LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

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_G\METHODS\8270-BG102516.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 | 2.978 | 18 | 24 | 44 | rVB | 8044158 | 27117561 | 100.00% | 20.992% |
| 2 | 3.131 | 44 | 50 | 67 | rVB | 8123490 | 17407351 | 64.19% | 13.475% |
| 3 | 3.278 | 67 | 75 | 100 | rVB | 6956731 | 20081453 | 74.05% | 15.545% |
| 4 | 3.537 | 113 | 119 | 125 | rBV2 | 227748 | 480472 | 1.77% | 0.372% |
| 5 | 3.601 | 125 | 130 | 141 | rVB2 | 251417 | 524791 | 1.94% | 0.406% |
| 6 | 5.329 | 417 | 424 | 435 | rBV | 631056 | 1090557 | 4.02% | 0.844% |
| 7 | 5.799 | 497 | 504 | 517 | rBV | 2851790 | 4876936 | 17.98% | 3.775% |
| 8 | 7.403 | 769 | 777 | 787 | rVB | 2973318 | 5394541 | 19.89% | 4.176% |
| 9 | 7.796 | 835 | 844 | 855 | rVB | 2840387 | 5132788 | 18.93% | 3.973% |
| 10 | 8.266 | 917 | 924 | 934 | rBV2 | 491232 | 863300 | 3.18% | 0.668% |
| 11 | 8.595 | 971 | 980 | 992 | rVB | 2118414 | 3841867 | 14.17% | 2.974% |
| 12 | 9.441 | 1115 | 1124 | 1133 | rBV | 1803226 | 3388676 | 12.50% | 2.623% |
| 13 | 11.092 | 1394 | 1405 | 1413 | rBV | 633842 | 1155606 | 4.26% | 0.895% |
| 14 | 13.507 | 1806 | 1816 | 1825 | rBV | 4609419 | 7575781 | 27.94% | 5.864% |
| 15 | 14.318 | 1948 | 1954 | 1962 | rBV | 972781 | 1445488 | 5.33% | 1.119% |
| 16 | 14.882 | 2043 | 2050 | 2058 | rBV | 1038209 | 1672114 | 6.17% | 1.294% |
| 17 | 16.369 | 2294 | 2303 | 2314 | rBV | 4212122 | 6818105 | 25.14% | 5.278% |
| 18 | 17.626 | 2510 | 2517 | 2526 | rBV | 1316240 | 2078203 | 7.66% | 1.609% |
| 19 | 18.472 | 2656 | 2661 | 2670 | rBV2 | 197369 | 307588 | 1.13% | 0.238% |
| 20 | 20.205 | 2949 | 2956 | 2962 | rBV | 8359593 | 11670362 | 43.04% | 9.034% |
| 21 | 21.498 | 3171 | 3176 | 3185 | rBV5 | 191638 | 367370 | 1.35% | 0.284% |
| 22 | 21.921 | 3241 | 3248 | 3255 | rBV | 1570733 | 2738064 | 10.10% | 2.120% |
| 23 | 23.642 | 3535 | 3541 | 3552 | rBV | 216741 | 434576 | 1.60% | 0.336% |
| 24 | 25.346 | 3819 | 3831 | 3843 | rVB3 | 867998 | 2717228 | 10.02% | 2.103% |

Sum of corrected areas: 129180778

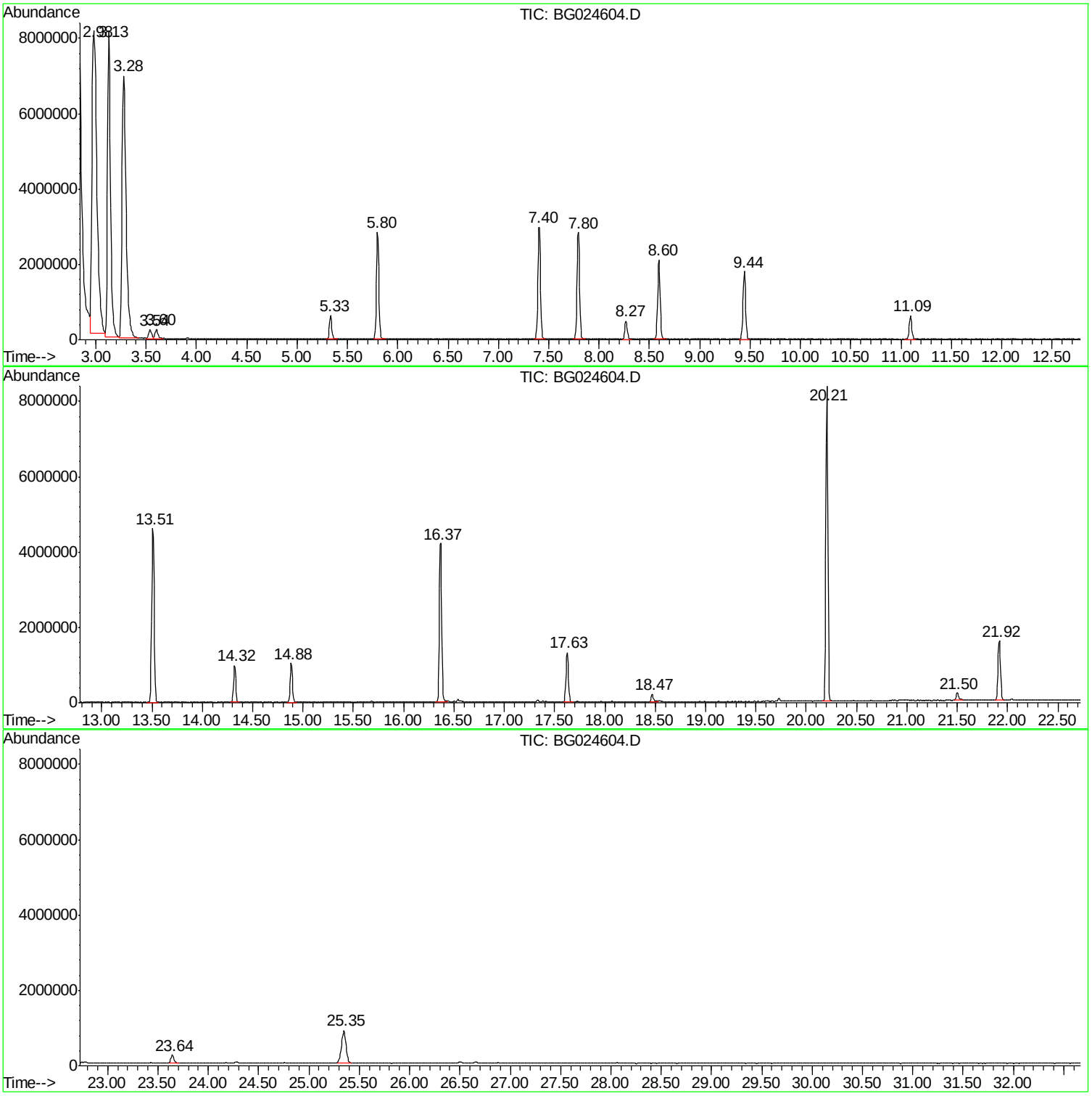
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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 G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

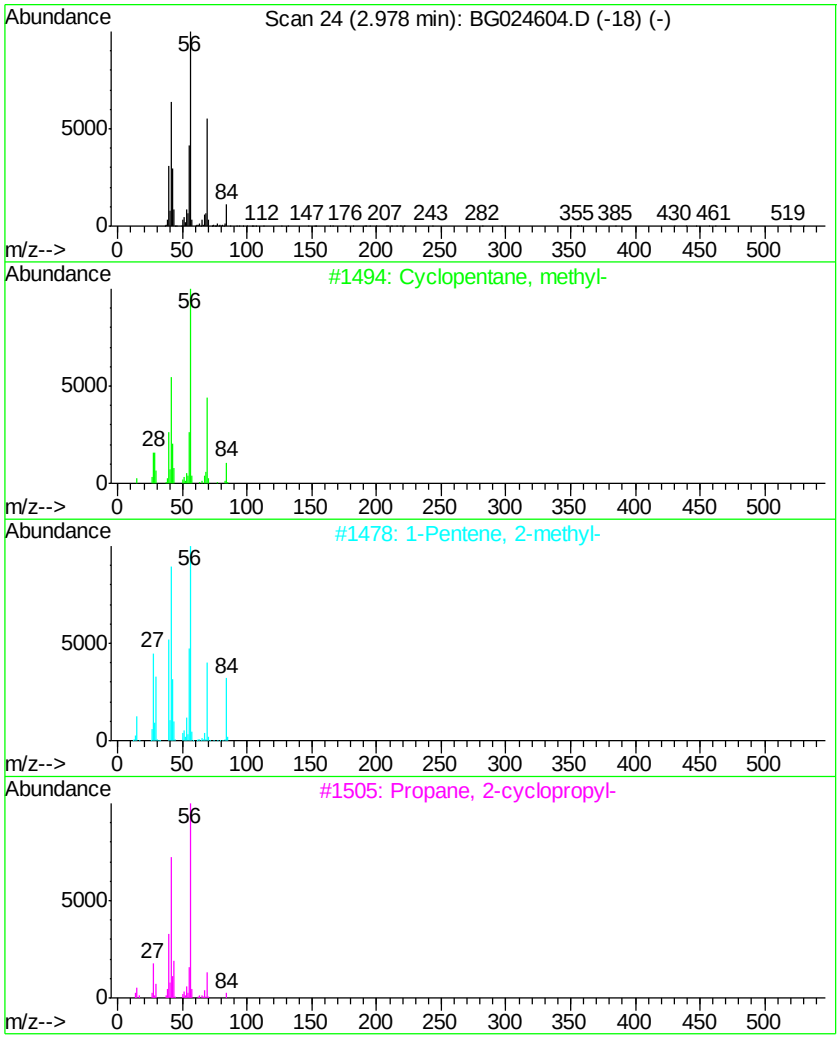
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

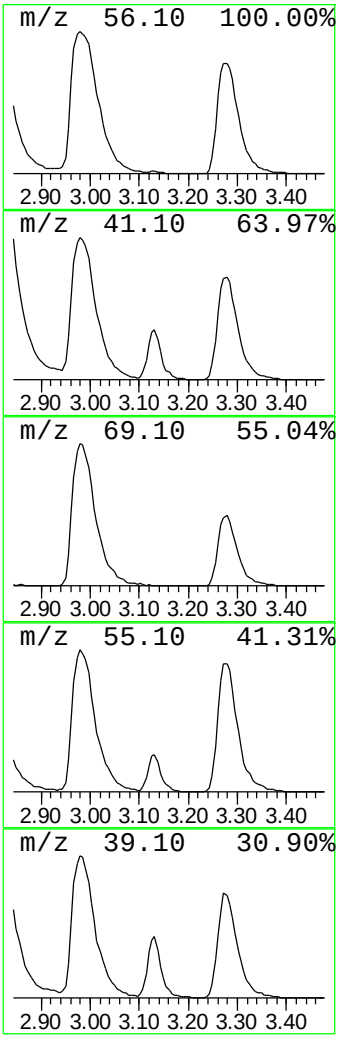
**********

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.98 | 628.23 ng | 27117600 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentane, methyl- | 84 | C6H12 | 000096-37-7 | 91 |
| 2 | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 64 |
| 3 | Propane, 2-cyclopropyl- | 84 | C6H12 | 003638-35-5 | 59 |
| 4 | 1-Hexene, 3,4-dimethyl- | 112 | C8H16 | 016745-94-1 | 59 |
| 5 | Cyclopropane, propyl- | 84 | C6H12 | 002415-72-7 | 56 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

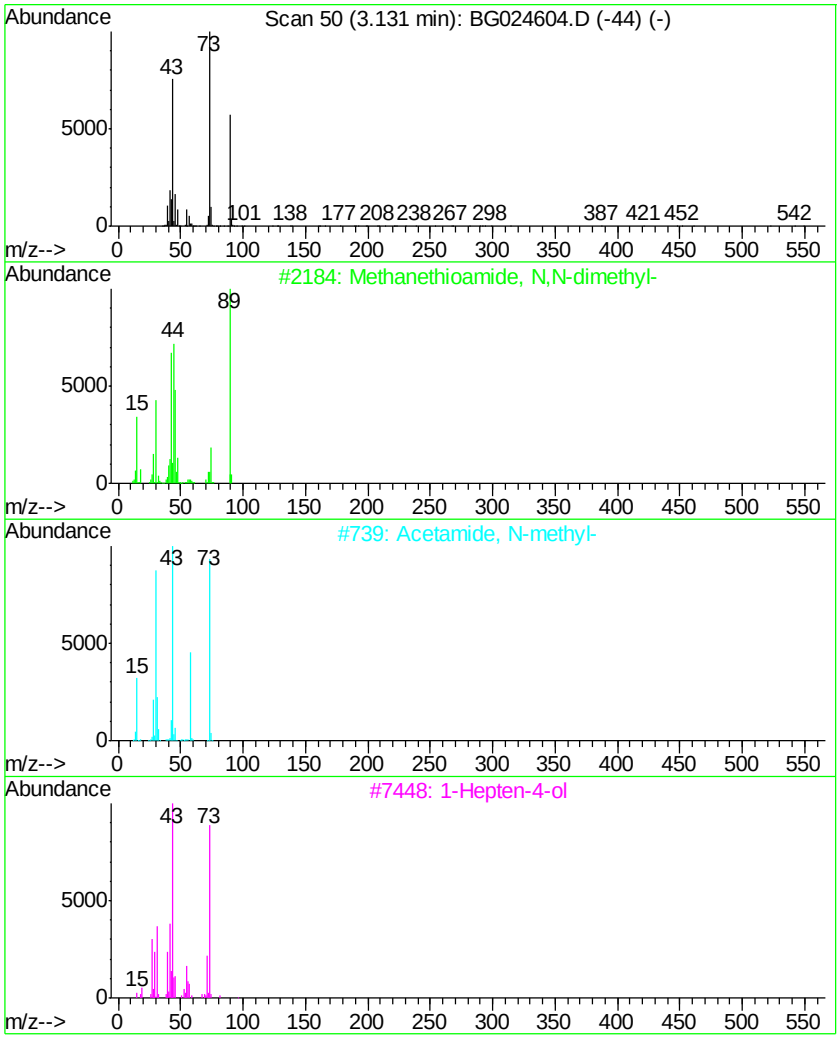
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

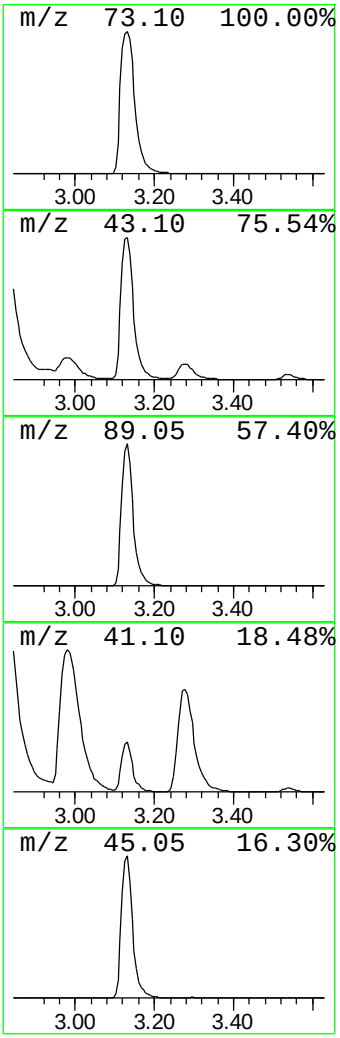
**********

Peak Number 2 unknown3.13 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.13 | 403.28 ng | 17407400 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methanethioamide, N,N-dimethyl- | 89 | C3H7NS | 000758-16-7 | 32 |
| 2 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 25 |
| 3 | 1-Hepten-4-ol | 114 | C7H14O | 003521-91-3 | 23 |
| 4 | Thiopropionamide | 89 | C3H7NS | 000631-58-3 | 9 |
| 5 | Thiazole, tetrahydro- | 89 | C3H7NS | 000504-78-9 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

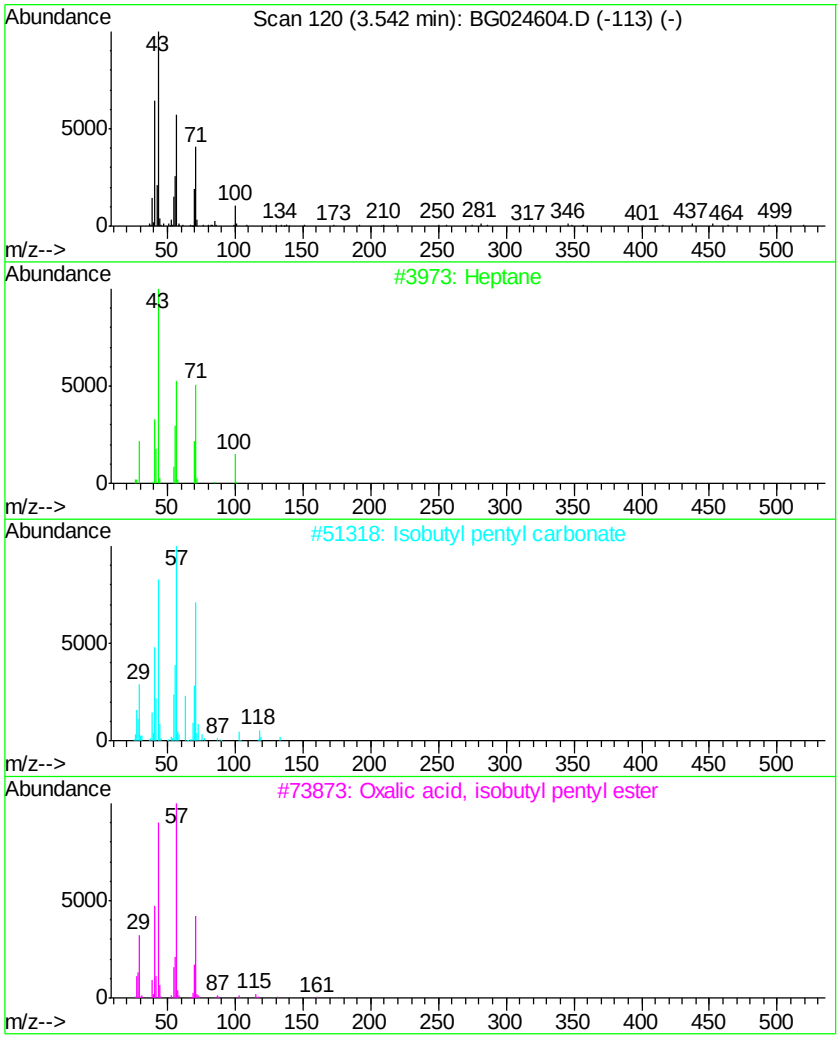
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

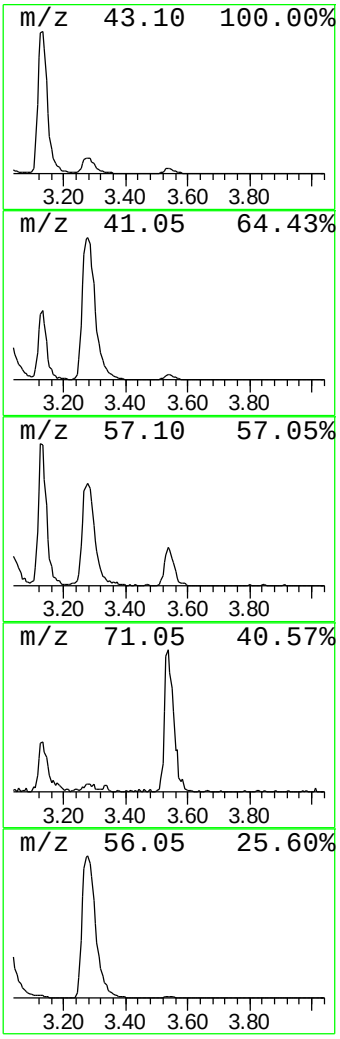
**********

Peak Number 4 Heptane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.54 | 11.13 ng | 480472 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane | 100 | C7H16 | 000142-82-5 | 87 |
| 2 | Isobutyl pentyl carbonate | 188 | C10H20O3 | 178442-32-5 | 45 |
| 3 | Oxalic acid, isobutyl pentyl ester | 216 | C11H20O4 | 1000309-37-0 | 40 |
| 4 | Hexane, 3-methyl- | 100 | C7H16 | 000589-34-4 | 38 |
| 5 | Pentane, 2,3,4-trimethyl- | 114 | C8H18 | 000565-75-3 | 28 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

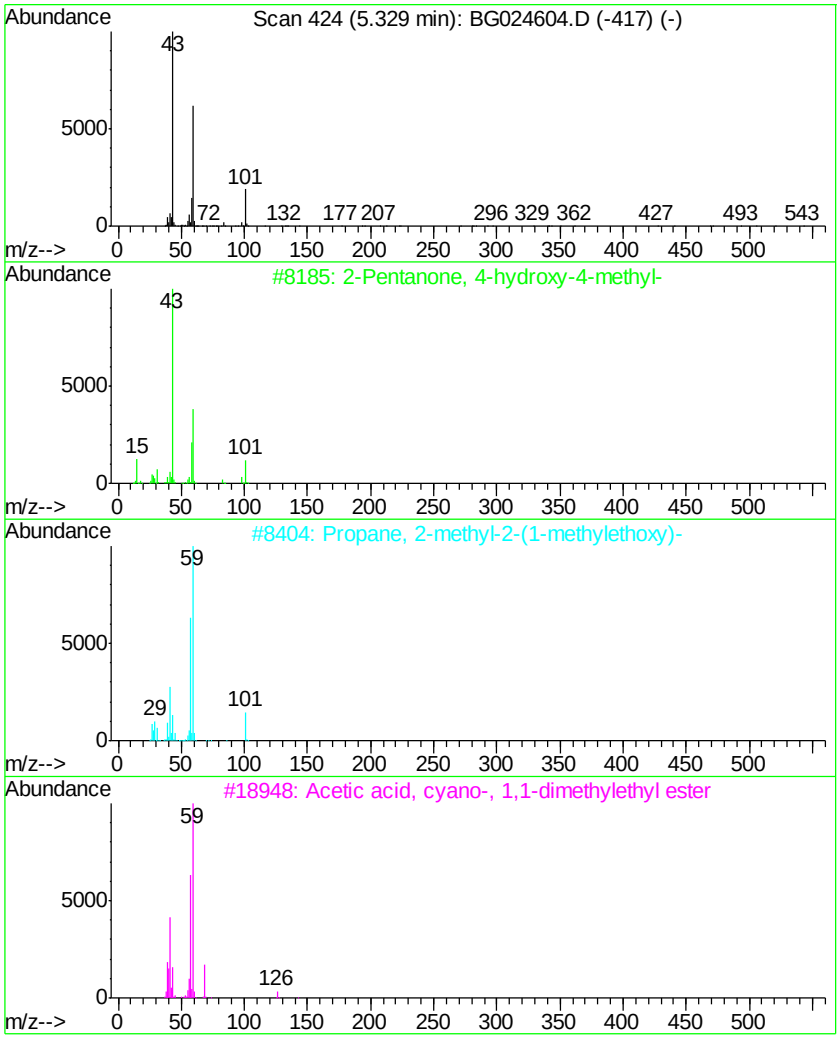
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

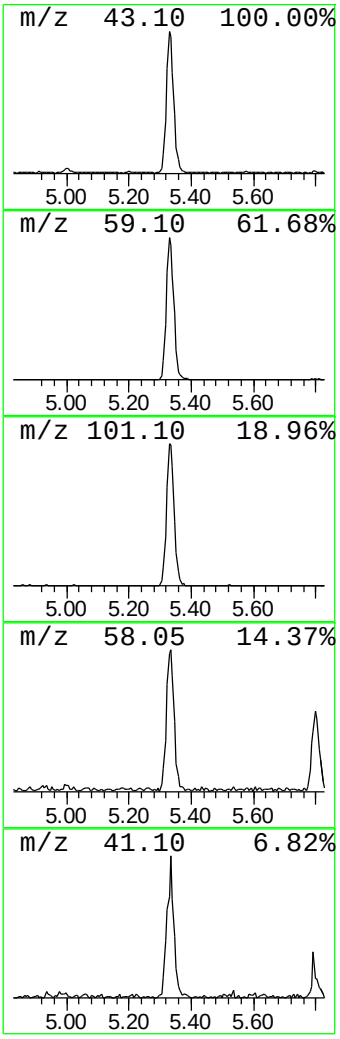
**********

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.33 | 25.26 ng | 1090560 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 37 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 28 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

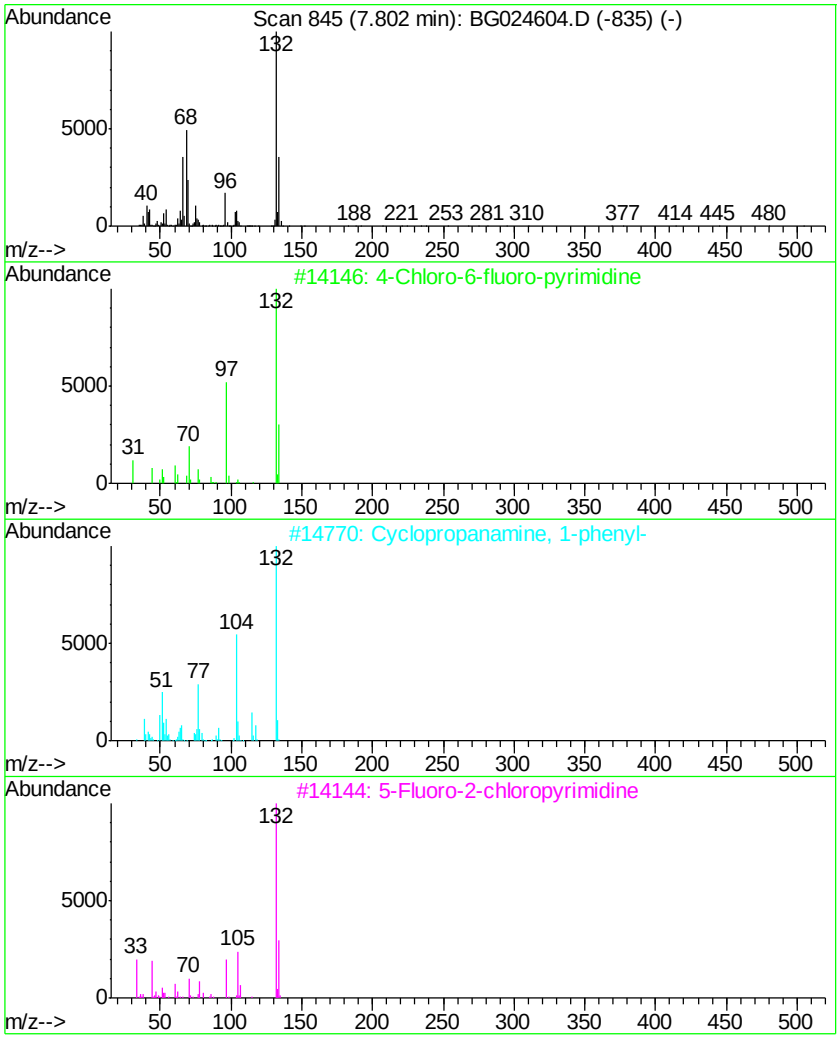
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

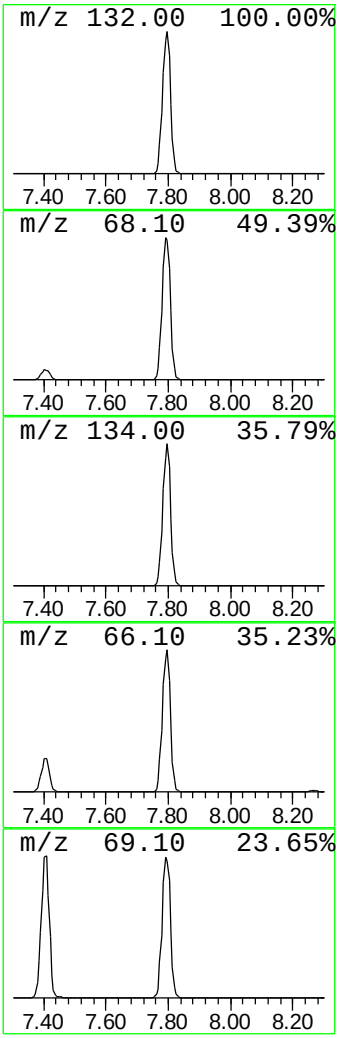
**********

Peak Number 7 unknown7.80 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.80 | 118.91 ng | 5132790 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 22 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 5 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 12 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

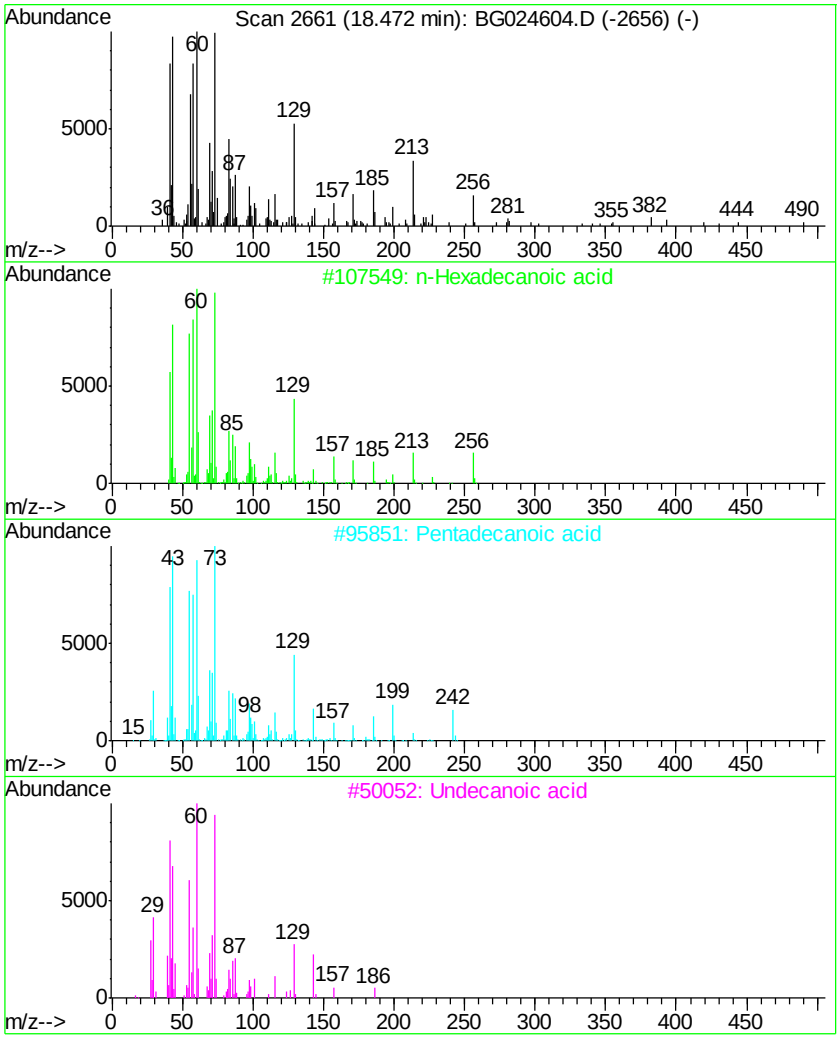
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

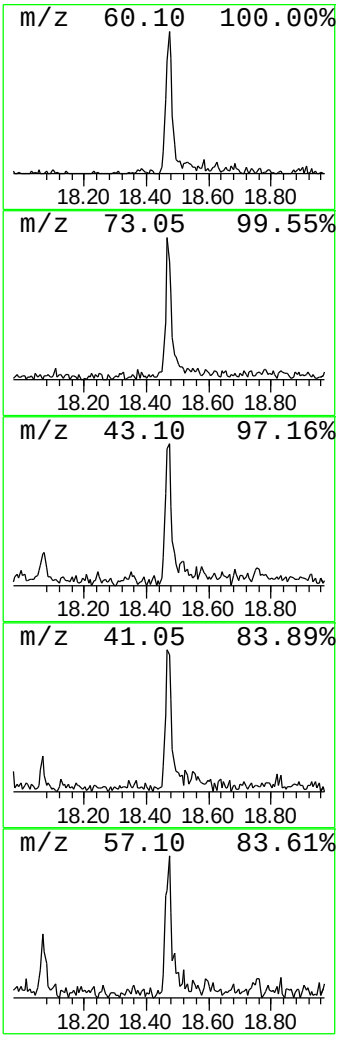
**********

Peak Number 9 n-Hexadecanoic acid Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.47 | 2.96 ng | 307588 | Phenanthrene-d10 | 17.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 74 |
| 3 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 60 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 55 |



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Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

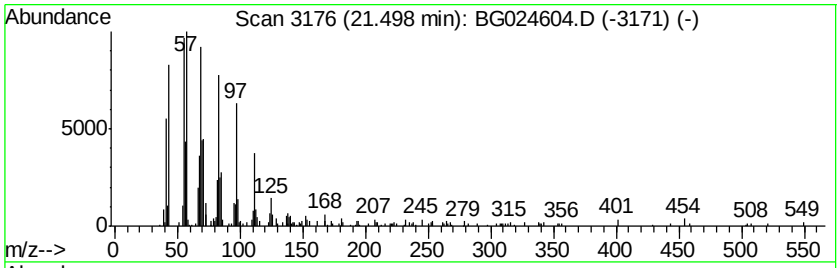
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

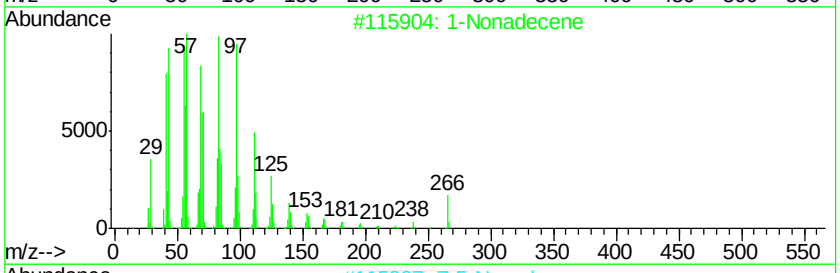
**********

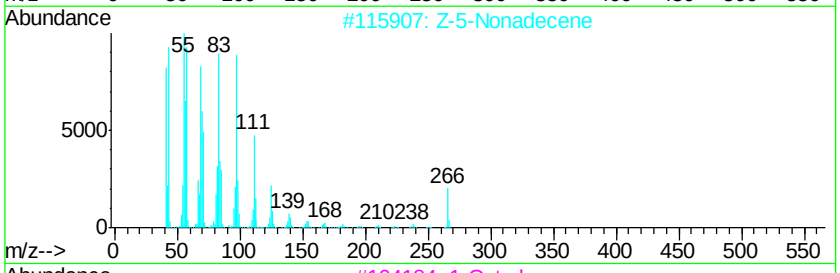
Peak Number 10 1-Nonadecene Concentration Rank 11

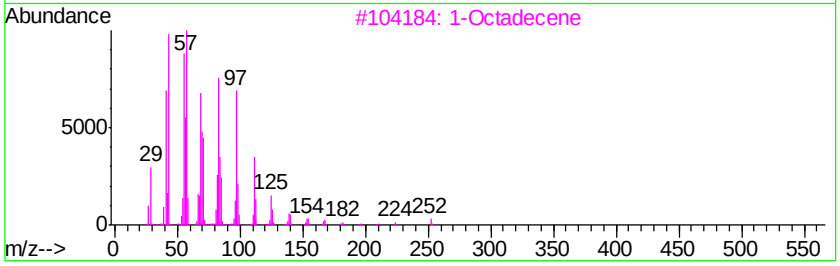
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.50 | 2.68 ng | 367370 | Chrysene-d12 | 21.92 |

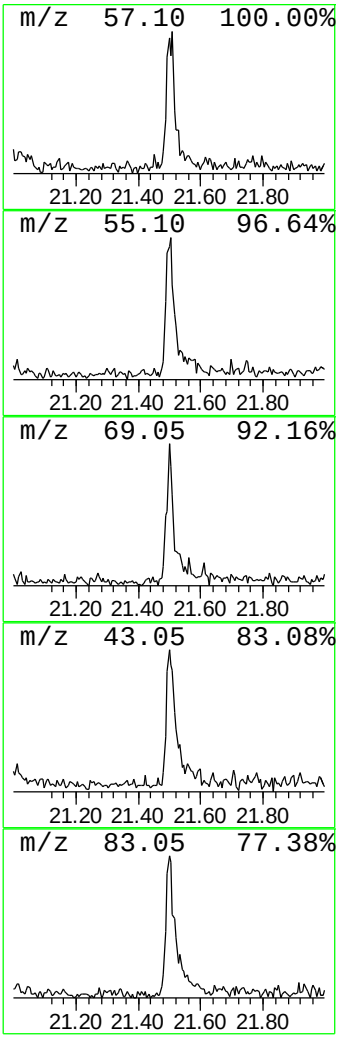
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 98 |
| 2 | Z-5-Nonadecene | 266 | C19H38 | 1000131-11-8 | 96 |
| 3 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 95 |
| 4 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 95 |
| 5 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |



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Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

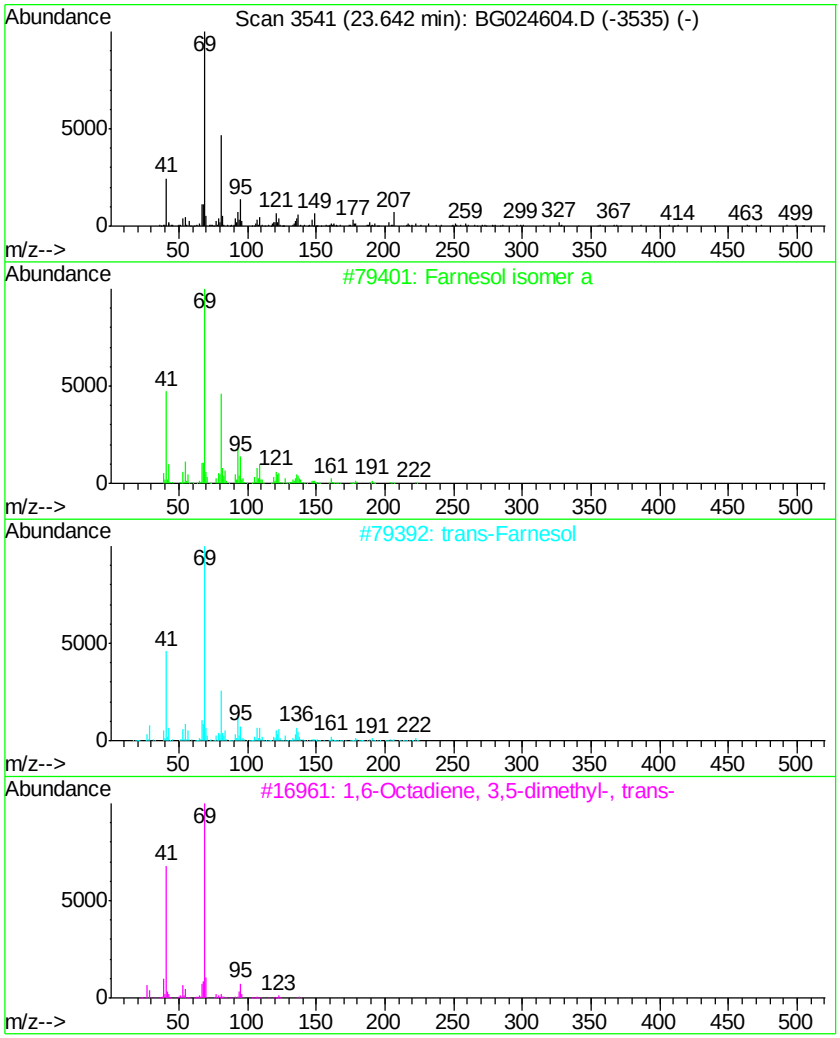
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

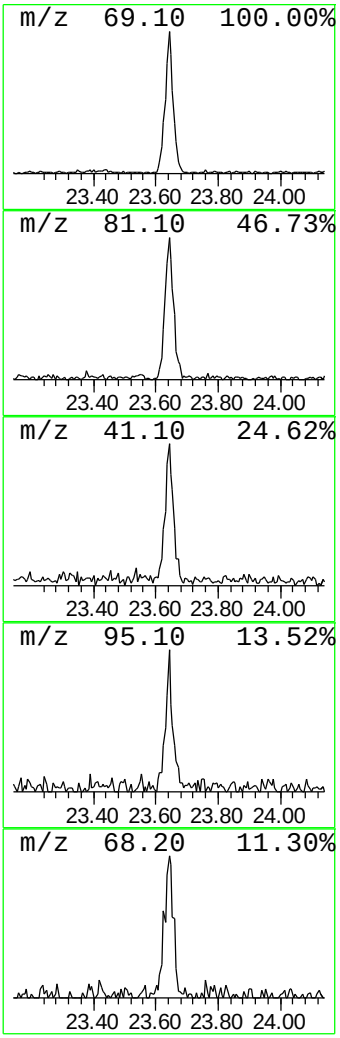
**********

Peak Number 11 Farnesol isomer a Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.64 | 3.20 ng | 434576 | Perylene-d12 | 25.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Farnesol isomer a | 222 | C15H26O | 1000108-92-4 | 74 |
| 2 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 64 |
| 3 | 1,6-Octadiene, 3,5-dimethyl-, tr... | 138 | C10H18 | 074630-87-8 | 64 |
| 4 | 1,5-Heptadiene, 3,3,6-trimethyl- | 138 | C10H18 | 035387-63-4 | 59 |
| 5 | 1,3-Dioxolan-2-one, 3-methyl-3-(... | 264 | C16H24O3 | 336879-76-6 | 59 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110116\
Data File : BG024604.D
Acq On : 1 Nov 2016 22:22
Operator : UM/SJ
Sample : H5489-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-71-6.5-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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 |
| Cyclopentane, met... | 2.98 | 628.2 | ng | 27117600 | 1 | 8.27 | 863300 | 20.0 |
| unknown3.13 | 3.13 | 403.3 | ng | 17407400 | 1 | 8.27 | 863300 | 20.0 |
| Heptane | 3.54 | 11.1 | ng | 480472 | 1 | 8.27 | 863300 | 20.0 |
| 2-Pentanone, 4-hy... | 5.33 | 25.3 | ng | 1090560 | 1 | 8.27 | 863300 | 20.0 |
| unknown7.80 | 7.80 | 118.9 | ng | 5132790 | 1 | 8.27 | 863300 | 20.0 |
| n-Hexadecanoic acid | 18.47 | 3.0 | ng | 307588 | 4 | 17.63 | 2078200 | 20.0 |
| 1-Nonadecene | 21.50 | 2.7 | ng | 367370 | 5 | 21.92 | 2738060 | 20.0 |
| Farnesol isomer a | 23.64 | 3.2 | ng | 434576 | 6 | 25.35 | 2717230 | 20.0 |