LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

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_M\METHODS\8270-BM050517.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 | 4.422 | 221 | 227 | 233 | rBV | 259332 | 365612 | 5.19% | 1.290% |
| 2 | 4.899 | 303 | 308 | 322 | rVB | 295549 | 427869 | 6.07% | 1.510% |
| 3 | 5.093 | 336 | 341 | 348 | rVB | 69850 | 103293 | 1.47% | 0.364% |
| 4 | 5.357 | 378 | 386 | 399 | rBV | 510921 | 794344 | 11.27% | 2.802% |
| 5 | 6.951 | 651 | 657 | 671 | rVB | 362715 | 609493 | 8.65% | 2.150% |
| 6 | 7.304 | 708 | 717 | 730 | rBV | 1016100 | 1613122 | 22.89% | 5.691% |
| 7 | 7.769 | 789 | 796 | 808 | rVB | 306259 | 512477 | 7.27% | 1.808% |
| 8 | 8.087 | 842 | 850 | 861 | rBV | 1333018 | 2176320 | 30.88% | 7.678% |
| 9 | 8.939 | 988 | 995 | 1007 | rBV | 1251058 | 2121460 | 30.10% | 7.484% |
| 10 | 10.563 | 1263 | 1271 | 1277 | rBV | 388472 | 670287 | 9.51% | 2.365% |
| 11 | 13.033 | 1684 | 1691 | 1700 | rBV | 2992527 | 4209003 | 59.72% | 14.849% |
| 12 | 13.886 | 1828 | 1836 | 1840 | rBV | 74510 | 114054 | 1.62% | 0.402% |
| 13 | 14.421 | 1919 | 1927 | 1936 | rBV2 | 558670 | 863208 | 12.25% | 3.045% |
| 14 | 15.357 | 2080 | 2086 | 2094 | rBV7 | 35223 | 82921 | 1.18% | 0.293% |
| 15 | 15.921 | 2176 | 2182 | 2194 | rBV2 | 1453935 | 2260912 | 32.08% | 7.976% |
| 16 | 16.462 | 2266 | 2274 | 2282 | rBV | 99561 | 154085 | 2.19% | 0.544% |
| 17 | 17.180 | 2390 | 2396 | 2403 | rBV | 739245 | 1084127 | 15.38% | 3.825% |
| 18 | 17.545 | 2453 | 2458 | 2463 | rBV4 | 70944 | 105205 | 1.49% | 0.371% |
| 19 | 18.915 | 2686 | 2691 | 2698 | rBV | 177724 | 253845 | 3.60% | 0.896% |
| 20 | 19.268 | 2746 | 2751 | 2760 | rBV6 | 53149 | 79384 | 1.13% | 0.280% |
| 21 | 19.803 | 2836 | 2842 | 2849 | rBV | 6133961 | 7047653 | 100.00% | 24.864% |
| 22 | 21.050 | 3051 | 3054 | 3061 | rBV8 | 51501 | 83329 | 1.18% | 0.294% |
| 23 | 21.368 | 3103 | 3108 | 3113 | rBV | 1077553 | 1391214 | 19.74% | 4.908% |
| 24 | 23.662 | 3492 | 3498 | 3507 | rVB2 | 600022 | 1221563 | 17.33% | 4.310% |

Sum of corrected areas: 28344780

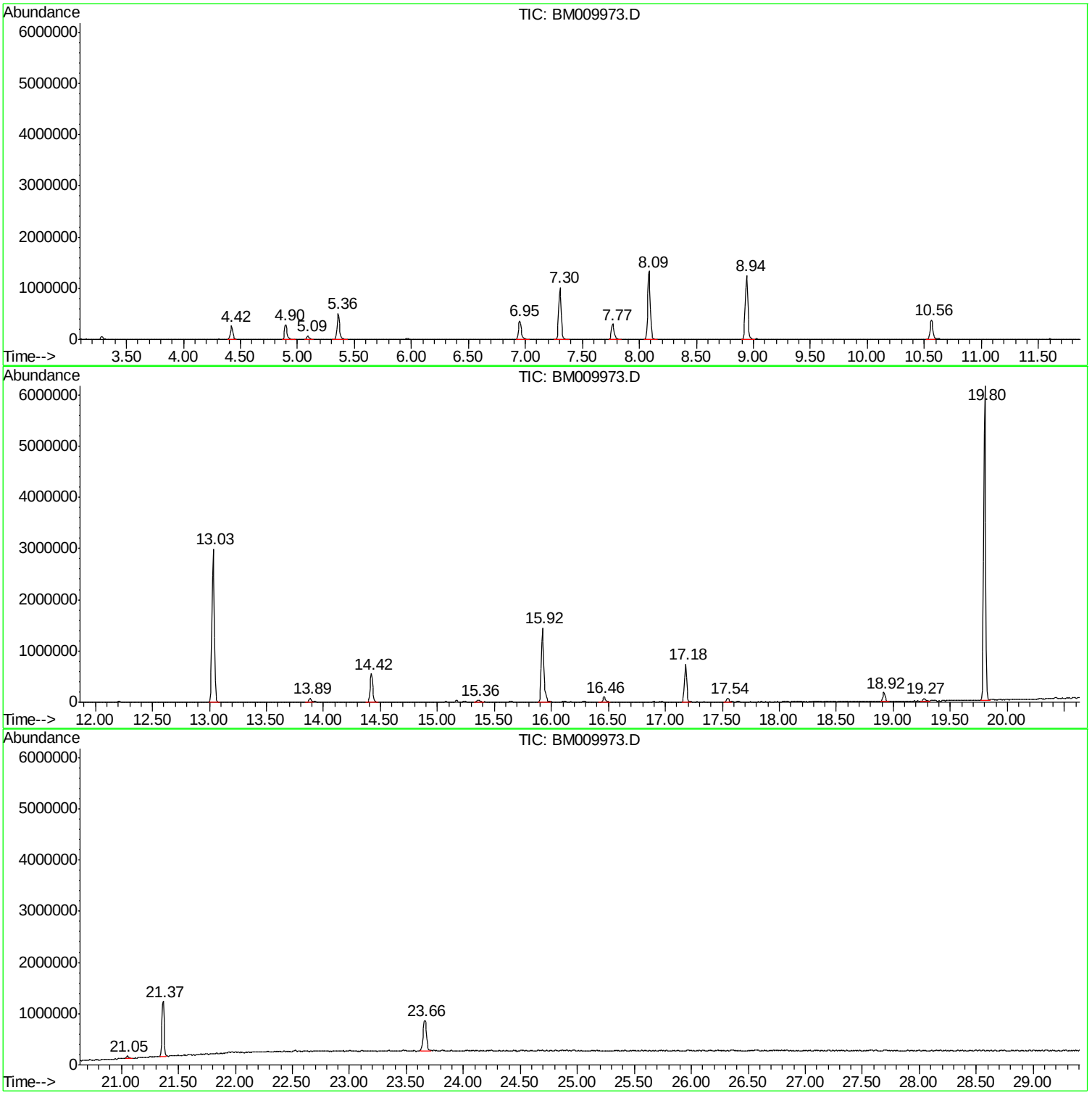
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

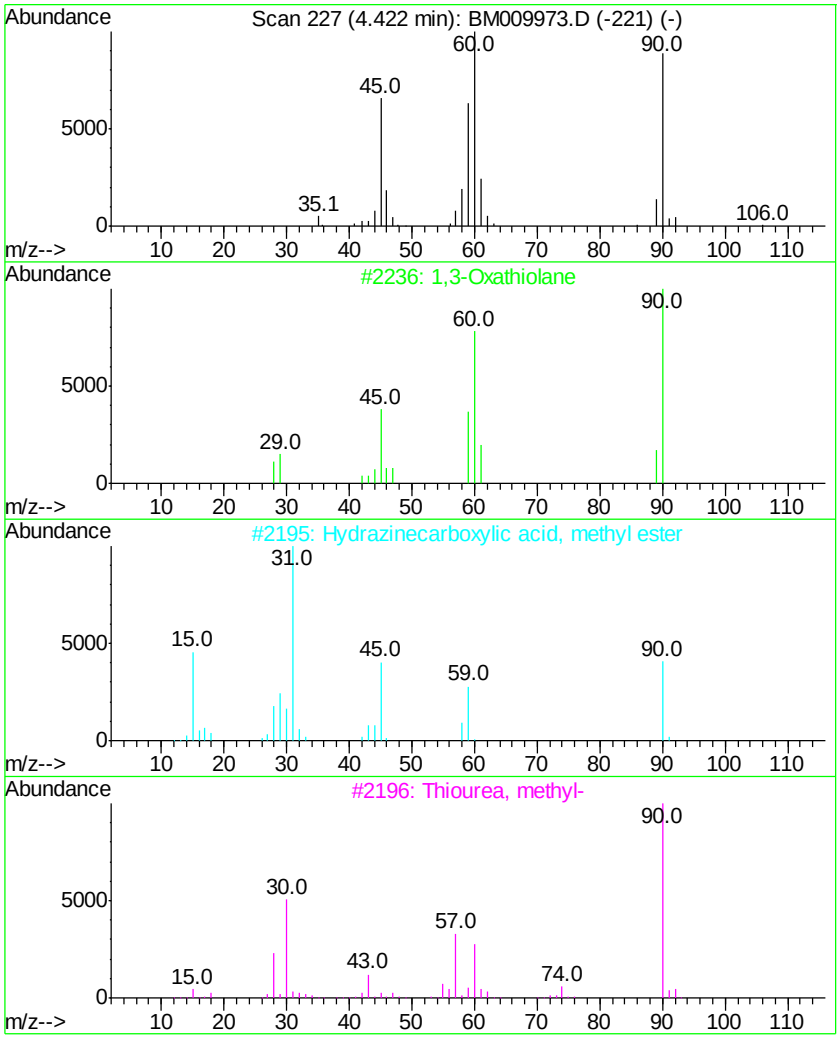
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

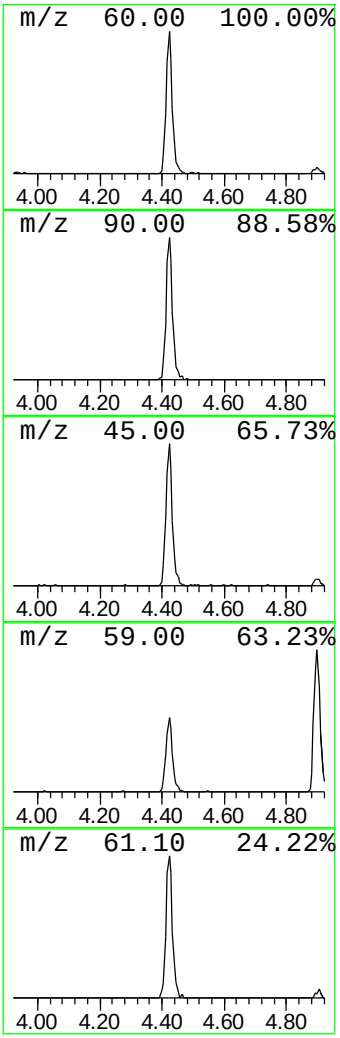
**********

Peak Number 1 1,3-Oxathiolane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.42 | 14.27 ng | 365612 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Oxathiolane | 90 | C3H6OS | 002094-97-5 | 59 |
| 2 | Hydrazinecarboxylic acid, methyl... | 90 | C2H6N2O2 | 006294-89-9 | 59 |
| 3 | Thiourea, methyl- | 90 | C2H6N2S | 000598-52-7 | 50 |
| 4 | 3-Thietanol | 90 | C3H6OS | 010304-16-2 | 40 |
| 5 | Thiirane | 60 | C2H4S | 000420-12-2 | 18 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

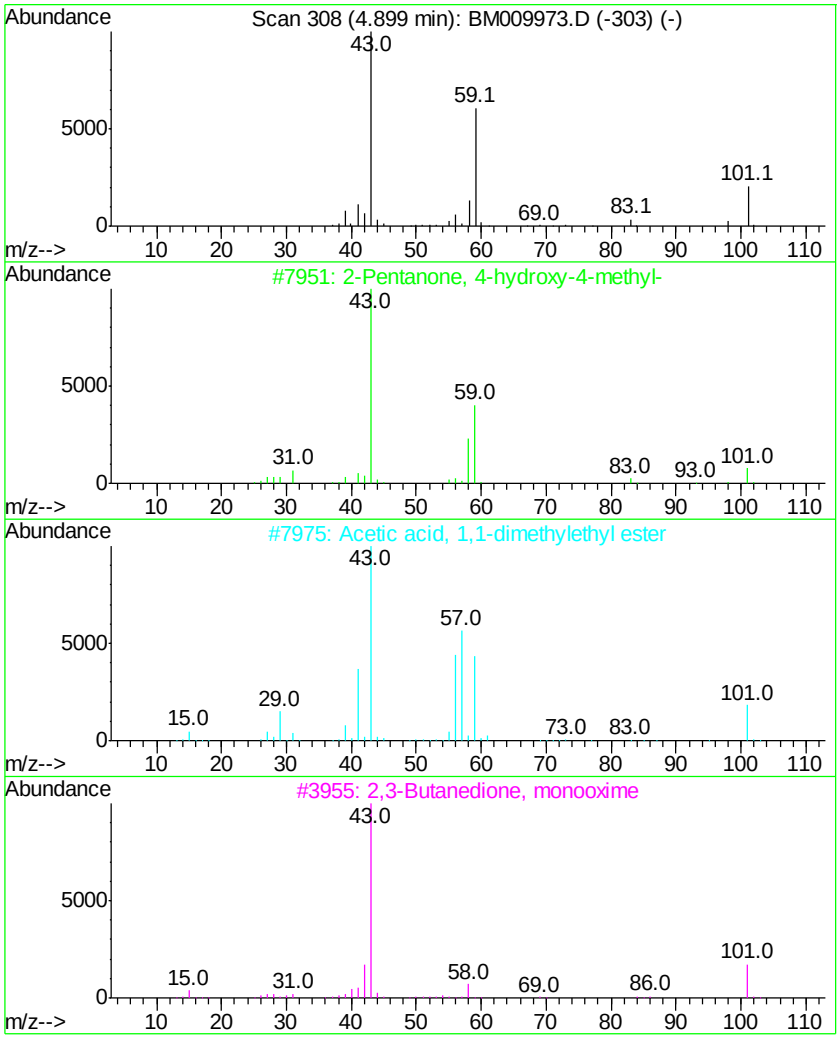
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

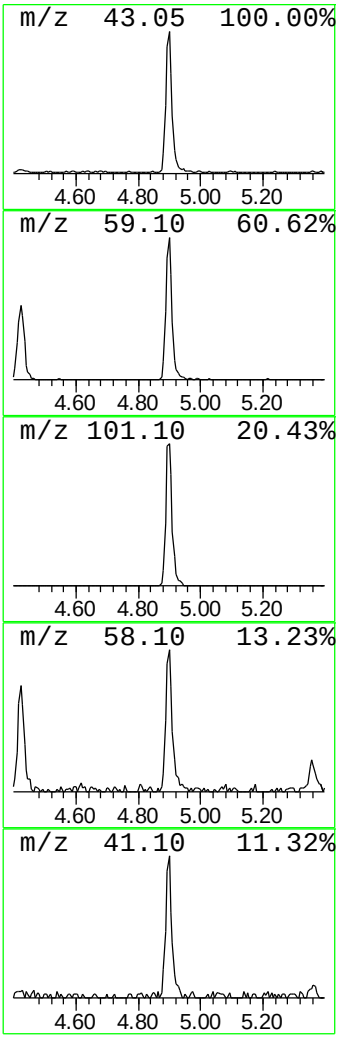
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.90 | 16.70 ng | 427869 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 32 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 25 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

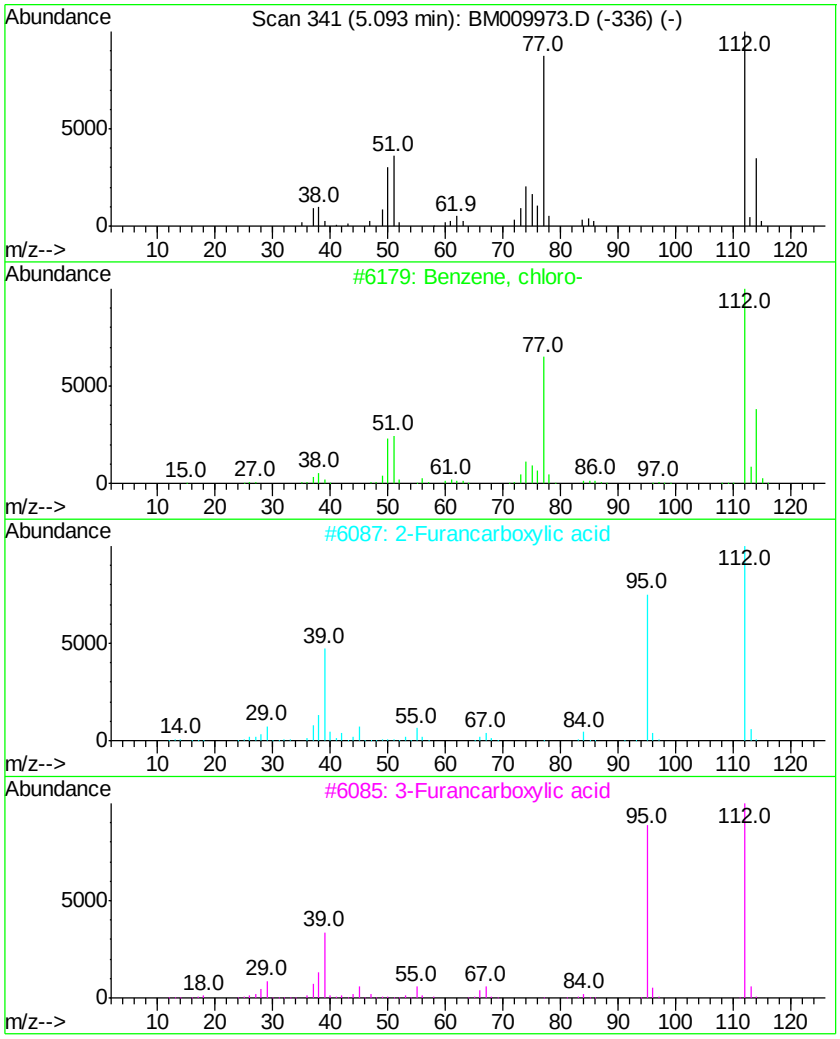
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

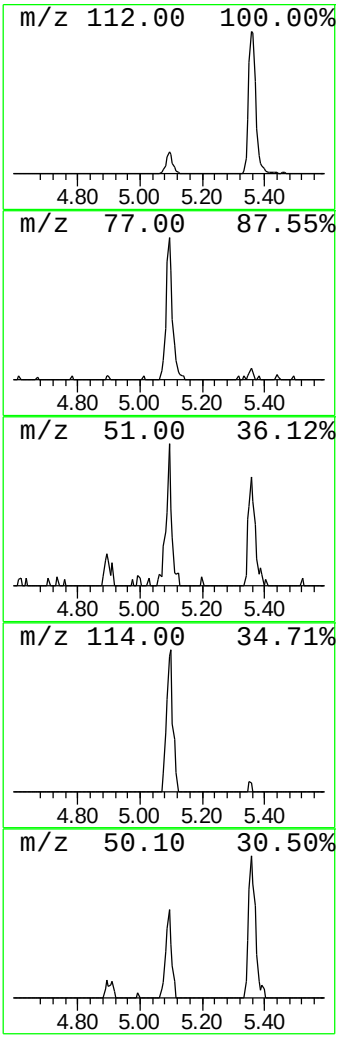
**********

Peak Number 3 Benzene, chloro- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 4.03 ng | 103293 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, chloro- | 112 | C6H5Cl | 000108-90-7 | 94 |
| 2 | 2-Furancarboxylic acid | 112 | C5H4O3 | 000088-14-2 | 27 |
| 3 | 3-Furancarboxylic acid | 112 | C5H4O3 | 000488-93-7 | 27 |
| 4 | Benzo-1,2,3-triazin-4(3H)-one, 3... | 162 | C7H6N4O | 041225-81-4 | 16 |
| 5 | Cevane-3,4,6,7,14,15,16,20-octol... | 793 | C41H63NO14 | 000143-57-7 | 10 |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

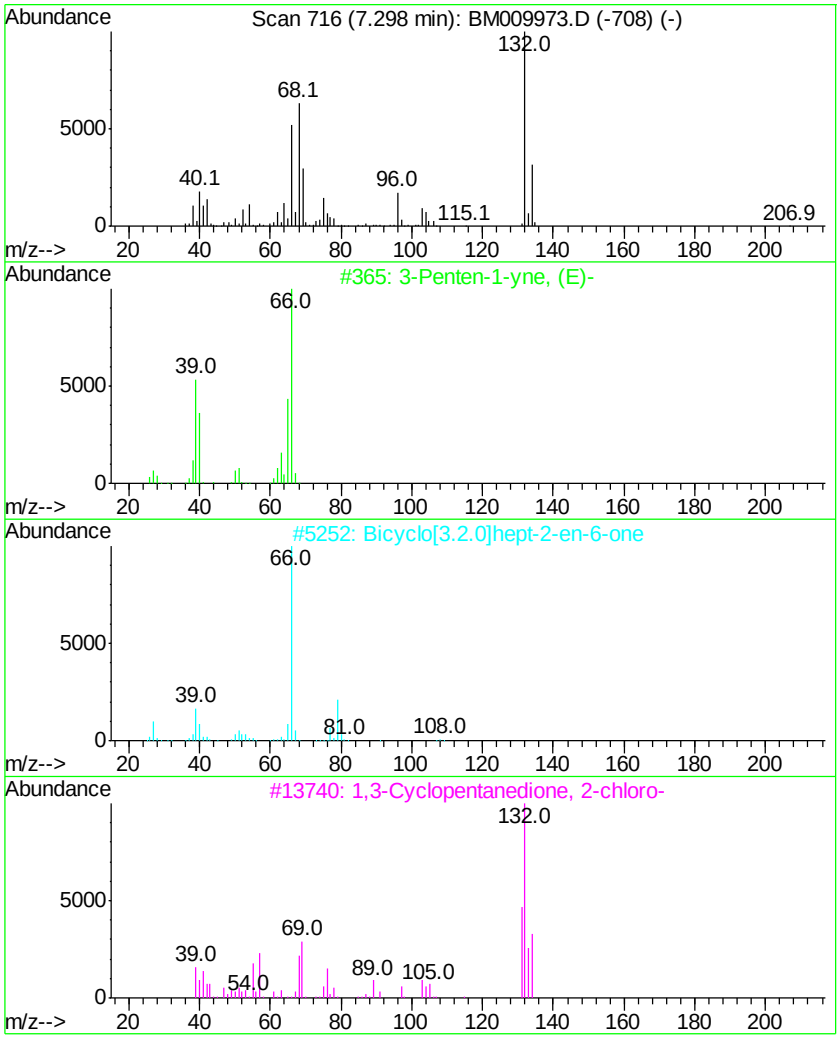
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

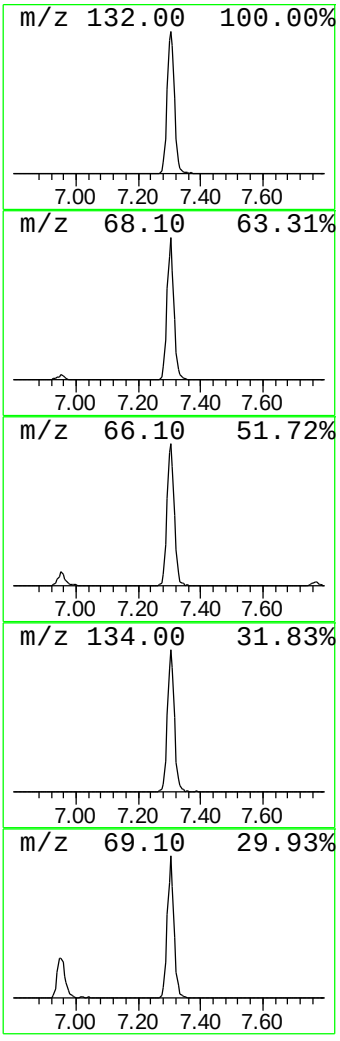
**********

Peak Number 4 unknown7.30 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.30 | 62.95 ng | 1613120 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-1-yne, (E)- | 66 | C5H6 | 002004-69-5 | 35 |
| 2 | Bicyclo[3.2.0]hept-2-en-6-one | 108 | C7H8O | 013173-09-6 | 35 |
| 3 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 27 |
| 4 | Bicyclo[2.2.1]hept-5-en-2-ol | 110 | C7H10O | 013080-90-5 | 25 |
| 5 | Silane, bicyclo[2.2.1]hept-5-en-... | 226 | C7H9Cl3Si | 014319-64-3 | 25 |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

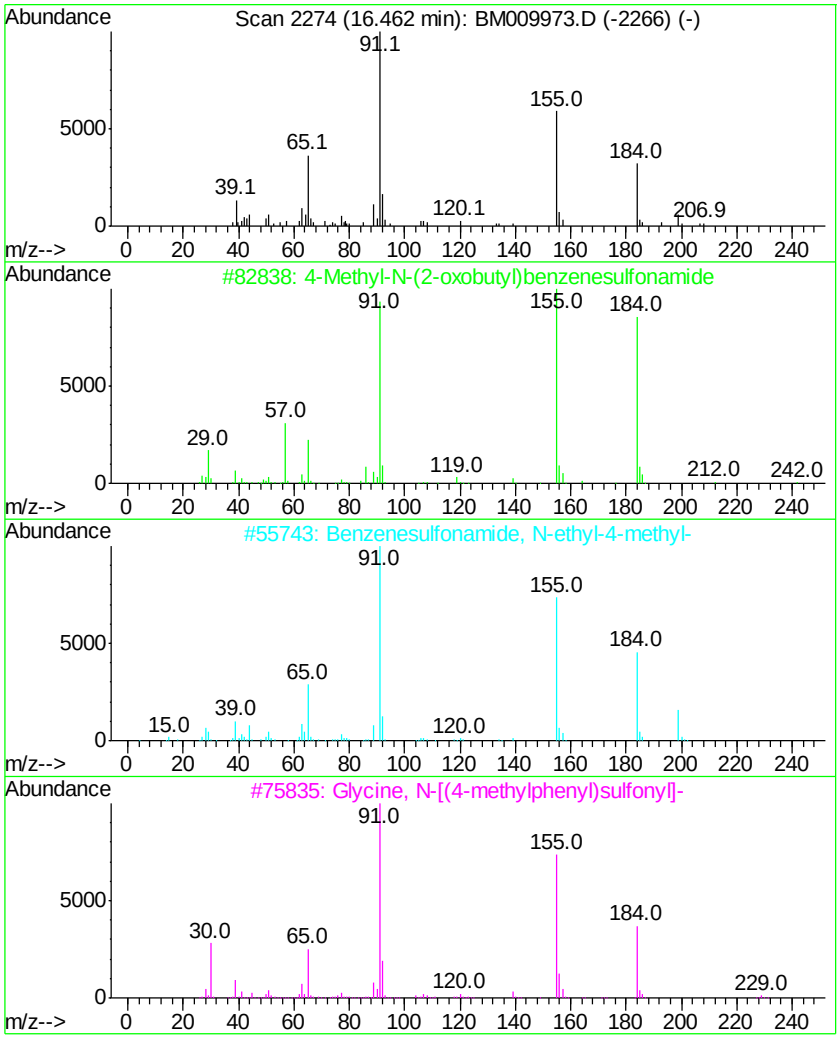
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

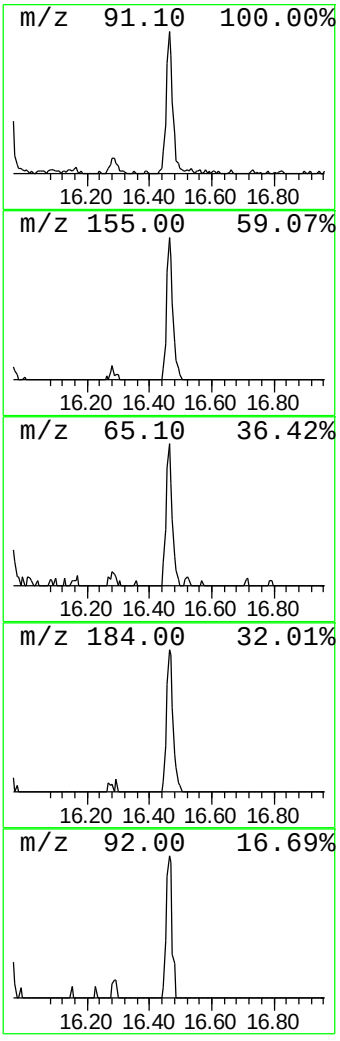
**********

Peak Number 6 4-Methyl-N-(2-oxobutyl)benz... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.46 | 2.84 ng | 154085 | Phenanthrene-d10 | 17.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Methyl-N-(2-oxobutyl)benzenesu... | 241 | C11H15NO3S | 1000192-14-5 | 83 |
| 2 | Benzenesulfonamide, N-ethyl-4-me... | 199 | C9H13NO2S | 000080-39-7 | 78 |
| 3 | Glycine, N-[(4-methylphenyl)sulf... | 229 | C9H11NO4S | 001080-44-0 | 64 |
| 4 | Benzene, 1-[(chloromethyl)sulfon... | 204 | C8H9ClO2S | 007569-26-8 | 59 |
| 5 | 4-Toluenesulfonylmethylisocyanide | 195 | C9H9NO2S | 036635-61-7 | 59 |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

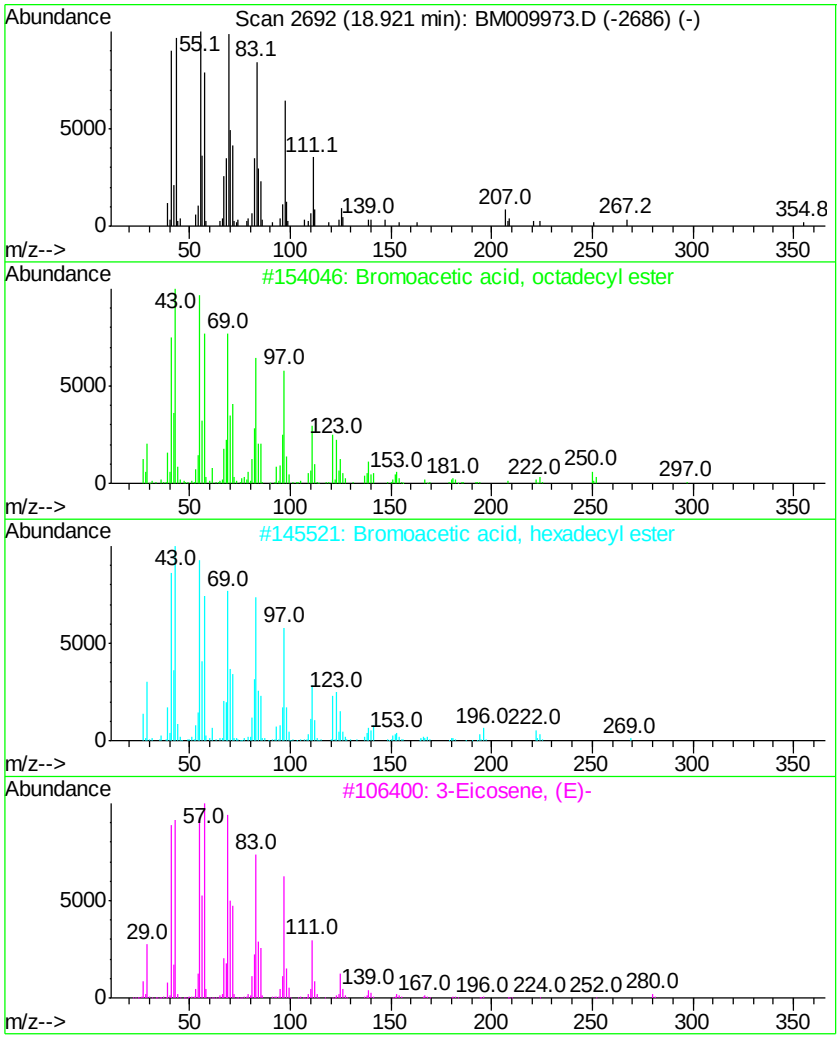
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

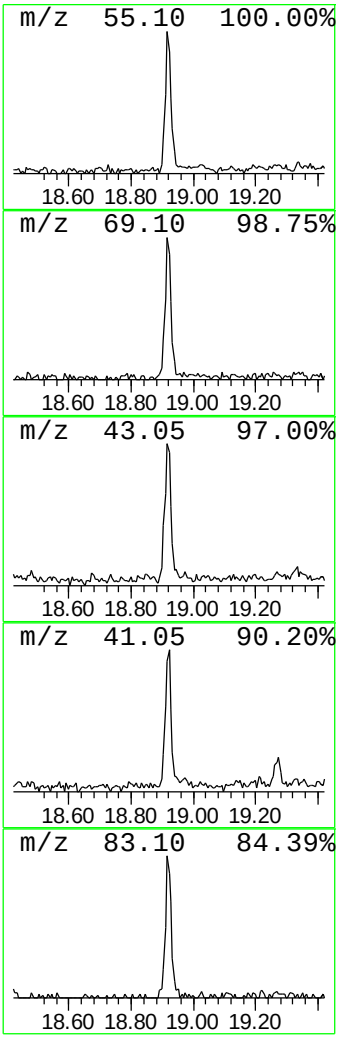
**********

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.92 | 4.68 ng | 253845 | Phenanthrene-d10 | 17.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bromoacetic acid, octadecyl ester | 390 | C20H39BrO2 | 018992-03-5 | 91 |
| 2 | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 91 |
| 3 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 83 |
| 4 | 1-Tetracosanol | 354 | C24H50O | 000506-51-4 | 76 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 74 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051017\
Data File : BM009973.D
Acq On : 10 May 2017 16:33
Operator : SJ/MA
Sample : I3058-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_M
**ClientSampleId :** LF001MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.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 |
| 1,3-Oxathiolane | 4.42 | 14.3 | ng | 365612 | 1 | 7.77 | 512477 | 20.0 |
| 2-Pentanone, 4-hy... | 4.90 | 16.7 | ng | 427869 | 1 | 7.77 | 512477 | 20.0 |
| Benzene, chloro- | 5.09 | 4.0 | ng | 103293 | 1 | 7.77 | 512477 | 20.0 |
| unknown7.30 | 7.30 | 63.0 | ng | 1613120 | 1 | 7.77 | 512477 | 20.0 |
| 4-Methyl-N-(2-oxo... | 16.46 | 2.8 | ng | 154085 | 4 | 17.18 | 1084130 | 20.0 |
| Bromoacetic acid,... | 18.92 | 4.7 | ng | 253845 | 4 | 17.18 | 1084130 | 20.0 |