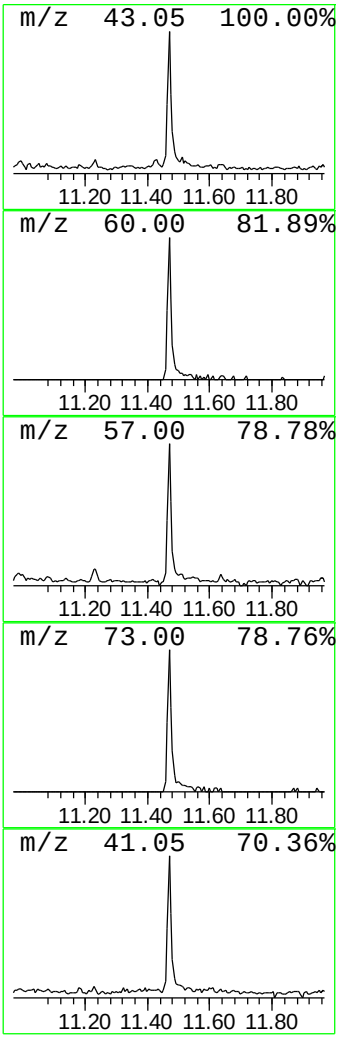
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.47 | 3.78 ng | 143841 | Phenanthrene-d10 | 10.91 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 90 |
| 3 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 86 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 64 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

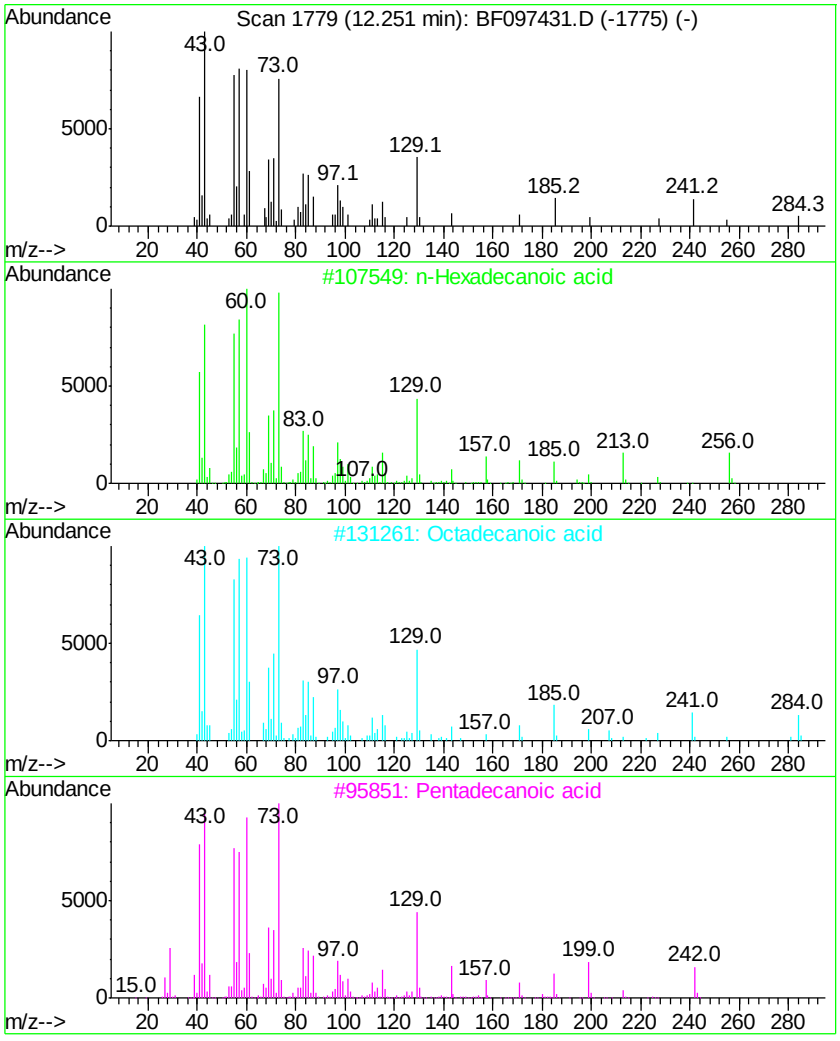
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

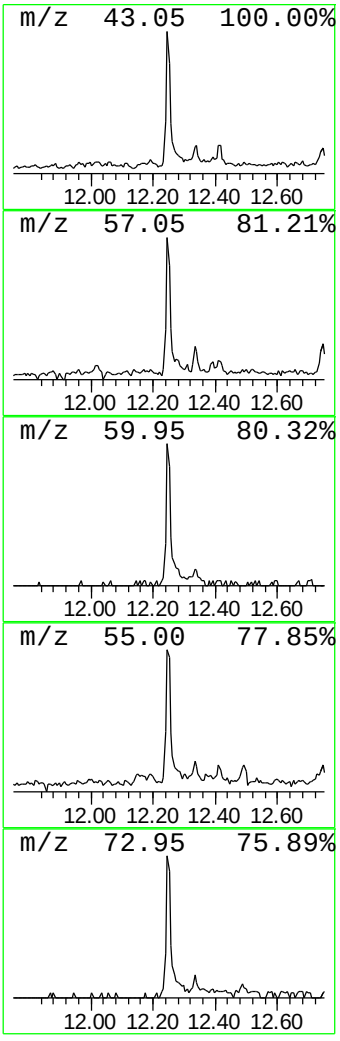
**********

Peak Number 6 Octadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.25 | 4.49 ng | 133561 | Chrysene-d12 | 13.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 91 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 5 | Oxalic acid, cyclobutyl pentadec... | 354 | C21H38O4 | 1000309-70-5 | 15 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

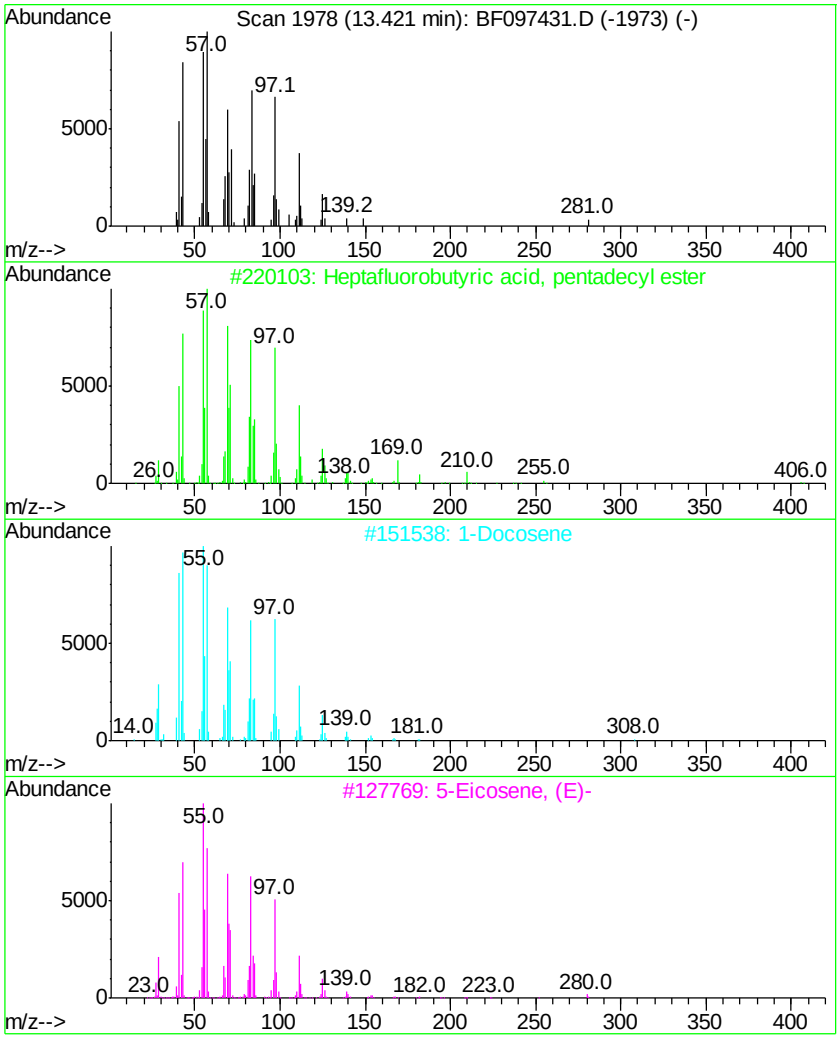
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

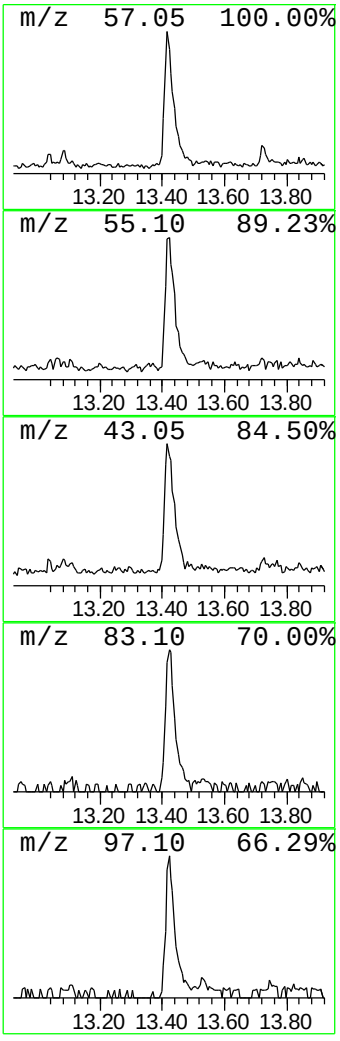
**********

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.42 | 6.65 ng | 197880 | Chrysene-d12 | 13.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 3 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 91 |
| 4 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 91 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

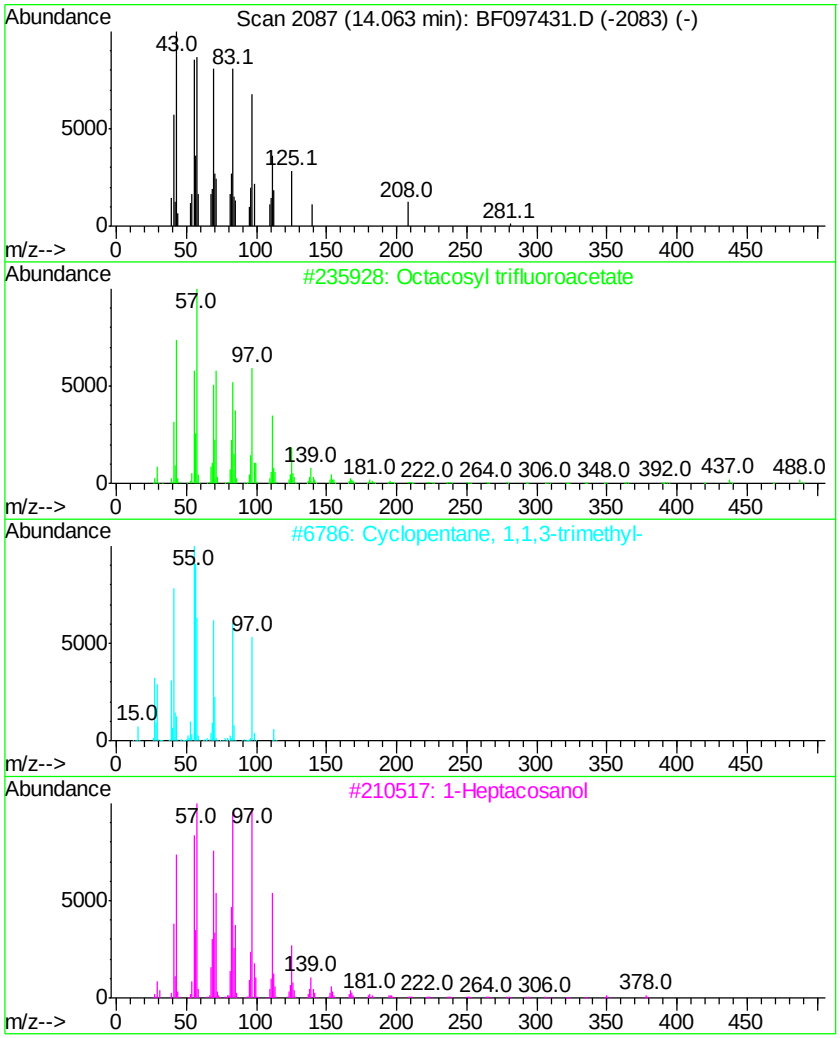
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

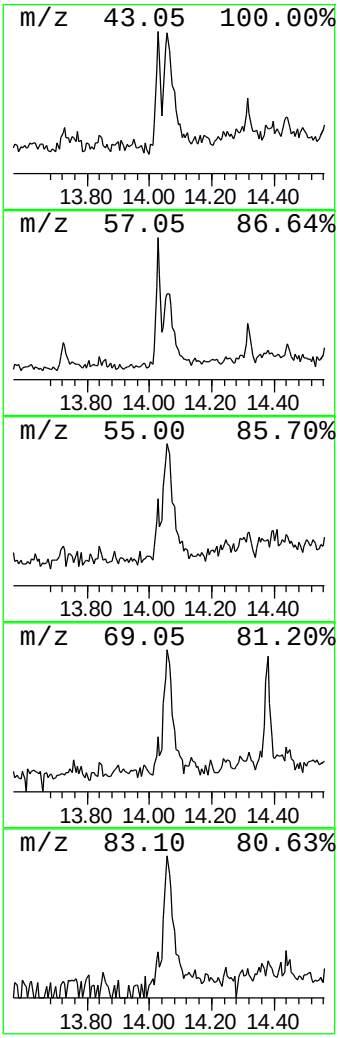
**********

Peak Number 8 Octacosyl trifluoroacetate Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.06 | 3.06 ng | 91012 | Chrysene-d12 | 13.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 62 |
| 2 | Cyclopentane, 1,1,3-trimethyl- | 112 | C8H16 | 004516-69-2 | 62 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 62 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 52 |
| 5 | 2-Hexenal, (E)- | 98 | C6H10O | 006728-26-3 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

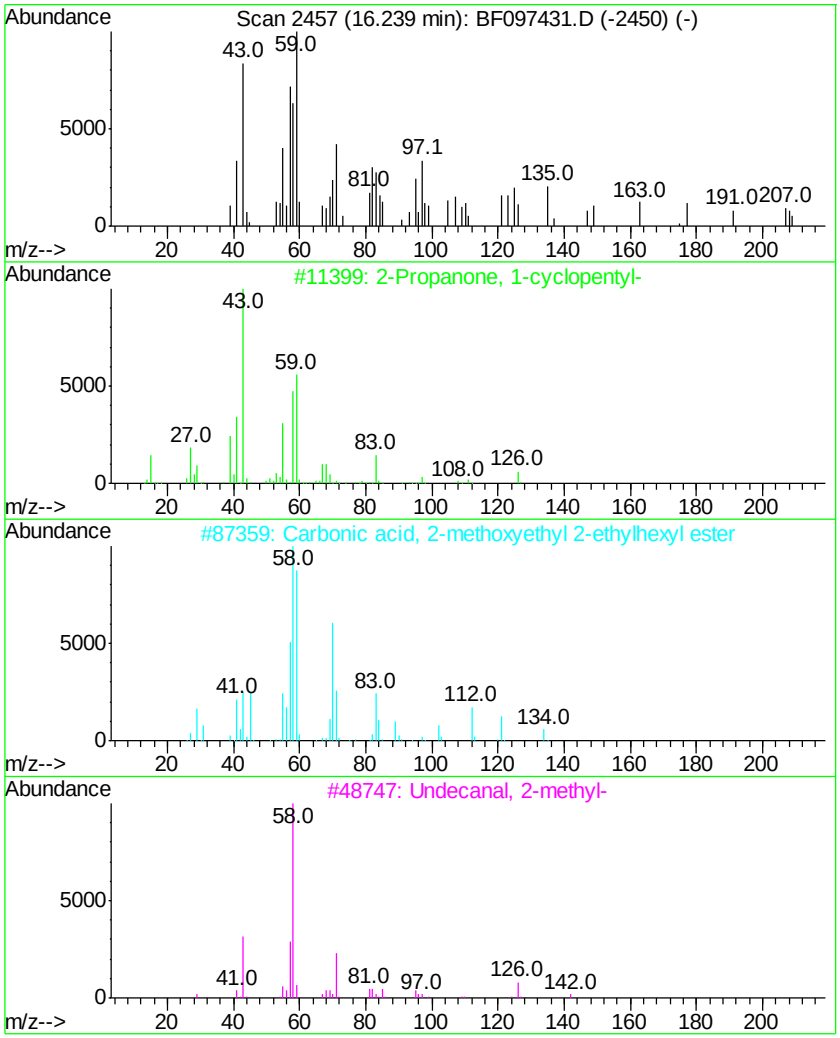
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

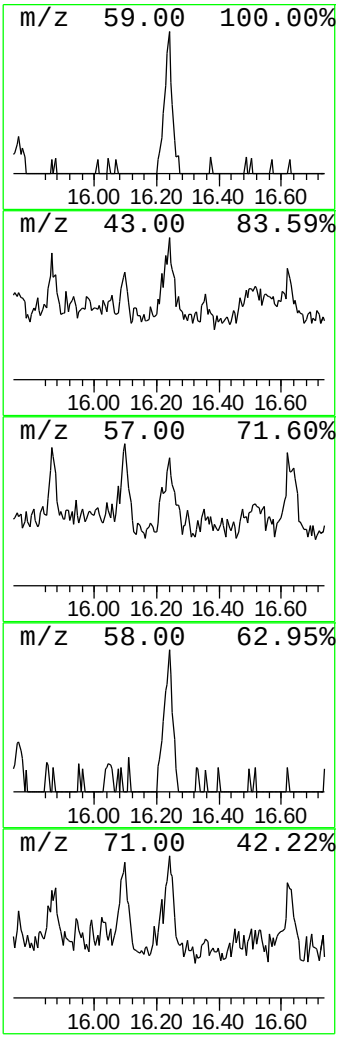
**********

Peak Number 9 unknown16.24 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.24 | 2.33 ng | 60154 | Perylene-d12 | 14.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanone, 1-cyclopentyl- | 126 | C8H14O | 001122-98-1 | 35 |
| 2 | Carbonic acid, 2-methoxyethyl 2-... | 232 | C12H24O4 | 1000357-86-9 | 25 |
| 3 | Undecanal, 2-methyl- | 184 | C12H24O | 000110-41-8 | 22 |
| 4 | 4,5-Dimethyl-3-heptanol | 144 | C9H20O | 019549-76-9 | 16 |
| 5 | 7-Octen-2-one | 126 | C8H14O | 003664-60-6 | 14 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097431.D
Acq On : 7 Aug 2017 16:09
Operator : SJ/JU
Sample : I4625-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CLINTON-AVE-COMP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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 |
| 2-Pentanone, 4-hy... | 4.54 | 8.0 | ng | 244707 | 1 | 6.41 | 610428 | 20.0 |
| unknown6.19 | 6.19 | 68.3 | ng | 2085080 | 1 | 6.41 | 610428 | 20.0 |
| Hexadecane | 10.36 | 2.2 | ng | 84002 | 4 | 10.91 | 761308 | 20.0 |
| n-Hexadecanoic acid | 11.47 | 3.8 | ng | 143841 | 4 | 10.91 | 761308 | 20.0 |
| Octadecanoic acid | 12.25 | 4.5 | ng | 133561 | 5 | 13.53 | 595031 | 20.0 |
| Heptafluorobutyri... | 13.42 | 6.7 | ng | 197880 | 5 | 13.53 | 595031 | 20.0 |
| Octacosyl trifluo... | 14.06 | 3.1 | ng | 91012 | 5 | 13.53 | 595031 | 20.0 |
| unknown16.24 | 16.24 | 2.3 | ng | 60154 | 6 | 14.87 | 517043 | 20.0 |