LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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 | 3.128 | 43 | 49 | 68 | rVB | 6616620 | 11351325 | 100.00% | 18.464% |
| 2 | 5.332 | 417 | 424 | 431 | rBV | 407518 | 681324 | 6.00% | 1.108% |
| 3 | 5.796 | 495 | 503 | 512 | rBV | 1958303 | 3300683 | 29.08% | 5.369% |
| 4 | 7.406 | 768 | 777 | 788 | rBV | 2062837 | 3780111 | 33.30% | 6.149% |
| 5 | 7.793 | 834 | 843 | 851 | rBV | 1931812 | 3461569 | 30.49% | 5.631% |
| 6 | 8.269 | 915 | 924 | 934 | rVB2 | 337768 | 632330 | 5.57% | 1.029% |
| 7 | 8.592 | 972 | 979 | 987 | rVB | 1406288 | 2530724 | 22.29% | 4.117% |
| 8 | 9.439 | 1114 | 1123 | 1133 | rBV | 1264119 | 2334897 | 20.57% | 3.798% |
| 9 | 11.095 | 1397 | 1405 | 1413 | rBV | 432208 | 830718 | 7.32% | 1.351% |
| 10 | 13.504 | 1807 | 1815 | 1823 | rBV | 2885798 | 4733866 | 41.70% | 7.700% |
| 11 | 14.321 | 1946 | 1954 | 1960 | rBV | 1055117 | 1547635 | 13.63% | 2.517% |
| 12 | 14.885 | 2043 | 2050 | 2056 | rBV | 748943 | 1230926 | 10.84% | 2.002% |
| 13 | 16.366 | 2294 | 2302 | 2313 | rBV | 3428461 | 5304679 | 46.73% | 8.629% |
| 14 | 17.623 | 2510 | 2516 | 2522 | rBV | 1134517 | 1754281 | 15.45% | 2.854% |
| 15 | 17.958 | 2565 | 2573 | 2580 | rBV2 | 340071 | 534886 | 4.71% | 0.870% |
| 16 | 18.469 | 2655 | 2660 | 2670 | rBV2 | 171740 | 288632 | 2.54% | 0.469% |
| 17 | 19.309 | 2798 | 2803 | 2822 | rBV | 1647818 | 2428548 | 21.39% | 3.950% |
| 18 | 19.662 | 2858 | 2863 | 2868 | rVB2 | 88572 | 124200 | 1.09% | 0.202% |
| 19 | 20.202 | 2949 | 2955 | 2962 | rBV | 6279730 | 8767903 | 77.24% | 14.262% |
| 20 | 20.455 | 2993 | 2998 | 3003 | rBV6 | 67332 | 137366 | 1.21% | 0.223% |
| 21 | 20.813 | 3052 | 3059 | 3063 | rBV4 | 181456 | 290437 | 2.56% | 0.472% |
| 22 | 20.925 | 3072 | 3078 | 3083 | rBV4 | 74654 | 126607 | 1.12% | 0.206% |
| 23 | 21.495 | 3171 | 3175 | 3186 | rBV4 | 230498 | 402795 | 3.55% | 0.655% |
| 24 | 21.759 | 3215 | 3220 | 3225 | rVB | 124284 | 191323 | 1.69% | 0.311% |
| 25 | 21.918 | 3240 | 3247 | 3254 | rBV | 1381455 | 2358554 | 20.78% | 3.836% |
| 26 | 25.349 | 3820 | 3831 | 3844 | rVB2 | 745237 | 2350769 | 20.71% | 3.824% |

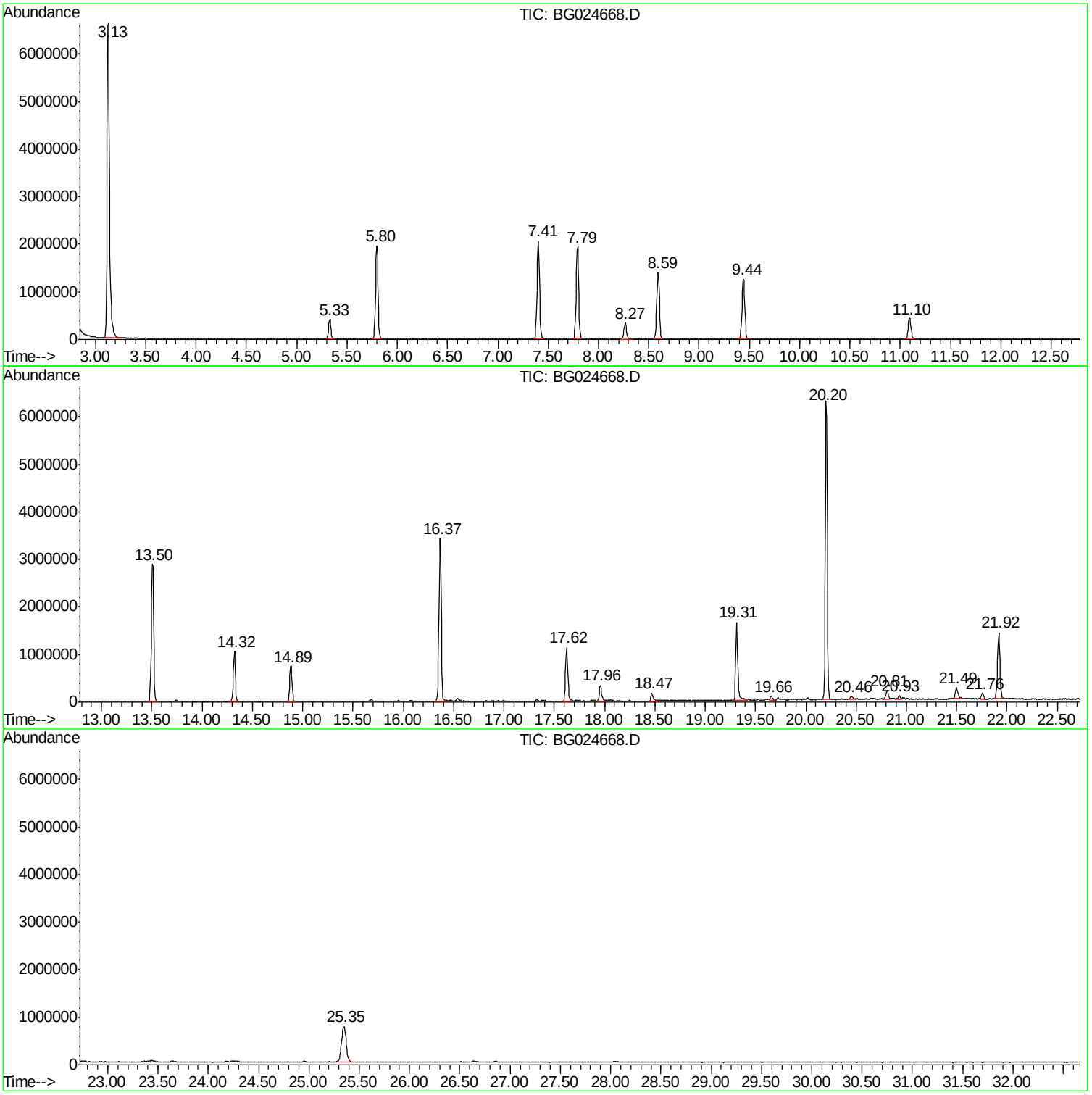
Sum of corrected areas: 61477088

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

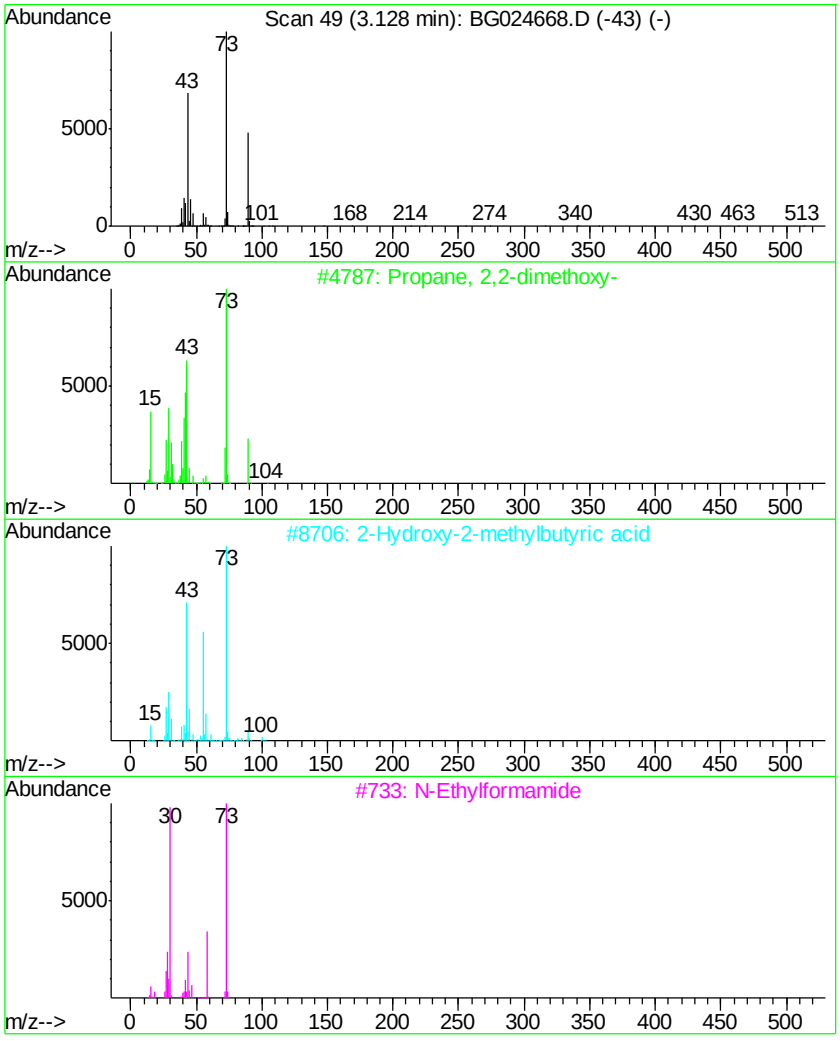
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

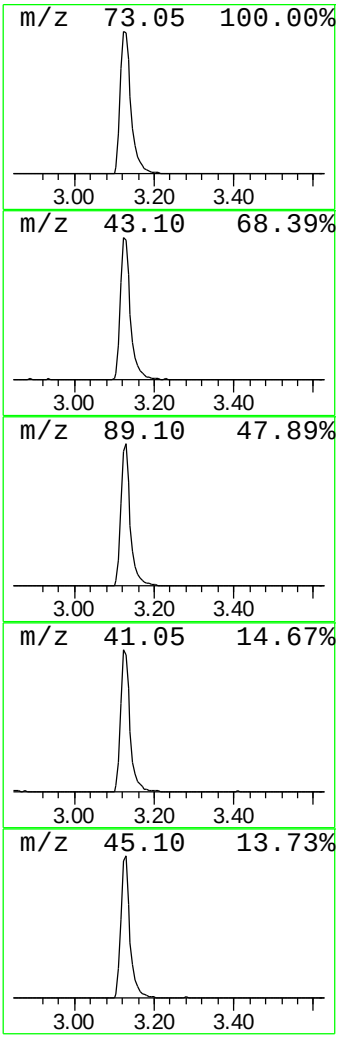
**********

Peak Number 1 unknown3.13 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.13 | 359.03 ng | 11351300 | 1,4-Dichlorobenzene-d4 | 8.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 28 |
| 2 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 17 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 4 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 9 |
| 5 | 1-(2-Methoxyethoxy)-2-methyl-2-p... | 162 | C8H18O3 | 1000364-24-4 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

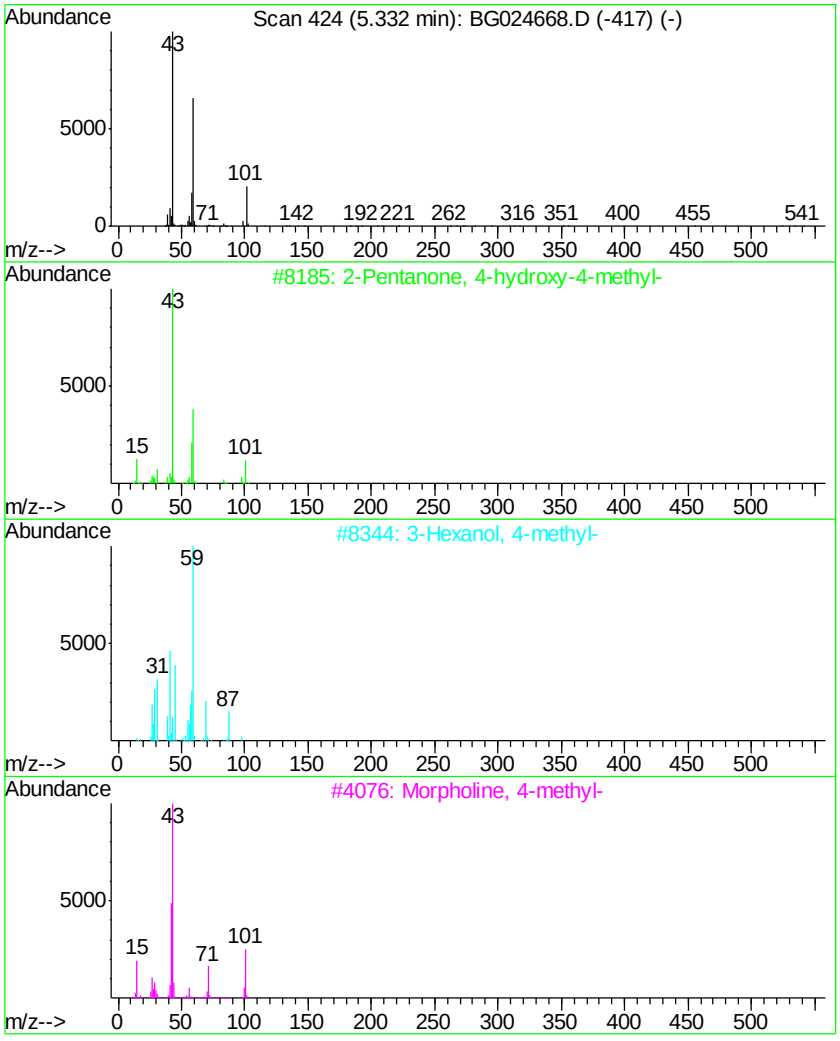
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

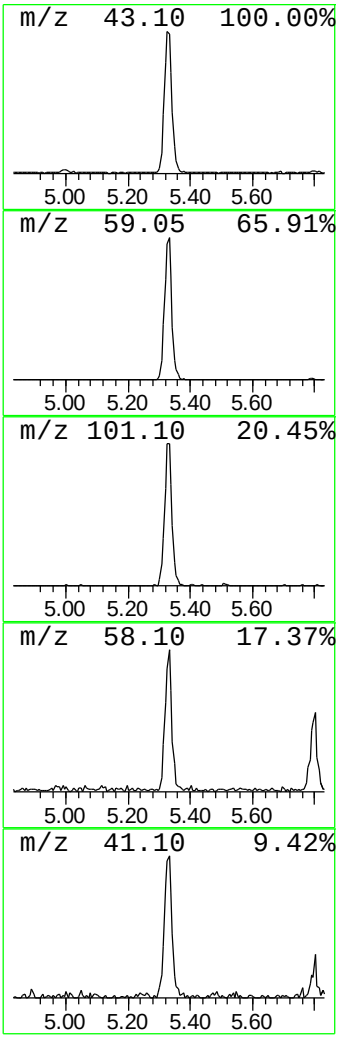
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.33 | 21.55 ng | 681324 | 1,4-Dichlorobenzene-d4 | 8.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 25 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 3-Heptadecanol | 256 | C17H36O | 084534-30-5 | 9 |
| 5 | 2,5,8,11-Tetraoxadodecane | 178 | C8H18O4 | 000112-49-2 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

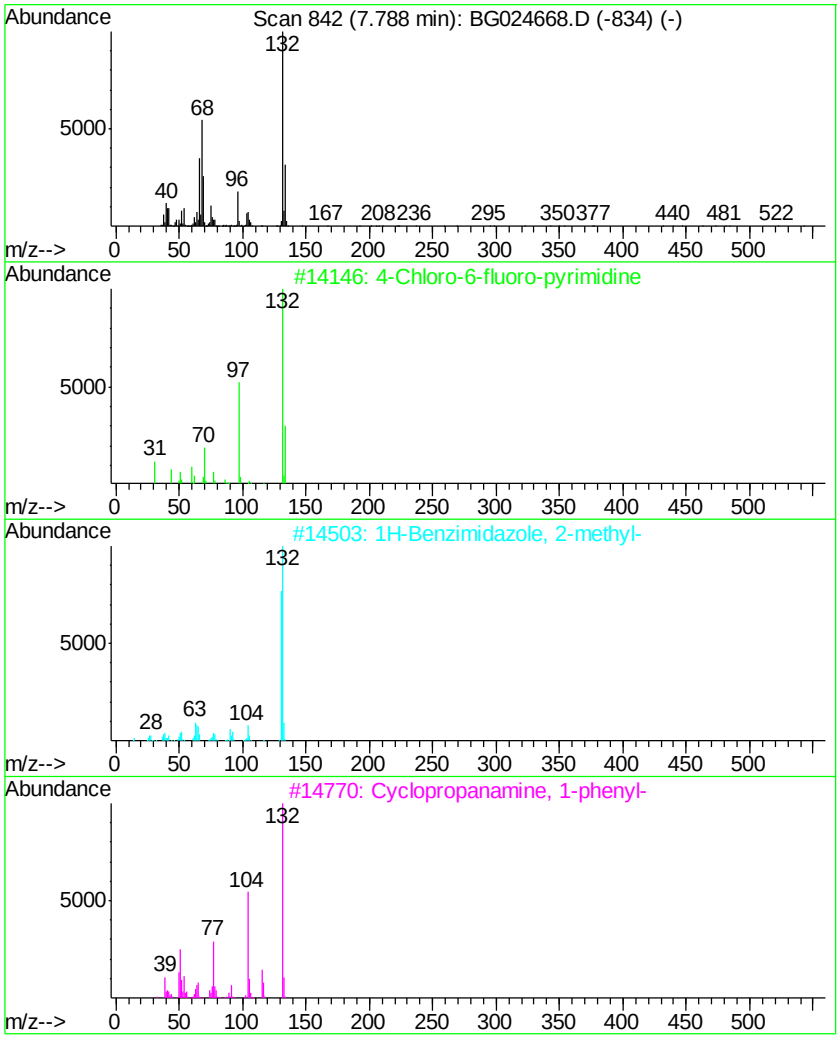
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

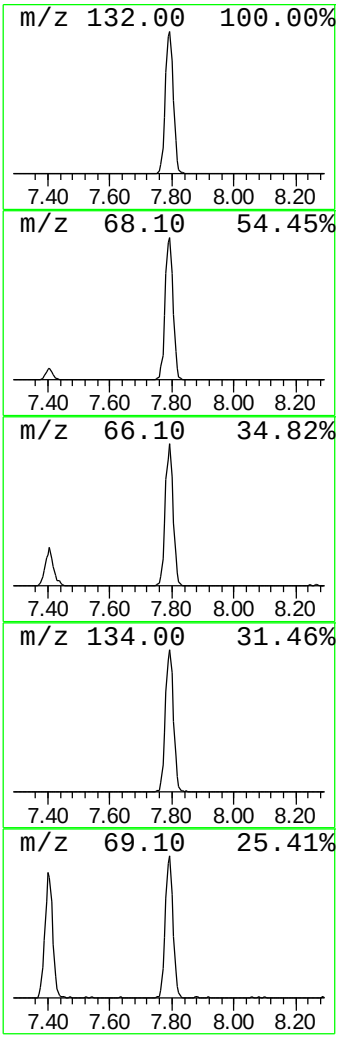
**********

Peak Number 3 unknown7.79 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.79 | 109.49 ng | 3461570 | 1,4-Dichlorobenzene-d4 | 8.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 22 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 16 |
| 5 | 3-(3,4-Dihydro-1H-isoquinolin-2-... | 377 | C24H27NO3 | 1000295-80-7 | 12 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

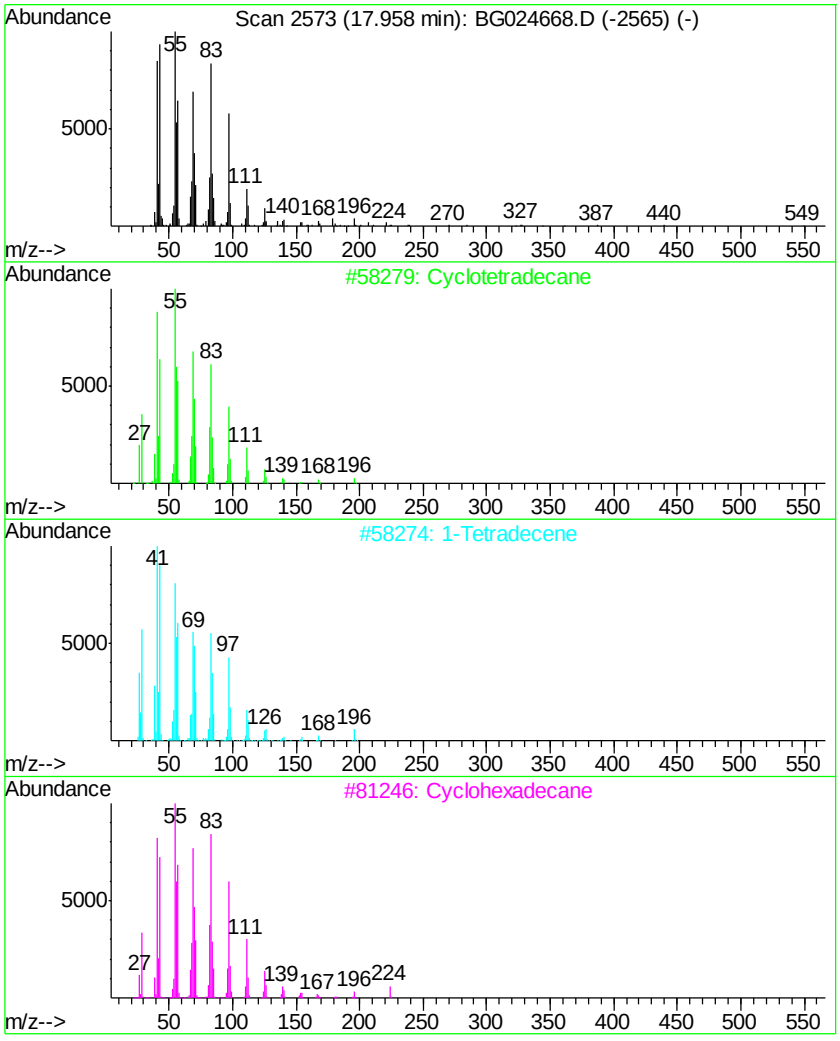
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

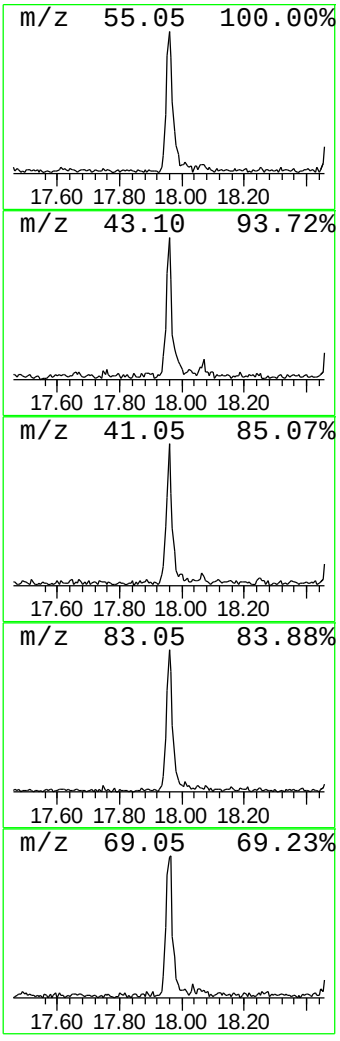
**********

Peak Number 5 Cyclotetradecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.96 | 6.10 ng | 534886 | Phenanthrene-d10 | 17.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 96 |
| 2 | 1-Tetradecene | 196 | C14H28 | 001120-36-1 | 93 |
| 3 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 91 |
| 4 | 7-Tetradecene, (E)- | 196 | C14H28 | 041446-63-3 | 87 |
| 5 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 70 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

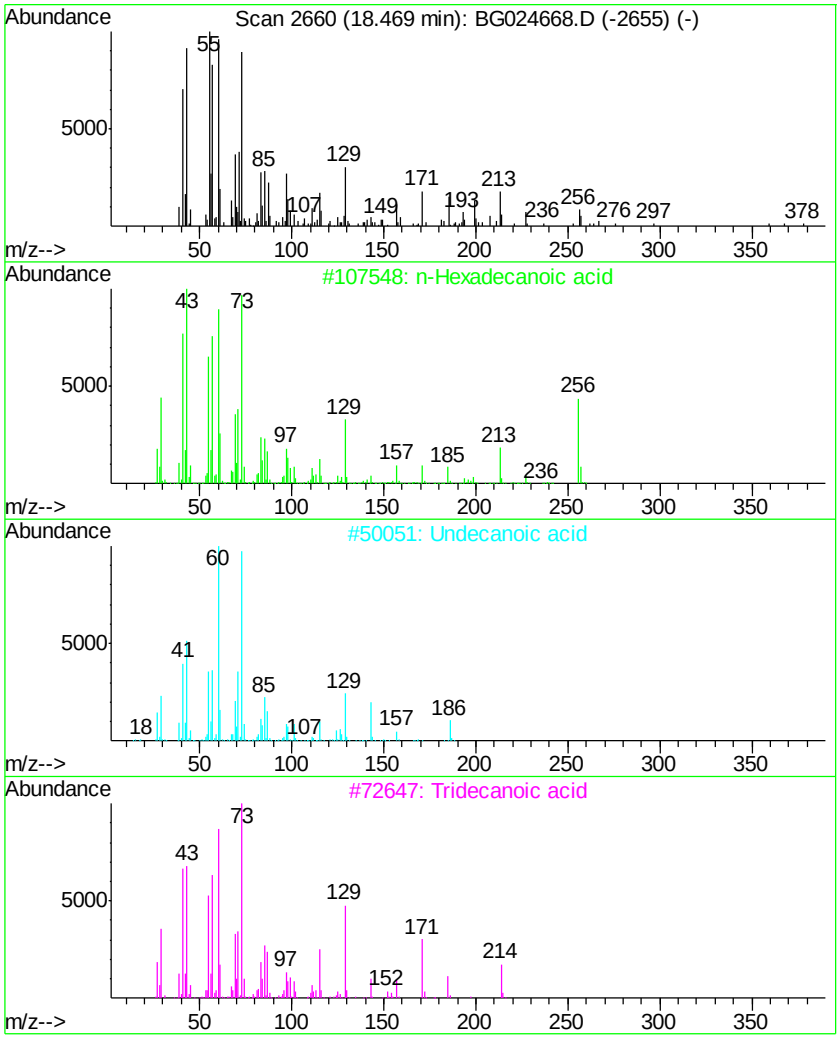
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

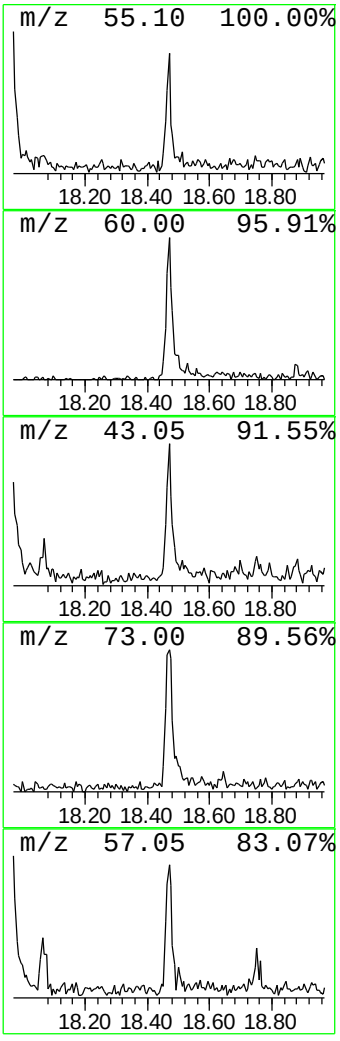
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.47 | 3.29 ng | 288632 | Phenanthrene-d10 | 17.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 83 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 78 |
| 4 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 72 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 64 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

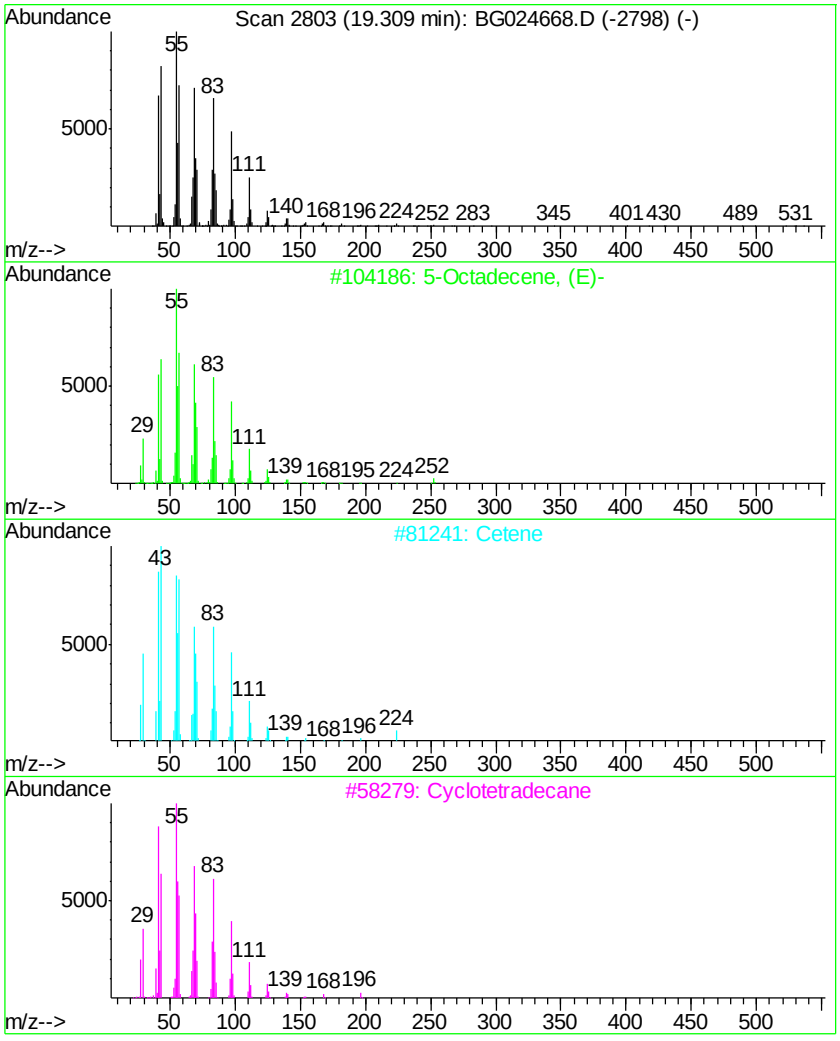
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

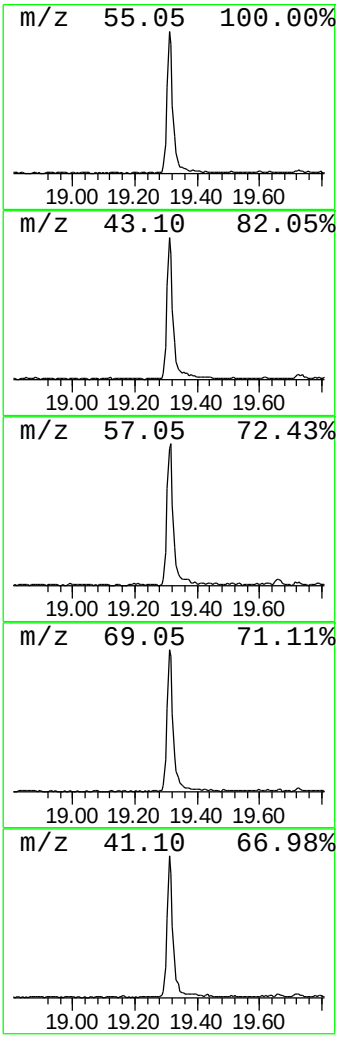
**********

Peak Number 7 5-Octadecene, (E)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.31 | 27.69 ng | 2428550 | Phenanthrene-d10 | 17.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 98 |
| 2 | Cetene | 224 | C16H32 | 000629-73-2 | 98 |
| 3 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 95 |
| 4 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 94 |
| 5 | Tetradecyl trifluoroacetate | 310 | C16H29F3O2 | 006222-02-2 | 91 |



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Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

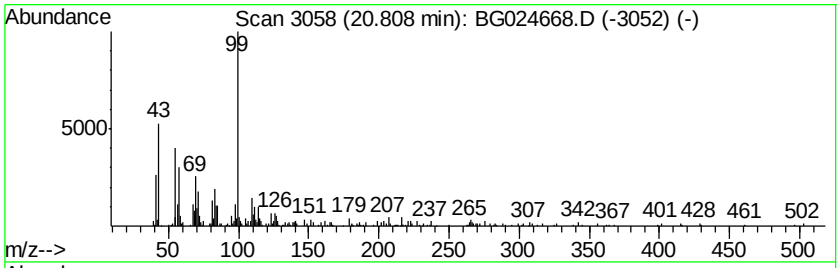
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

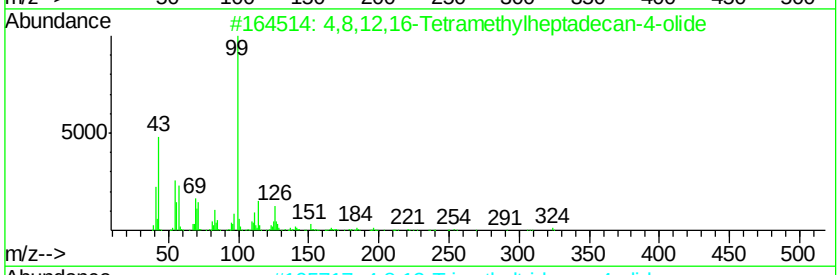
**********

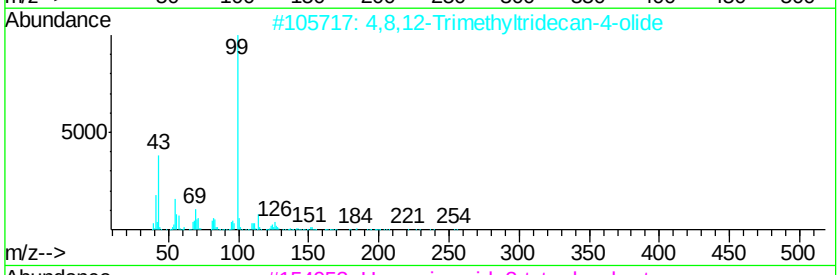
Peak Number 8 4,8,12,16-Tetramethylheptad... Concentration Rank 9

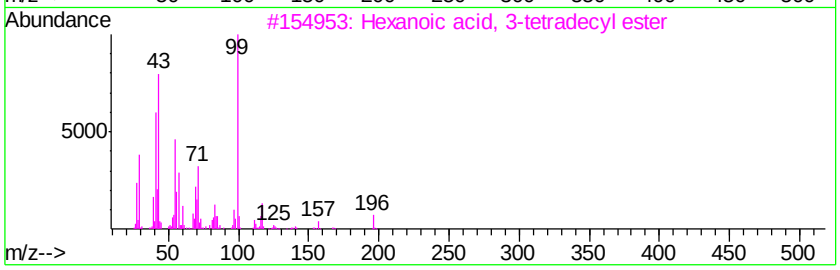
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.81 | 2.46 ng | 290437 | Chrysene-d12 | 21.92 |

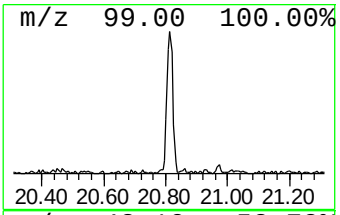
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4,8,12,16-Tetramethylheptadecan-... | 324 | C21H40O2 | 096168-15-9 | 80 |
| 2 | 4,8,12-Trimethyltridecan-4-olide | 254 | C16H30O2 | 220904-24-5 | 50 |
| 3 | Hexanoic acid, 3-tetradecyl ester | 312 | C20H40O2 | 1000279-29-7 | 47 |
| 4 | Hexanoic acid, 4-hexadecyl ester | 340 | C22H44O2 | 1000282-83-8 | 47 |
| 5 | Tripropyl phosphate | 224 | C9H21O4P | 000513-08-6 | 47 |

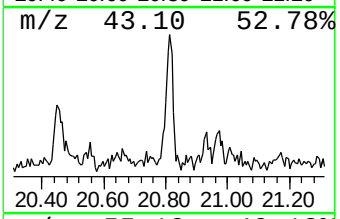


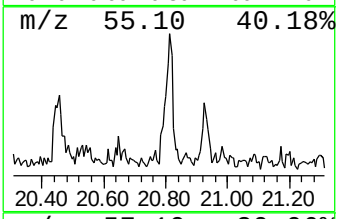



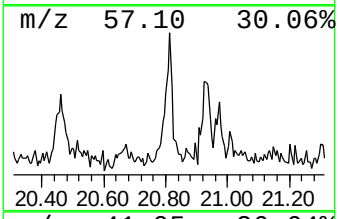



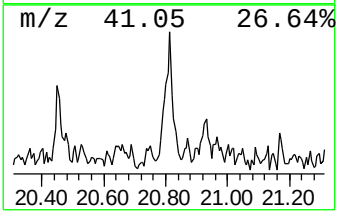



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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

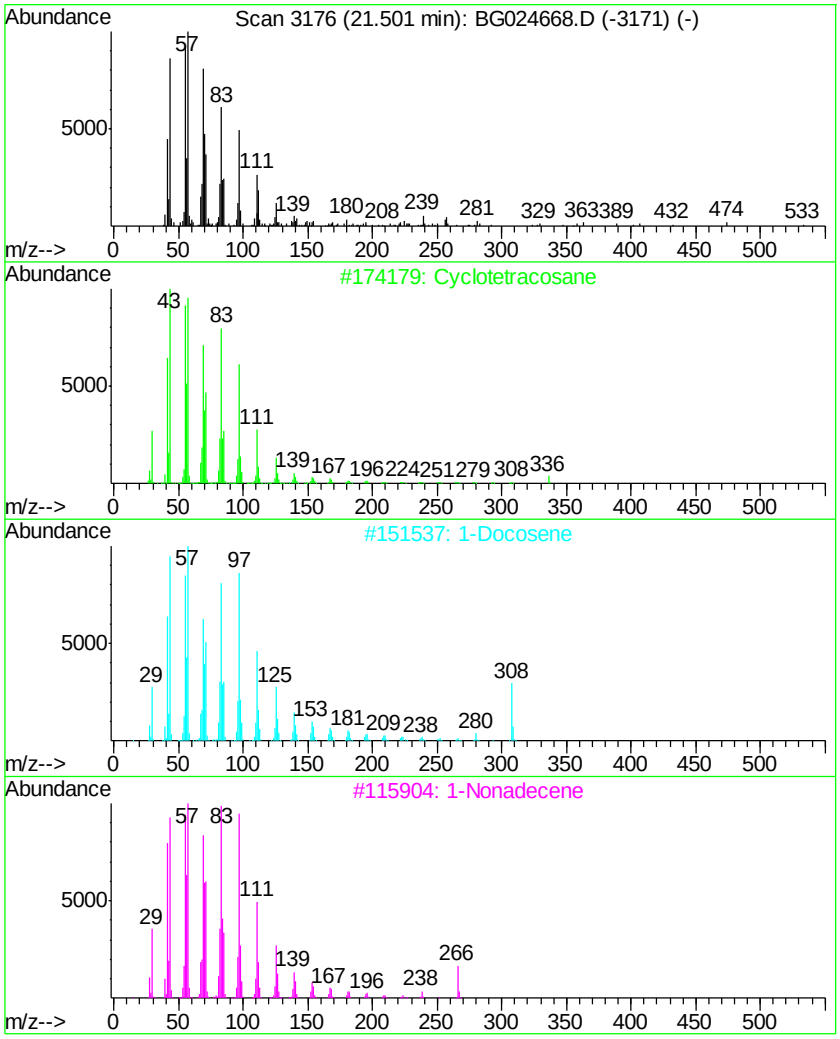
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

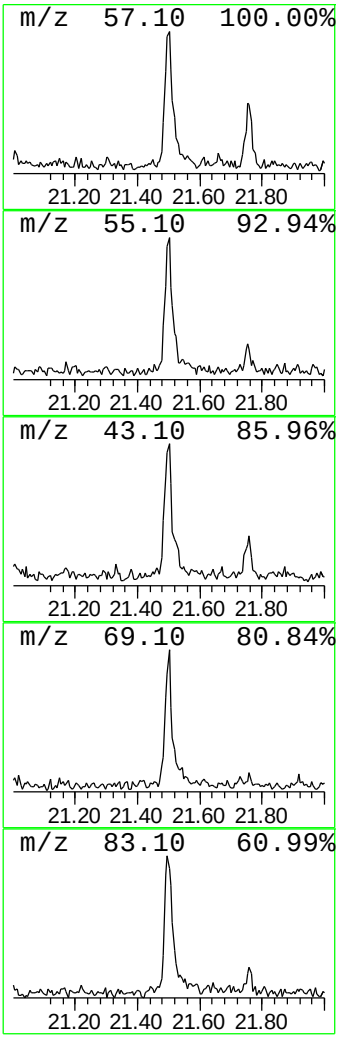
**********

Peak Number 9 Cyclotetracosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.50 | 3.42 ng | 402795 | Chrysene-d12 | 21.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 94 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 94 |
| 3 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 4 | Acetic acid, chloro-, octadecyl ... | 346 | C20H39ClO2 | 005348-82-3 | 90 |
| 5 | Z-5-Nonadecene | 266 | C19H38 | 1000131-11-8 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024668.D
Acq On : 4 Nov 2016 4:49
Operator : UM/SJ
Sample : H5509-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-96-17.5-18.0

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 |
| unknown3.13 | 3.13 | 359.0 | ng | 11351300 | 1 | 8.26 | 632330 | 20.0 |
| 2-Pentanone, 4-hy... | 5.33 | 21.6 | ng | 681324 | 1 | 8.26 | 632330 | 20.0 |
| unknown7.79 | 7.79 | 109.5 | ng | 3461570 | 1 | 8.26 | 632330 | 20.0 |
| Cyclotetradecane | 17.96 | 6.1 | ng | 534886 | 4 | 17.62 | 1754280 | 20.0 |
| n-Hexadecanoic acid | 18.47 | 3.3 | ng | 288632 | 4 | 17.62 | 1754280 | 20.0 |
| 5-Octadecene, (E)- | 19.31 | 27.7 | ng | 2428550 | 4 | 17.62 | 1754280 | 20.0 |
| 4,8,12,16-Tetrame... | 20.81 | 2.5 | ng | 290437 | 5 | 21.92 | 2358550 | 20.0 |
| Cyclotetracosane | 21.50 | 3.4 | ng | 402795 | 5 | 21.92 | 2358550 | 20.0 |