LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

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-BF110817.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 | 2.187 | 14 | 17 | 27 | rVB3 | 23114 | 36723 | 1.48% | 0.160% |
| 2 | 3.987 | 316 | 323 | 327 | rVB | 28279 | 35587 | 1.43% | 0.155% |
| 3 | 4.493 | 406 | 409 | 417 | rBV | 77246 | 92193 | 3.71% | 0.403% |
| 4 | 5.110 | 510 | 514 | 524 | rBV | 429745 | 504148 | 20.27% | 2.202% |
| 5 | 5.504 | 576 | 581 | 584 | rBV | 2467221 | 2364462 | 95.07% | 10.327% |
| 6 | 6.510 | 746 | 752 | 762 | rBV | 2392864 | 2487118 | 100.00% | 10.863% |
| 7 | 6.651 | 771 | 776 | 780 | rBV | 2400729 | 2400889 | 96.53% | 10.486% |
| 8 | 6.887 | 812 | 816 | 819 | rVB | 928238 | 805519 | 32.39% | 3.518% |
| 9 | 7.039 | 838 | 842 | 846 | rVB | 2106154 | 1870944 | 75.23% | 8.171% |
| 10 | 7.445 | 906 | 911 | 914 | rBV | 1634161 | 1497905 | 60.23% | 6.542% |
| 11 | 8.163 | 1029 | 1033 | 1037 | rVB | 1107076 | 1035074 | 41.62% | 4.521% |
| 12 | 8.716 | 1121 | 1127 | 1131 | rBV | 203380 | 162776 | 6.54% | 0.711% |
| 13 | 9.239 | 1211 | 1216 | 1219 | rBV | 2834817 | 2486098 | 99.96% | 10.858% |
| 14 | 9.292 | 1222 | 1225 | 1228 | rBV | 61335 | 60747 | 2.44% | 0.265% |
| 15 | 9.628 | 1278 | 1282 | 1286 | rBV | 370488 | 292403 | 11.76% | 1.277% |
| 16 | 9.922 | 1327 | 1332 | 1335 | rBV | 1151753 | 1015861 | 40.84% | 4.437% |
| 17 | 10.627 | 1447 | 1452 | 1456 | rBV | 457351 | 415652 | 16.71% | 1.815% |
| 18 | 10.710 | 1459 | 1466 | 1469 | rBV | 1187667 | 1152304 | 46.33% | 5.033% |
| 19 | 10.827 | 1481 | 1486 | 1488 | rBV | 39749 | 43315 | 1.74% | 0.189% |
| 20 | 10.857 | 1488 | 1491 | 1493 | rVB | 47207 | 37641 | 1.51% | 0.164% |
| 21 | 11.404 | 1581 | 1584 | 1588 | rBV | 968925 | 836395 | 33.63% | 3.653% |
| 22 | 12.986 | 1849 | 1853 | 1857 | rBV | 1784946 | 1751865 | 70.44% | 7.651% |
| 23 | 13.874 | 2001 | 2004 | 2012 | rBV | 110355 | 129373 | 5.20% | 0.565% |
| 24 | 14.045 | 2029 | 2033 | 2036 | rBV | 864052 | 764066 | 30.72% | 3.337% |
| 25 | 14.810 | 2159 | 2163 | 2165 | rVB3 | 25593 | 27253 | 1.10% | 0.119% |
| 26 | 15.151 | 2218 | 2221 | 2226 | rVB2 | 27972 | 32261 | 1.30% | 0.141% |
| 27 | 15.521 | 2279 | 2284 | 2289 | rVB | 430802 | 557666 | 22.42% | 2.436% |

Sum of corrected areas: 22896238

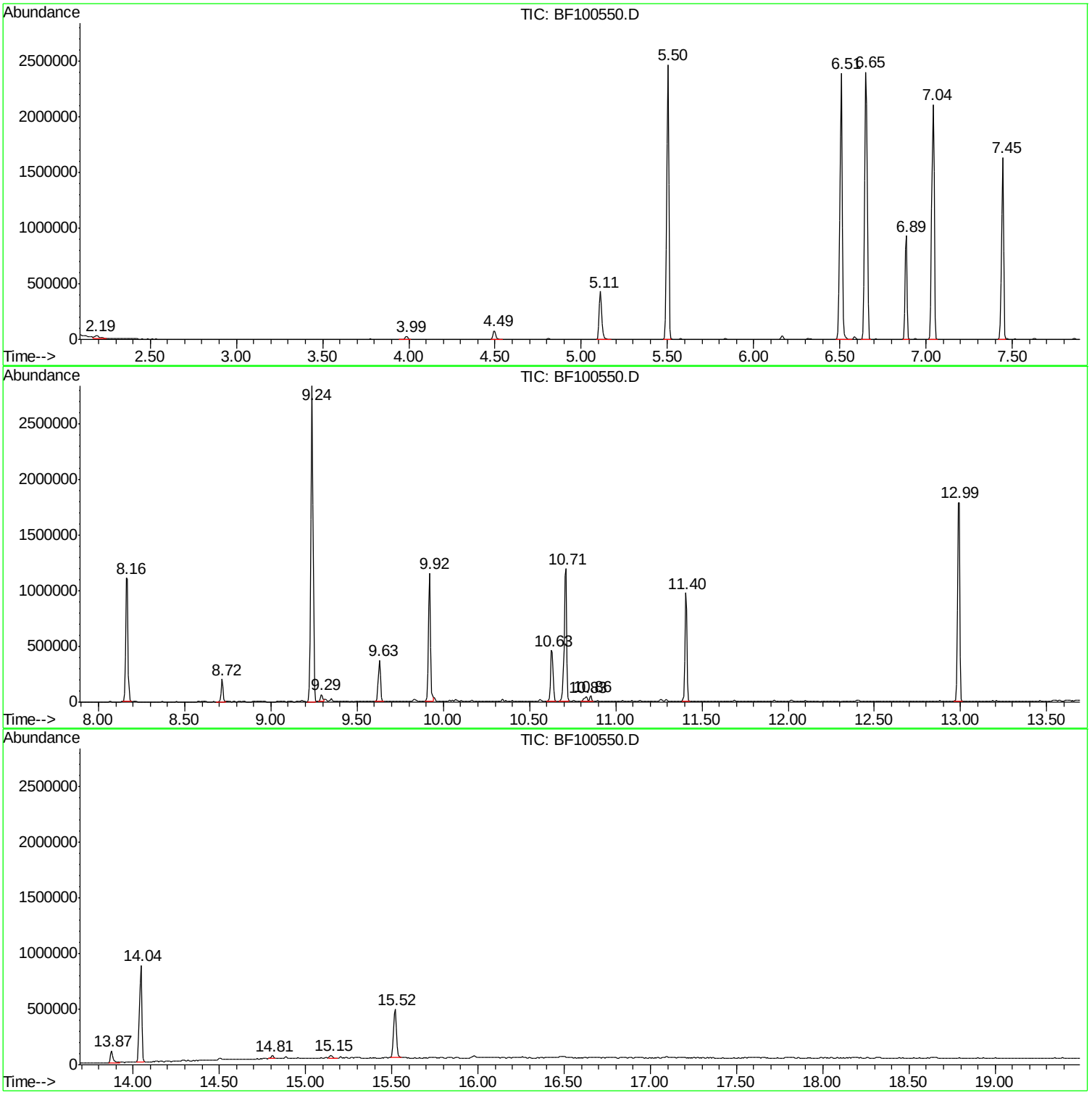
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

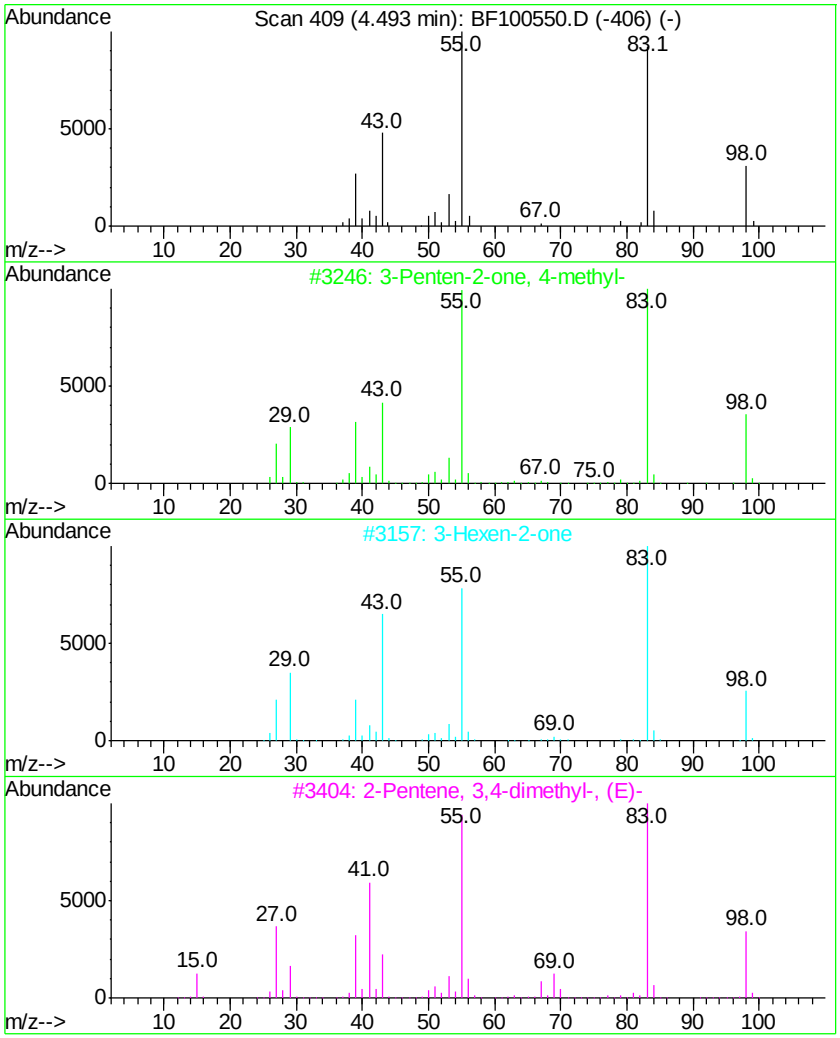
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

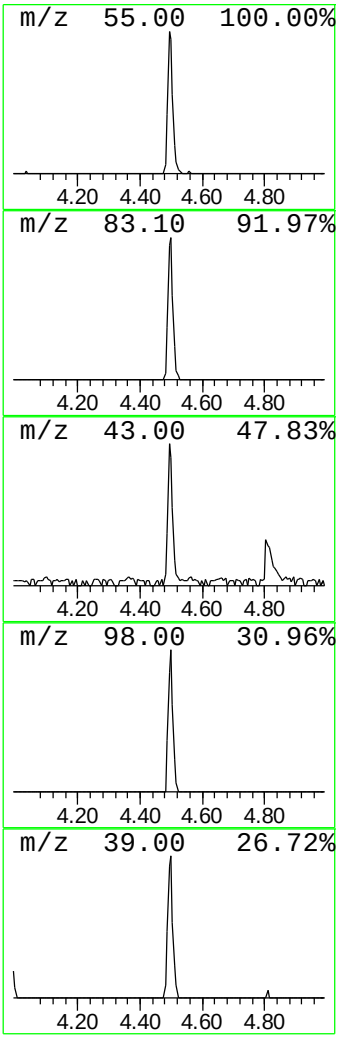
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.49 | 2.29 ng | 92193 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 87 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 86 |
| 4 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 83 |
| 5 | 2-Pentene, 3,4-dimethyl- | 98 | C7H14 | 024910-63-2 | 80 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

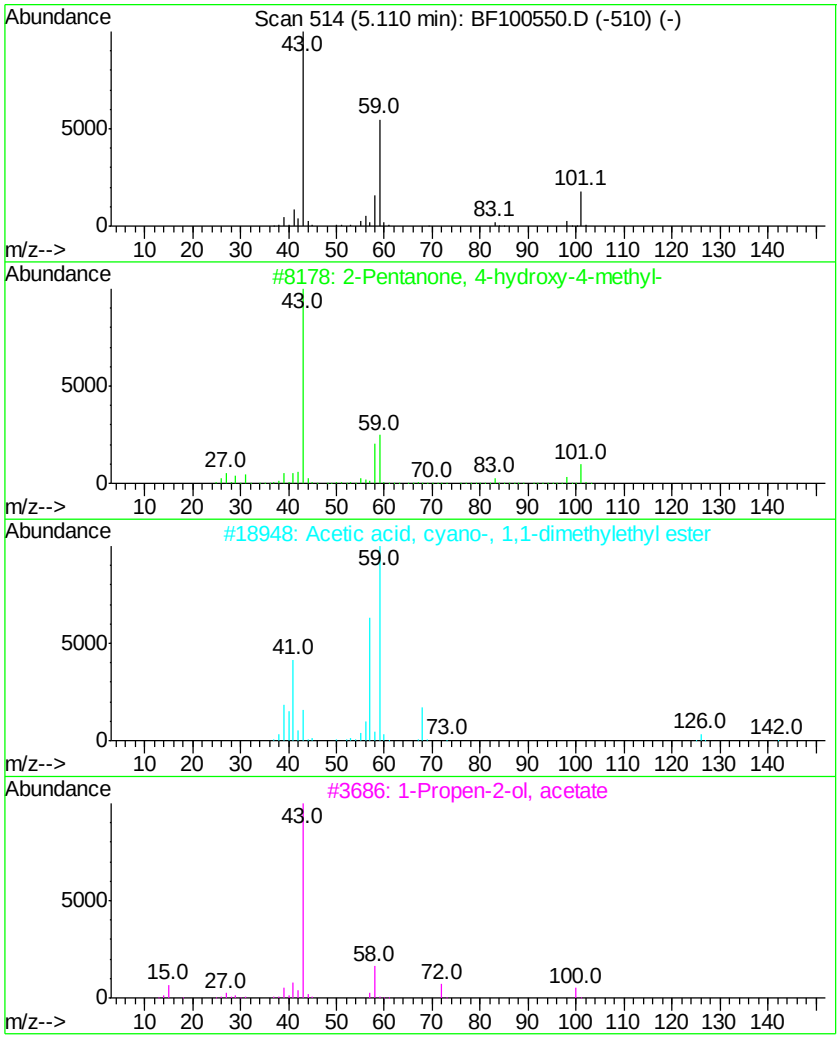
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

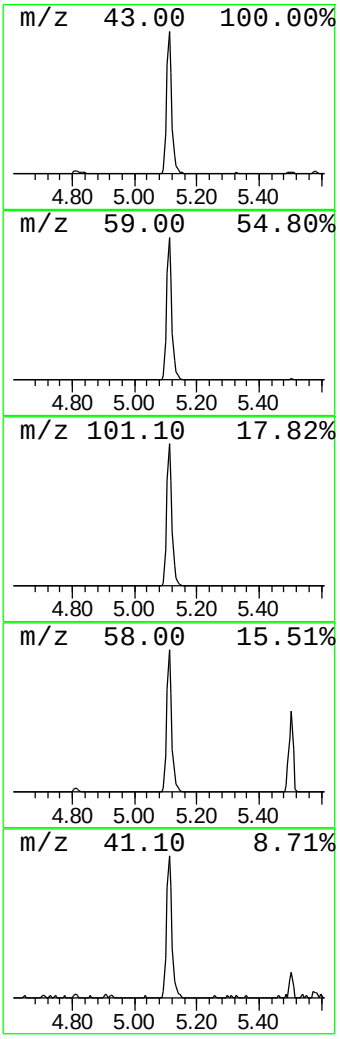
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 12.52 ng | 504148 | 1,4-Dichlorobenzene-d4 | 6.89 |

| 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, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 9 |



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

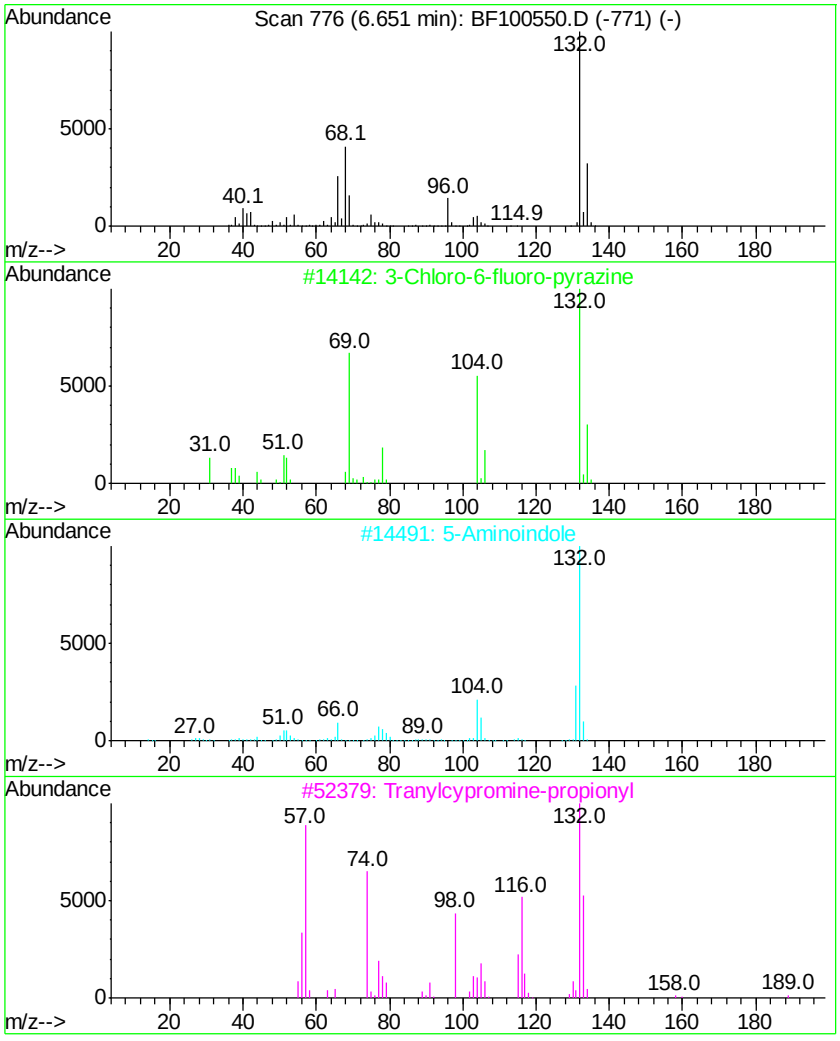
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

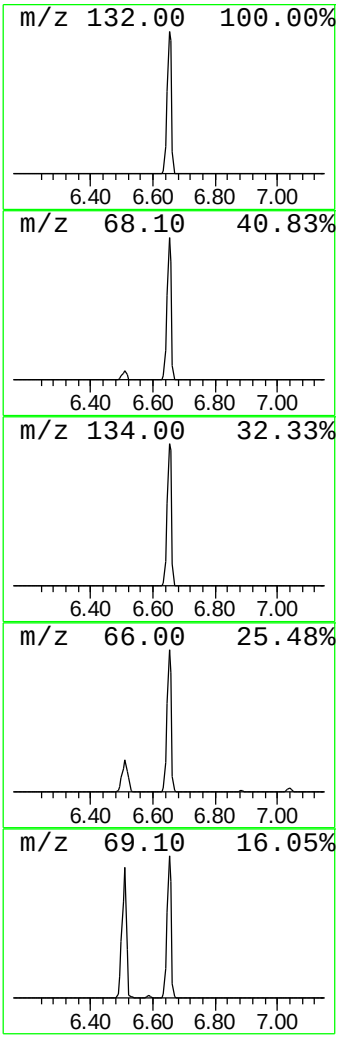
**********

Peak Number 3 unknown6.65 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.65 | 59.61 ng | 2400890 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

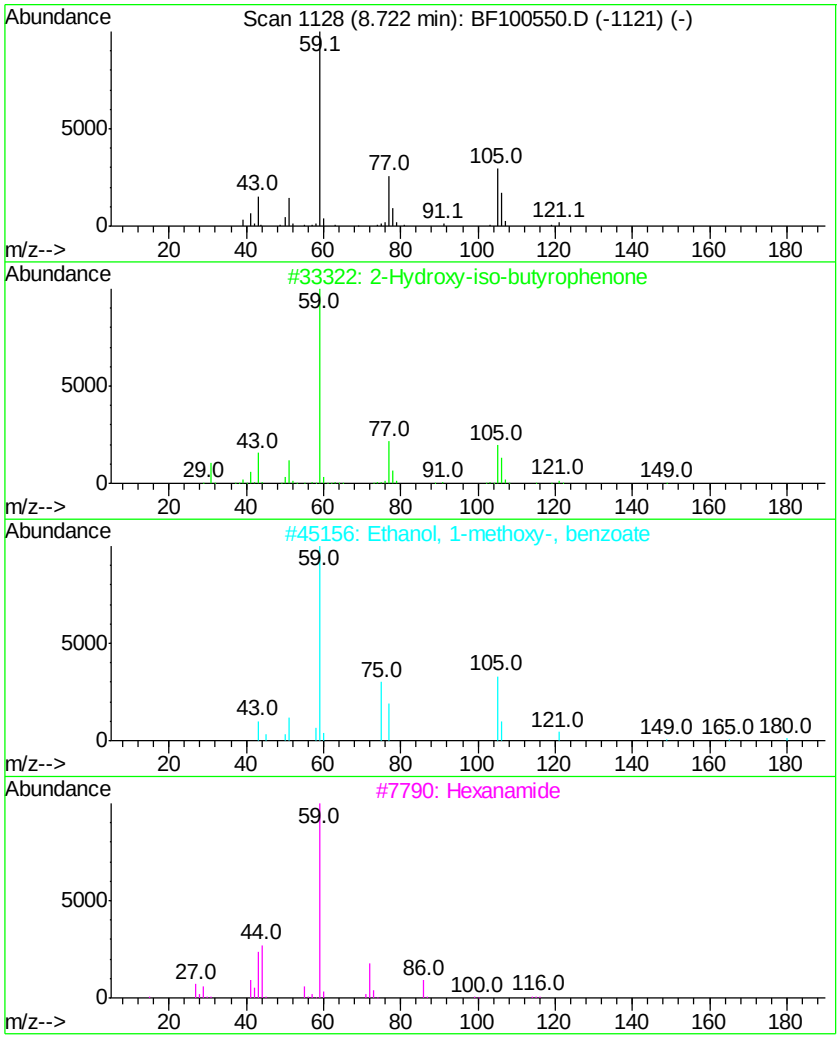
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

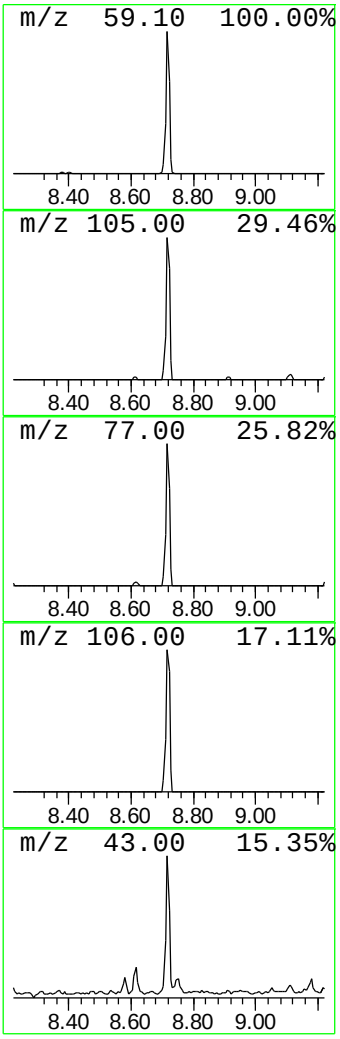
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.72 | 3.15 ng | 162776 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-iso-butyrophenone | 164 | C10H12O2 | 007473-98-5 | 90 |
| 2 | Ethanol, 1-methoxy-, benzoate | 180 | C10H12O3 | 051835-44-0 | 72 |
| 3 | Hexanamide | 115 | C6H13NO | 000628-02-4 | 9 |
| 4 | Propanoic acid, 2-hydroxy-2-meth... | 118 | C5H10O3 | 002110-78-3 | 9 |
| 5 | Propanoic acid, 2-hydroxy-2-meth... | 132 | C6H12O3 | 000080-55-7 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

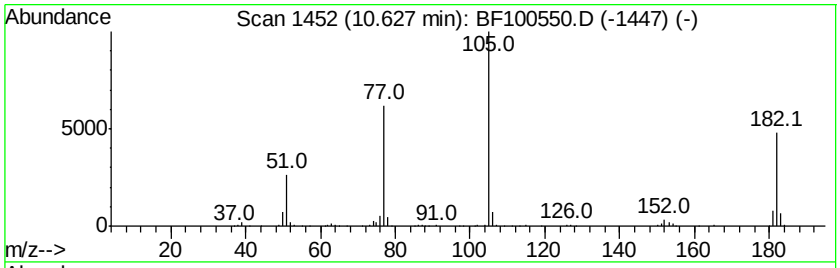
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

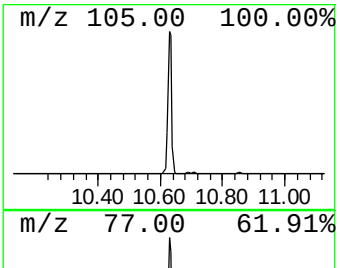
**********

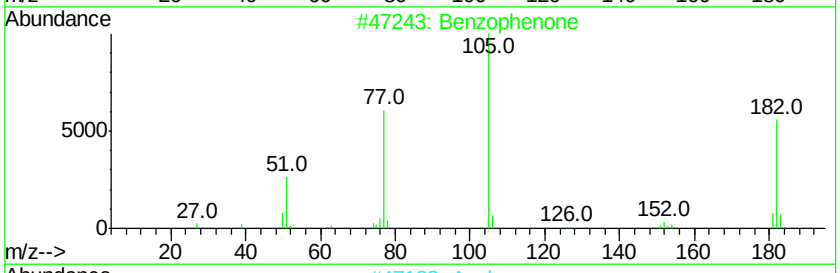
Peak Number 6 Benzophenone Concentration Rank 4

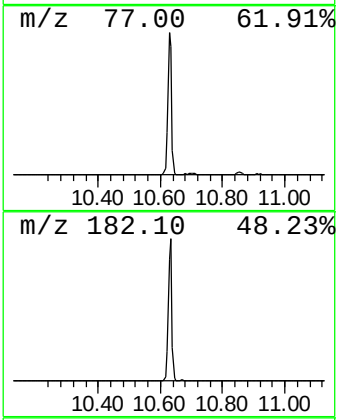
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.63 | 8.18 ng | 415652 | Acenaphthene-d10 | 9.92 |

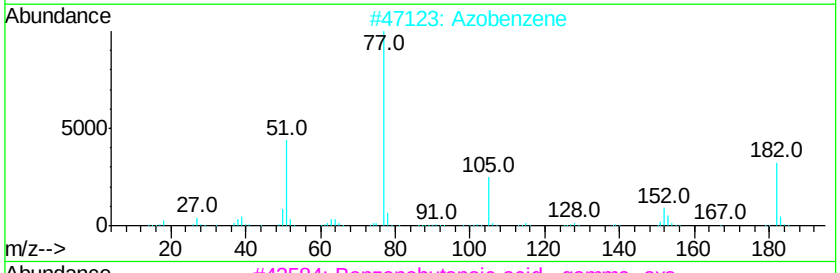
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 64 |
| 3 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 47 |
| 4 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 47 |
| 5 | Vinyl benzoate | 148 | C9H8O2 | 000769-78-8 | 47 |

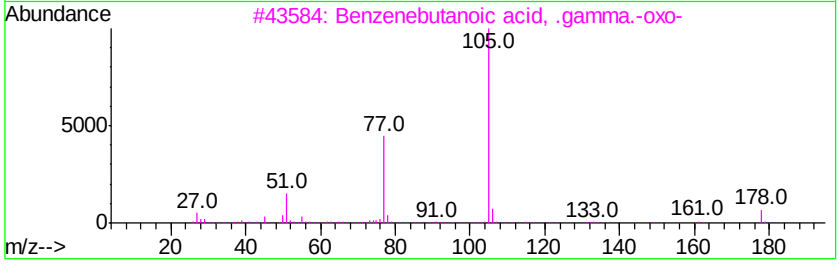


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Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

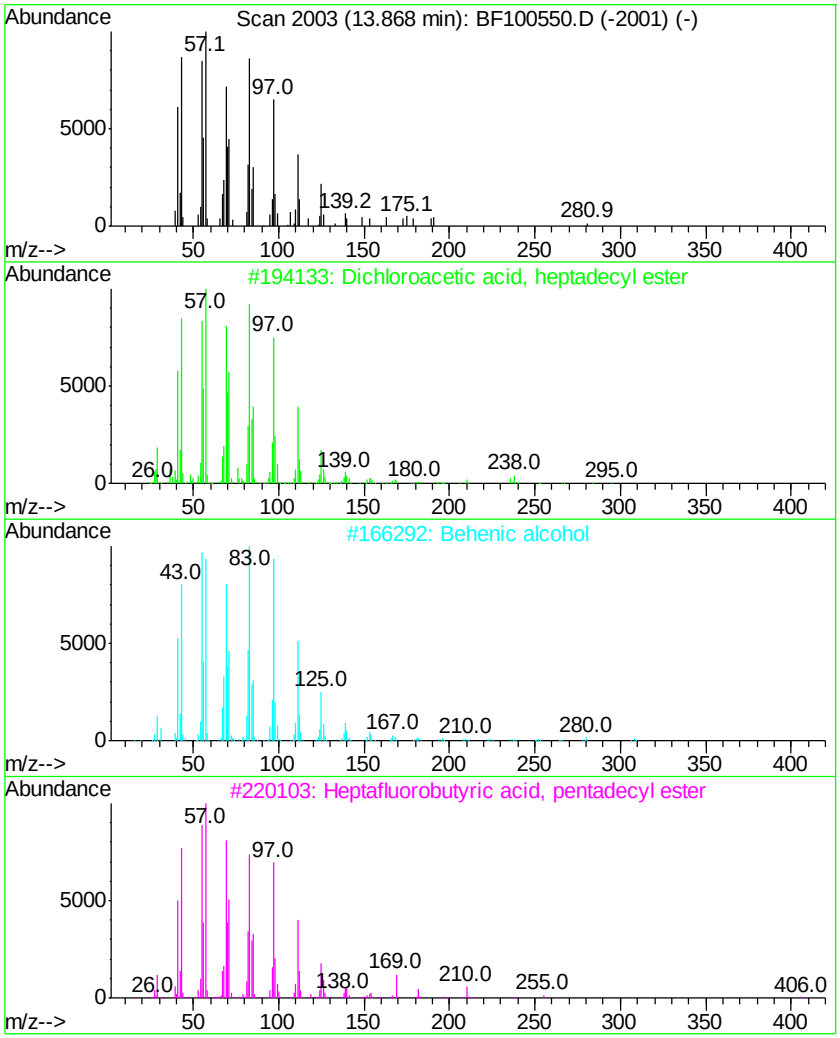
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

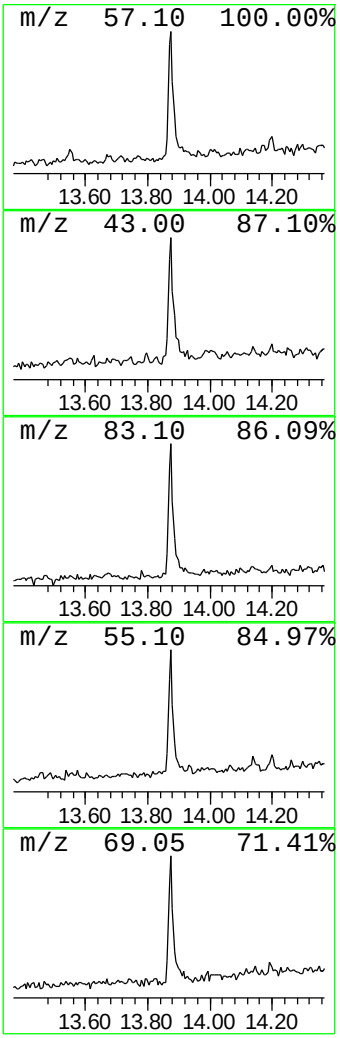
**********

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.87 | 3.39 ng | 129373 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 95 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 3 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 4 | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1 | 94 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF111417\
Data File : BF100550.D
Acq On : 14 Nov 2017 18:42
Operator : SJ/JU
Sample : I6388-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3N-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 |
| 3-Penten-2-one, 4... | 4.49 | 2.3 | ng | 92193 | 1 | 6.89 | 805519 | 20.0 |
| 2-Pentanone, 4-hy... | 5.11 | 12.5 | ng | 504148 | 1 | 6.89 | 805519 | 20.0 |
| unknown6.65 | 6.65 | 59.6 | ng | 2400890 | 1 | 6.89 | 805519 | 20.0 |
| 2-Hydroxy-iso-but... | 8.72 | 3.1 | ng | 162776 | 2 | 8.17 | 1035070 | 20.0 |
| Benzophenone | 10.63 | 8.2 | ng | 415652 | 3 | 9.92 | 1015860 | 20.0 |
| Dichloroacetic ac... | 13.87 | 3.4 | ng | 129373 | 5 | 14.04 | 764066 | 20.0 |