LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

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-BF102317.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 | 2.205 | 17 | 20 | 28 | rVB | 20861 | 27137 | 1.23% | 0.144% |
| 2 | 2.299 | 30 | 36 | 48 | rVB | 247392 | 358973 | 16.22% | 1.898% |
| 3 | 4.999 | 492 | 495 | 513 | rBV | 183272 | 268555 | 12.13% | 1.420% |
| 4 | 5.410 | 561 | 565 | 583 | rBV | 1565326 | 1637527 | 73.97% | 8.659% |
| 5 | 6.434 | 735 | 739 | 756 | rBV | 1527995 | 1720637 | 77.73% | 9.099% |
| 6 | 6.563 | 758 | 761 | 765 | rBV | 1902383 | 1738904 | 78.55% | 9.195% |
| 7 | 6.793 | 797 | 800 | 809 | rBV | 539162 | 448057 | 20.24% | 2.369% |
| 8 | 6.945 | 823 | 826 | 840 | rBV | 1510527 | 1383000 | 62.47% | 7.313% |
| 9 | 7.363 | 893 | 897 | 912 | rBV | 1199255 | 1058009 | 47.79% | 5.595% |
| 10 | 8.075 | 1015 | 1018 | 1028 | rBV | 799217 | 640831 | 28.95% | 3.389% |
| 11 | 8.634 | 1110 | 1113 | 1123 | rBB | 114249 | 96851 | 4.38% | 0.512% |
| 12 | 9.157 | 1197 | 1202 | 1205 | rBV | 2472115 | 2213726 | 100.00% | 11.706% |
| 13 | 9.551 | 1266 | 1269 | 1275 | rVB | 109524 | 80548 | 3.64% | 0.426% |
| 14 | 9.834 | 1314 | 1317 | 1321 | rBV | 868025 | 753211 | 34.02% | 3.983% |
| 15 | 10.551 | 1436 | 1439 | 1443 | rBV | 531253 | 419772 | 18.96% | 2.220% |
| 16 | 10.633 | 1449 | 1453 | 1456 | rBV | 1384062 | 1243913 | 56.19% | 6.578% |
| 17 | 11.328 | 1568 | 1571 | 1575 | rBV | 930121 | 788708 | 35.63% | 4.171% |
| 18 | 11.845 | 1657 | 1659 | 1669 | rBV2 | 59111 | 75524 | 3.41% | 0.399% |
| 19 | 12.551 | 1773 | 1779 | 1783 | rBV | 20786 | 26003 | 1.17% | 0.138% |
| 20 | 12.633 | 1790 | 1793 | 1800 | rBV3 | 34941 | 43031 | 1.94% | 0.228% |
| 21 | 12.916 | 1837 | 1841 | 1845 | rBV | 2172515 | 2143404 | 96.82% | 11.335% |
| 22 | 13.374 | 1916 | 1919 | 1925 | rVB4 | 23793 | 29565 | 1.34% | 0.156% |
| 23 | 13.445 | 1927 | 1931 | 1933 | rBV | 31022 | 30220 | 1.37% | 0.160% |
| 24 | 13.798 | 1987 | 1991 | 1996 | rBV | 84710 | 92549 | 4.18% | 0.489% |
| 25 | 13.939 | 2011 | 2015 | 2018 | rVB | 144131 | 115247 | 5.21% | 0.609% |
| 26 | 13.980 | 2018 | 2022 | 2026 | rBV | 712727 | 642790 | 29.04% | 3.399% |
| 27 | 14.598 | 2122 | 2127 | 2130 | rBV2 | 35976 | 64672 | 2.92% | 0.342% |
| 28 | 14.680 | 2139 | 2141 | 2144 | rVB | 43253 | 34888 | 1.58% | 0.184% |
| 29 | 14.768 | 2153 | 2156 | 2158 | rBV | 38108 | 32208 | 1.45% | 0.170% |
| 30 | 14.857 | 2168 | 2171 | 2177 | rVV2 | 32209 | 50709 | 2.29% | 0.268% |
| 31 | 14.910 | 2177 | 2180 | 2184 | rVV | 38597 | 45373 | 2.05% | 0.240% |
| 32 | 14.945 | 2184 | 2186 | 2193 | rVB | 31677 | 52228 | 2.36% | 0.276% |
| 33 | 15.057 | 2201 | 2205 | 2209 | rVB2 | 20995 | 30861 | 1.39% | 0.163% |
| 34 | 15.451 | 2267 | 2272 | 2280 | rVB | 418079 | 522793 | 23.62% | 2.765% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

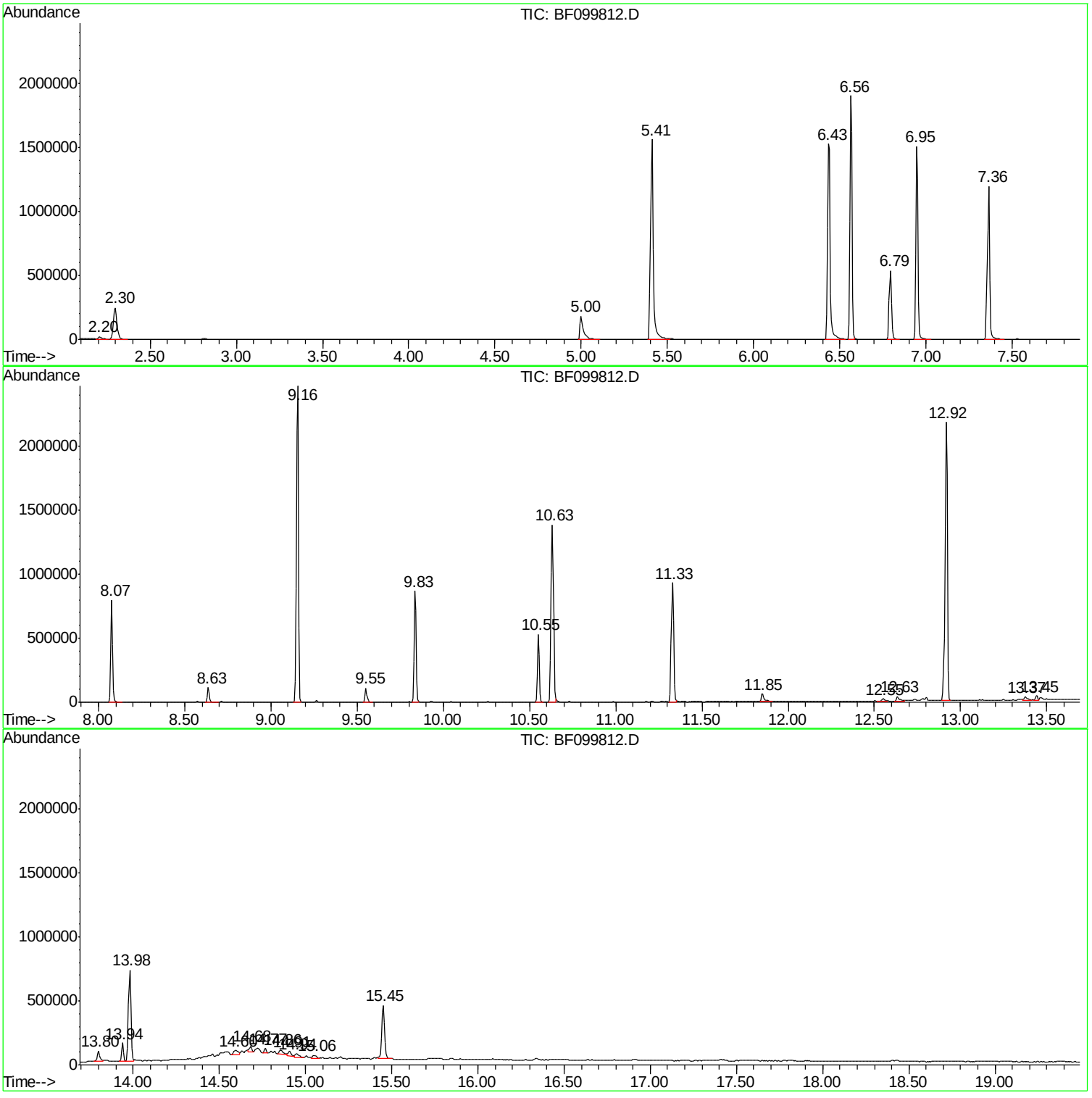
Sum of corrected areas: 18910424

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

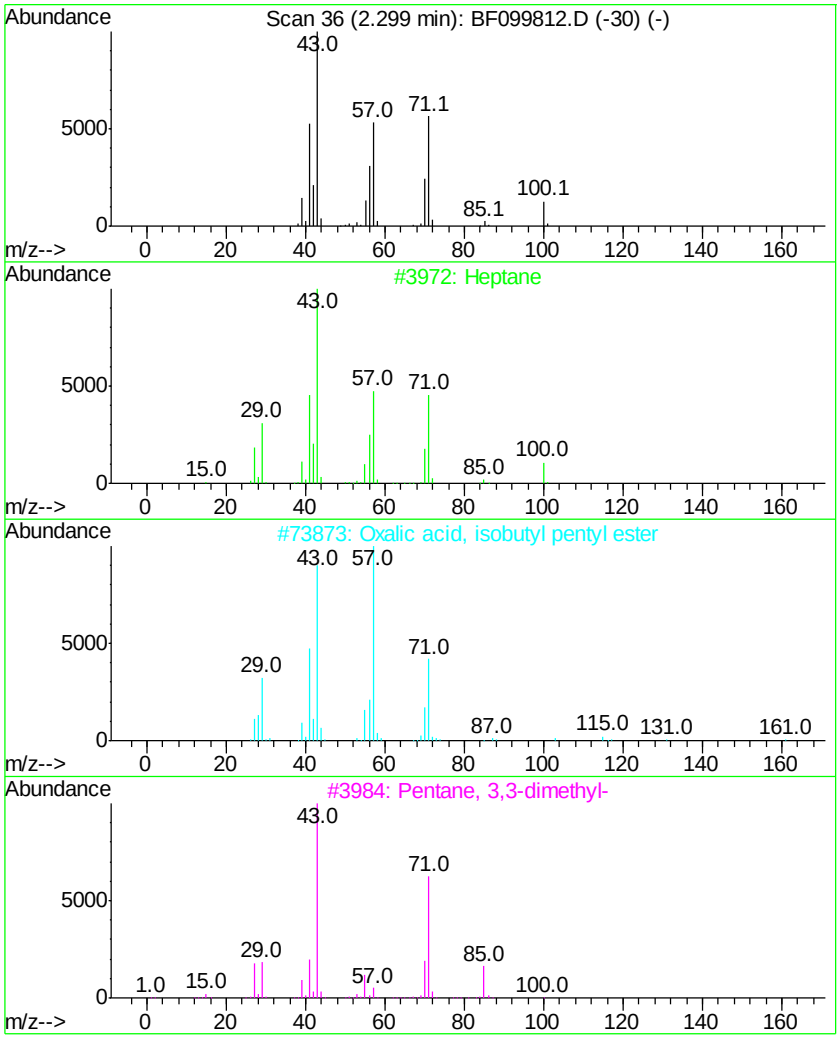
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

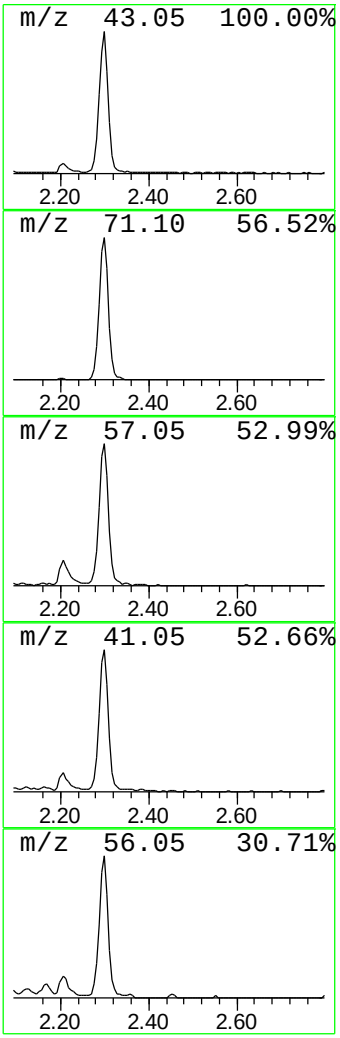
**********

Peak Number 1 Heptane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.30 | 16.02 ng | 358973 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane | 100 | C7H16 | 000142-82-5 | 95 |
| 2 | Oxalic acid, isobutyl pentyl ester | 216 | C11H20O4 | 1000309-37-0 | 53 |
| 3 | Pentane, 3,3-dimethyl- | 100 | C7H16 | 000562-49-2 | 47 |
| 4 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 43 |
| 5 | Isobutyl 3-methylbutan-2-yl carb... | 188 | C10H20O3 | 1000372-77-0 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

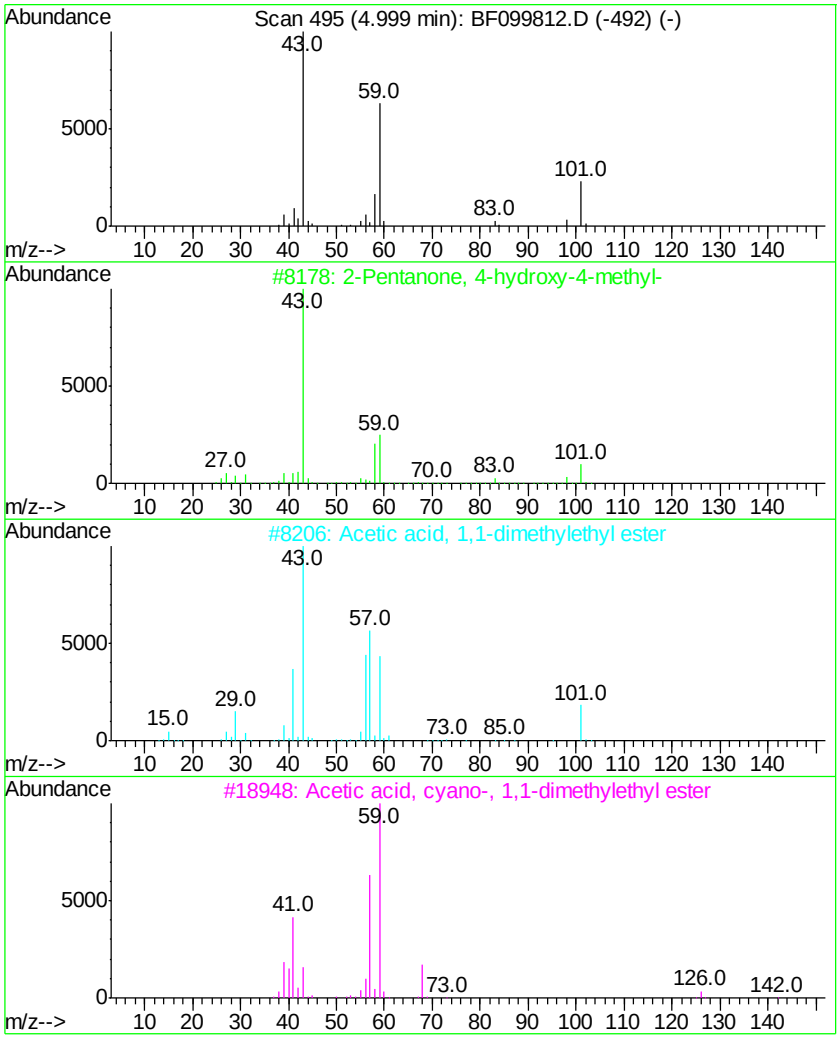
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

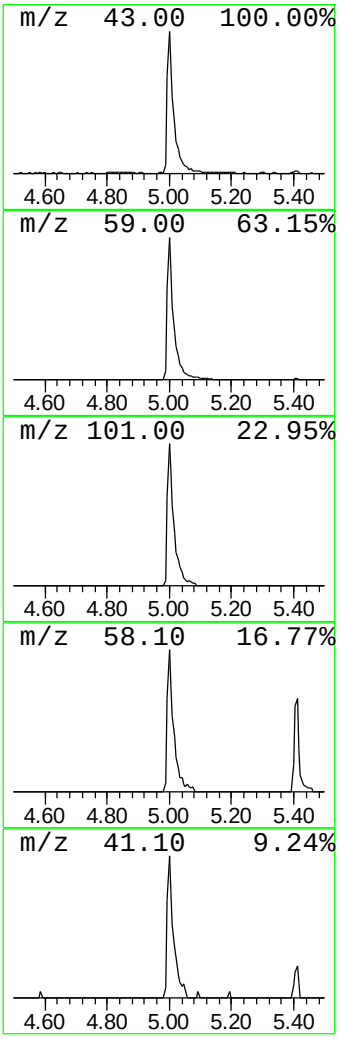
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.00 | 11.99 ng | 268555 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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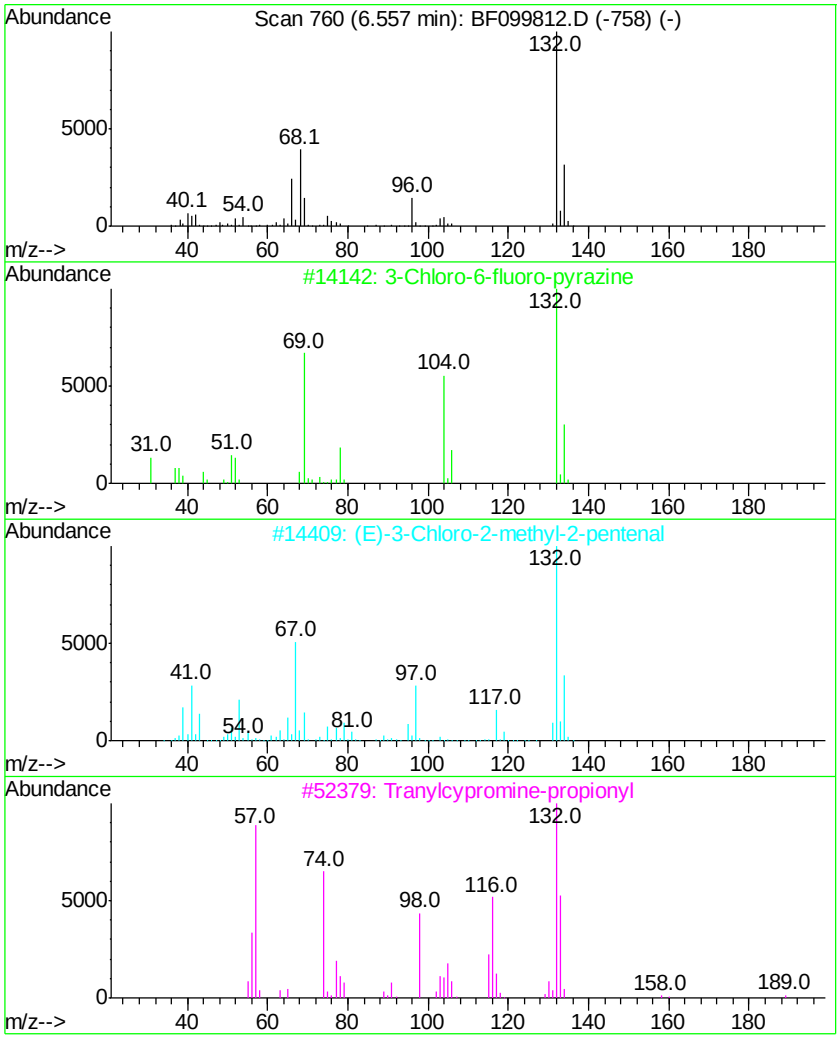
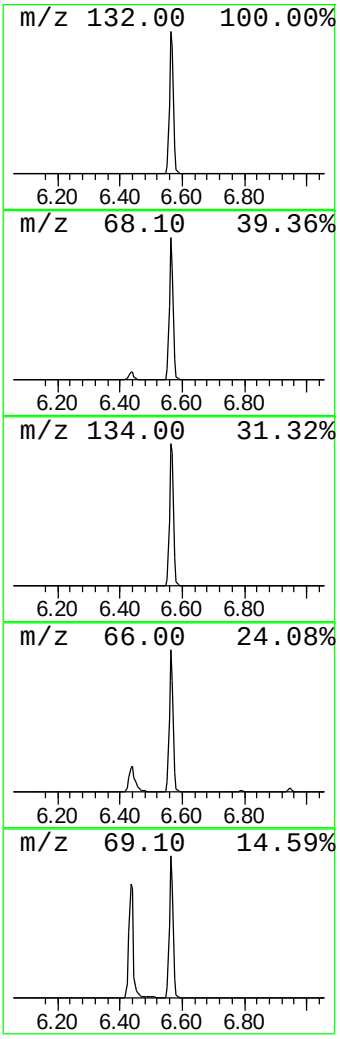
Peak Number 3 unknown6.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.56 | 77.62 ng | 1738900 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

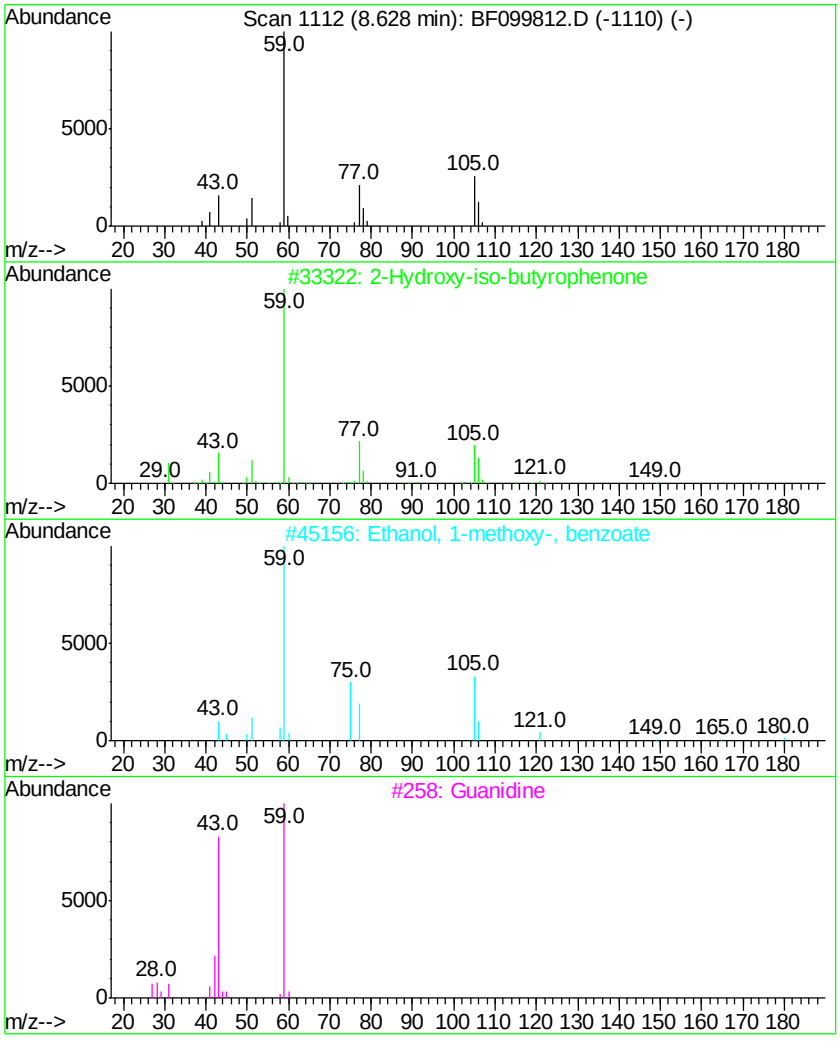
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

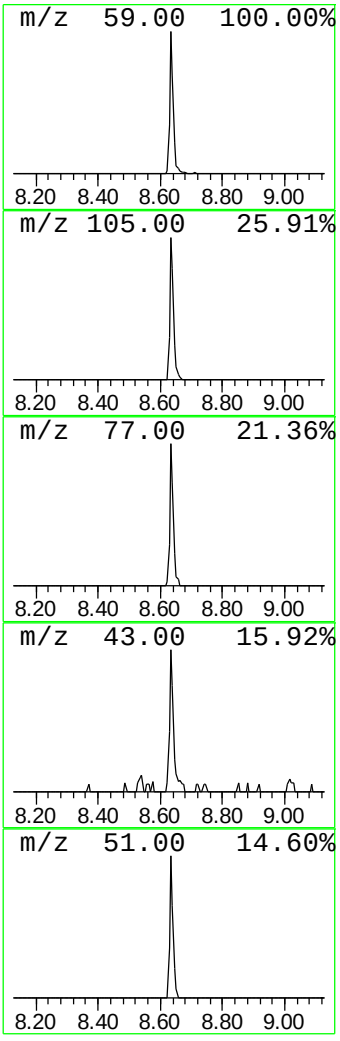
**********

Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.63 | 3.02 ng | 96851 | Naphthalene-d8 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-iso-butyrophenone | 164 | C10H12O2 | 007473-98-5 | 86 |
| 2 | Ethanol, 1-methoxy-, benzoate | 180 | C10H12O3 | 051835-44-0 | 64 |
| 3 | Guanidine | 59 | CH5N3 | 000113-00-8 | 7 |
| 4 | Formamide, N-methyl- | 59 | C2H5NO | 000123-39-7 | 5 |
| 5 | Acetamide | 59 | C2H5NO | 000060-35-5 | 5 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

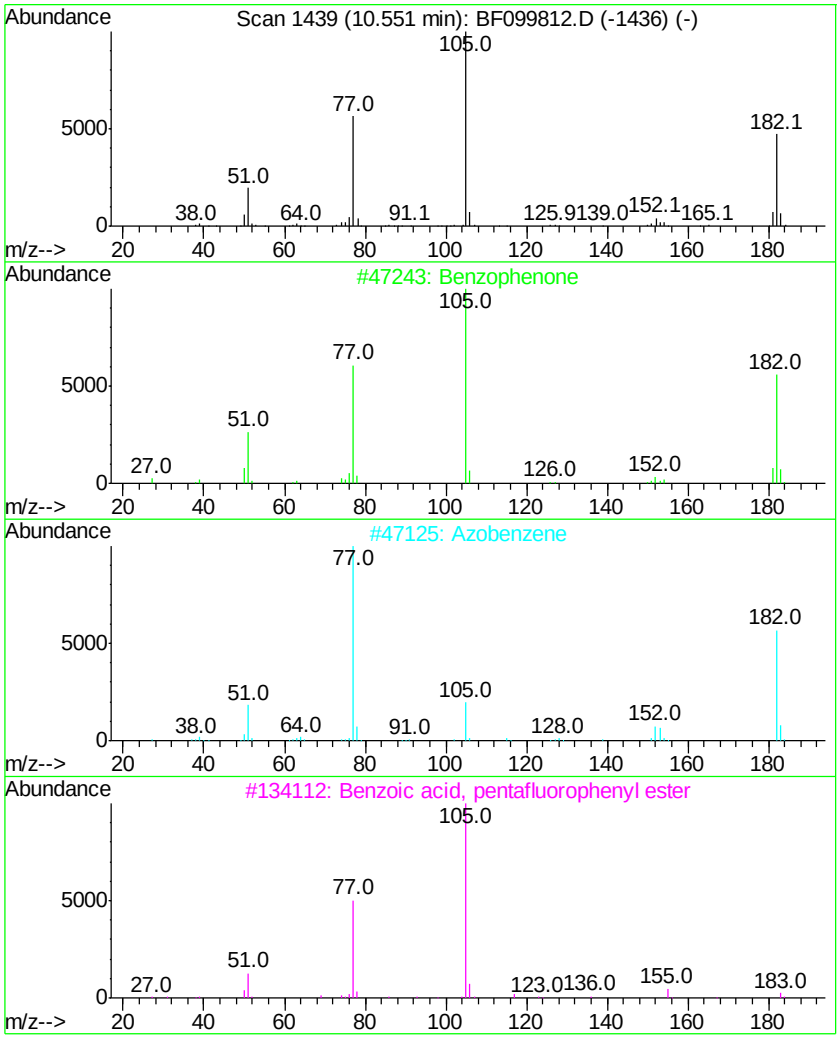
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

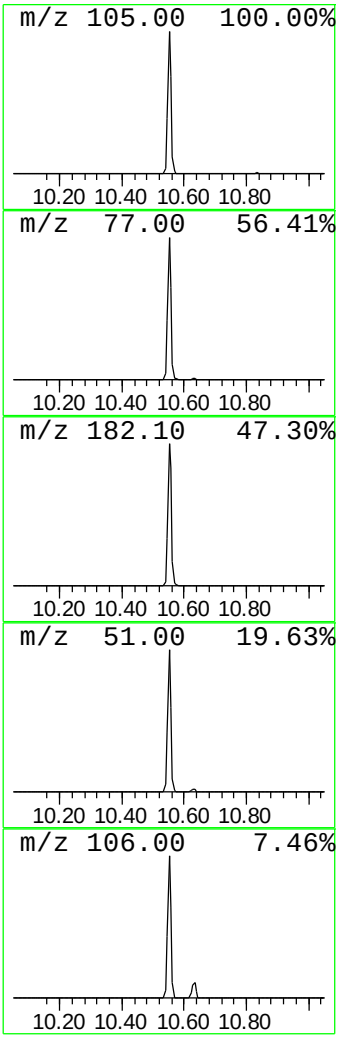
**********

Peak Number 6 Benzophenone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 11.15 ng | 419772 | Acenaphthene-d10 | 9.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 59 |
| 3 | Benzoic acid, pentafluorophenyl ... | 288 | C13H5F5O2 | 1000360-67-9 | 50 |
| 4 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 49 |
| 5 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 47 |



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Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

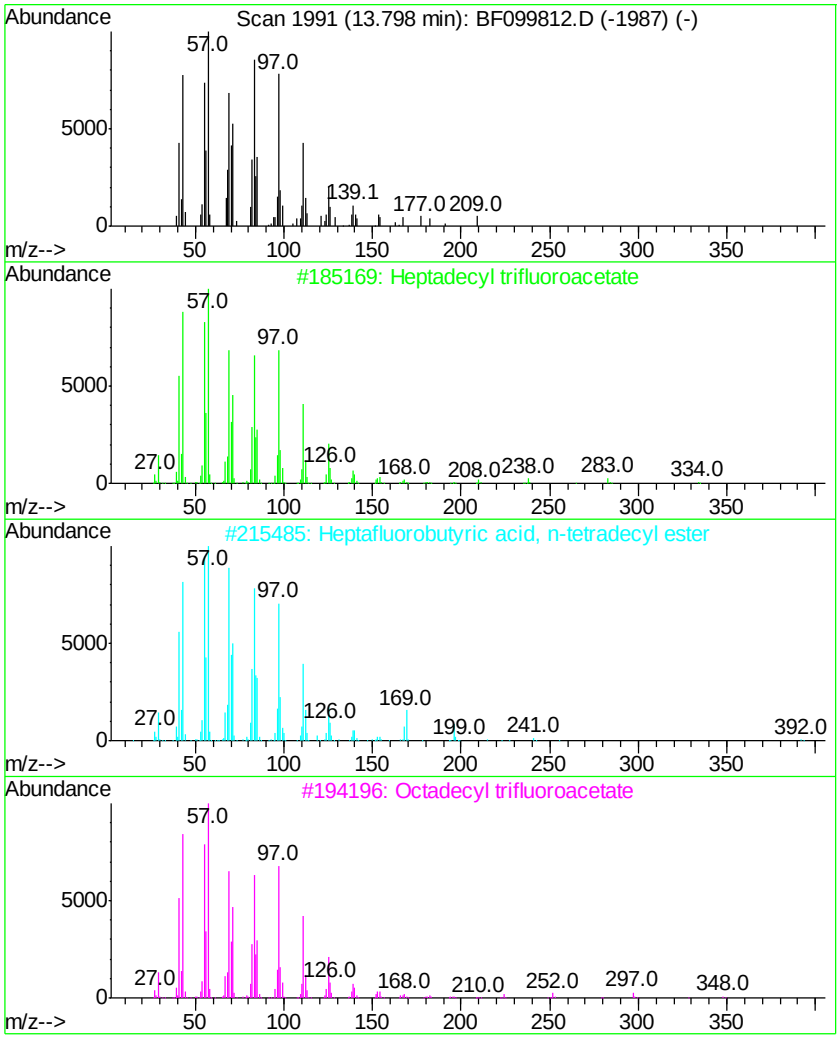
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

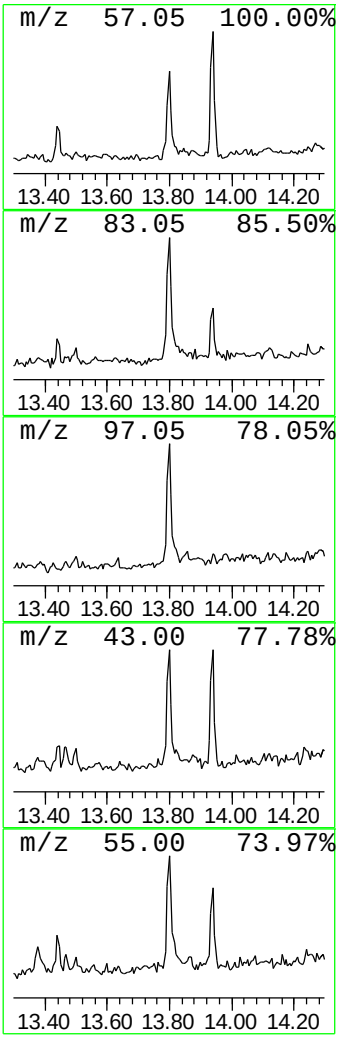
**********

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.80 | 2.88 ng | 92549 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 95 |
| 2 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 95 |
| 3 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 94 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 94 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |



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Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

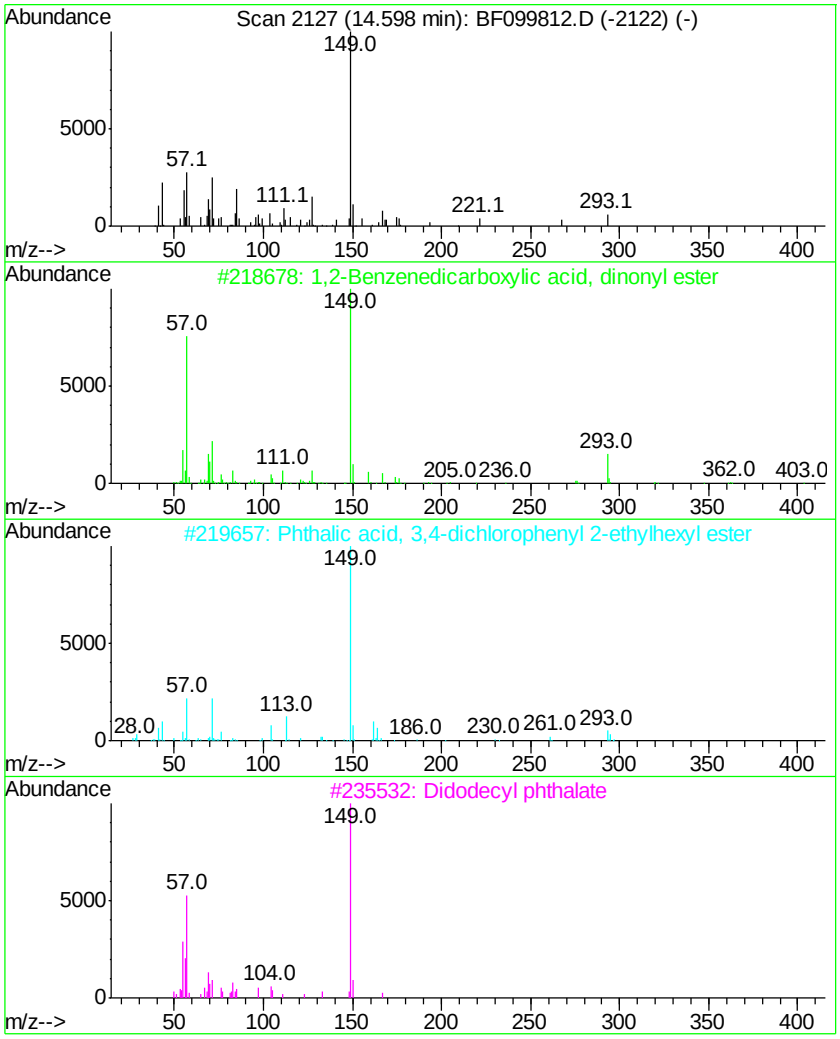
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

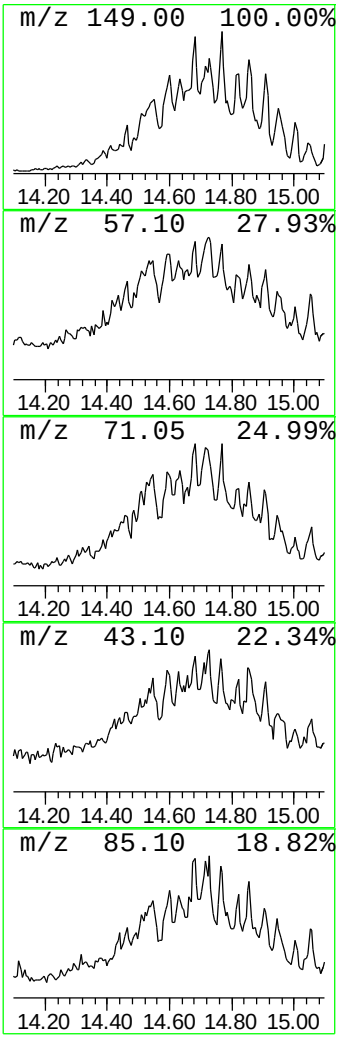
**********

Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.60 | 2.01 ng | 64672 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzenedicarboxylic acid, di... | 418 | C26H42O4 | 000084-76-4 | 59 |
| 2 | Phthalic acid, 3,4-dichlorophenyl... | 422 | C22H24Cl2O4 | 1000315-52-0 | 53 |
| 3 | Didodecyl phthalate | 502 | C32H54O4 | 002432-90-8 | 50 |
| 4 | Phthalic acid, 4-chloro-3-methyl... | 402 | C23H27ClO4 | 1000315-72-1 | 50 |
| 5 | Phthalic acid, hept-3-yl nonyl e... | 390 | C24H38O4 | 1000356-99-3 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102517\
Data File : BF099812.D
Acq On : 25 Oct 2017 14:42
Operator : SJ/JU
Sample : I6064-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 72-11935-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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 |
| Heptane | 2.30 | 16.0 | ng | 358973 | 1 | 6.79 | 448057 | 20.0 |
| 2-Pentanone, 4-hy... | 5.00 | 12.0 | ng | 268555 | 1 | 6.79 | 448057 | 20.0 |
| unknown6.56 | 6.56 | 77.6 | ng | 1738900 | 1 | 6.79 | 448057 | 20.0 |
| 2-Hydroxy-iso-but... | 8.63 | 3.0 | ng | 96851 | 2 | 8.07 | 640831 | 20.0 |
| Benzophenone | 10.55 | 11.2 | ng | 419772 | 3 | 9.83 | 753211 | 20.0 |
| Heptadecyl triflu... | 13.80 | 2.9 | ng | 92549 | 5 | 13.98 | 642790 | 20.0 |
| 1,2-Benzenedicarb... | 14.60 | 2.0 | ng | 64672 | 5 | 13.98 | 642790 | 20.0 |