# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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 | 3.194 | 13 | 18 | 32 | rVB | 129726 | 240814 | 11.25% | 1.558% |
| 2 | 5.620 | 423 | 431 | 443 | rBV | 535258 | 955218 | 44.61% | 6.179% |
| 3 | 7.219 | 695 | 703 | 716 | rBV | 581655 | 1120388 | 52.33% | 7.248% |
| 4 | 7.571 | 755 | 763 | 775 | rBV | 611108 | 1097164 | 51.24% | 7.097% |
| 5 | 8.023 | 832 | 840 | 848 | rBV | 180741 | 311539 | 14.55% | 2.015% |
| 6 | 8.347 | 888 | 895 | 903 | rBV | 442330 | 797295 | 37.24% | 5.158% |
| 7 | 9.187 | 1029 | 1038 | 1050 | rBV | 317508 | 641452 | 29.96% | 4.149% |
| 8 | 10.832 | 1310 | 1318 | 1331 | rBV | 203201 | 400844 | 18.72% | 2.593% |
| 9 | 13.276 | 1726 | 1734 | 1747 | rBV | 895645 | 1418132 | 66.23% | 9.174% |
| 10 | 14.099 | 1867 | 1874 | 1880 | rBV | 99902 | 153005 | 7.15% | 0.990% |
| 11 | 14.651 | 1960 | 1968 | 1976 | rBV2 | 394228 | 616700 | 28.80% | 3.989% |
| 12 | 16.143 | 2213 | 2222 | 2237 | rBV | 833146 | 1430130 | 66.79% | 9.251% |
| 13 | 17.395 | 2428 | 2435 | 2447 | rBV | 440184 | 769125 | 35.92% | 4.975% |
| 14 | 17.512 | 2451 | 2455 | 2459 | rVB5 | 22294 | 31726 | 1.48% | 0.205% |
| 15 | 18.288 | 2582 | 2587 | 2597 | rBV2 | 146195 | 265004 | 12.38% | 1.714% |
| 16 | 19.451 | 2781 | 2785 | 2789 | rBV | 20315 | 27609 | 1.29% | 0.179% |
| 17 | 19.557 | 2799 | 2803 | 2815 | rVB3 | 52280 | 94307 | 4.40% | 0.610% |
| 18 | 19.810 | 2843 | 2846 | 2850 | rVB3 | 18890 | 22639 | 1.06% | 0.146% |
| 19 | 20.004 | 2873 | 2879 | 2887 | rBV | 1513832 | 2141128 | 100.00% | 13.851% |
| 20 | 21.314 | 3099 | 3102 | 3113 | rVB7 | 56927 | 138872 | 6.49% | 0.898% |
| 21 | 21.660 | 3155 | 3161 | 3176 | rVB | 542196 | 1039065 | 48.53% | 6.722% |
| 22 | 21.848 | 3191 | 3193 | 3200 | rVB6 | 31549 | 37287 | 1.74% | 0.241% |
| 23 | 22.454 | 3292 | 3296 | 3301 | rBV | 42390 | 61460 | 2.87% | 0.398% |
| 24 | 22.512 | 3301 | 3306 | 3321 | rVB8 | 62521 | 161848 | 7.56% | 1.047% |
| 25 | 23.141 | 3409 | 3413 | 3421 | rBV5 | 59885 | 121007 | 5.65% | 0.783% |
| 26 | 23.934 | 3544 | 3548 | 3556 | rBV3 | 59920 | 112712 | 5.26% | 0.729% |
| 27 | 24.863 | 3696 | 3706 | 3718 | rVB2 | 400730 | 1137860 | 53.14% | 7.361% |
| 28 | 26.002 | 3894 | 3900 | 3907 | rVB4 | 46006 | 114234 | 5.34% | 0.739% |

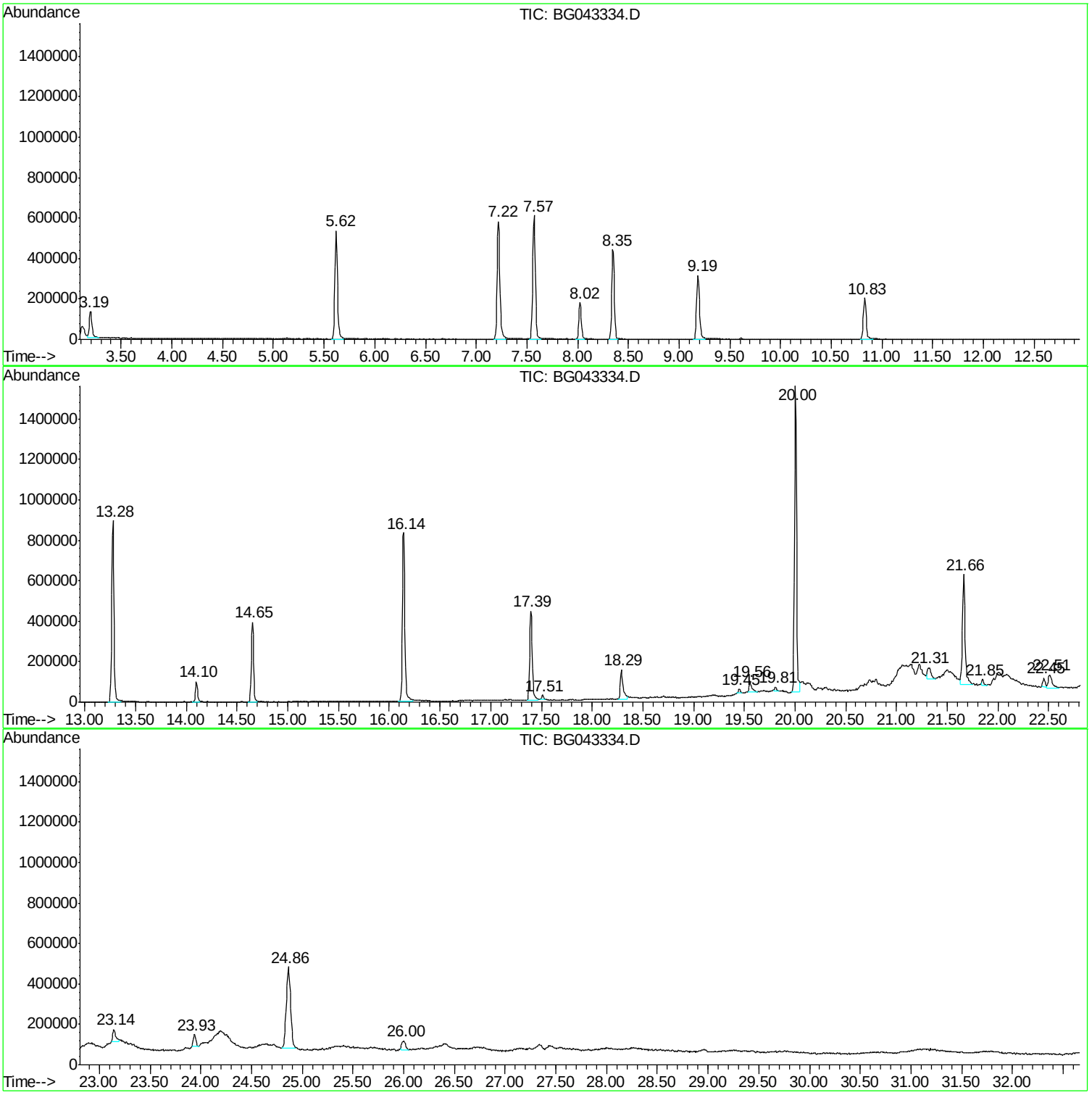
Sum of corrected areas: 15458564

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

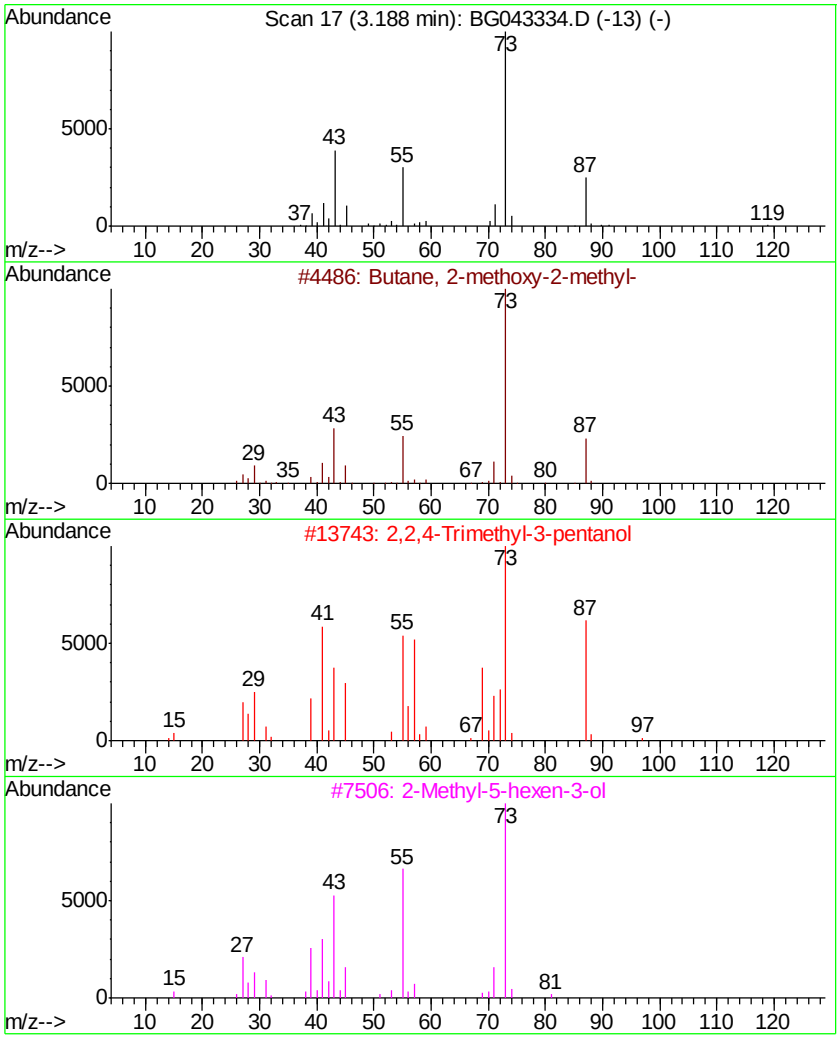
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

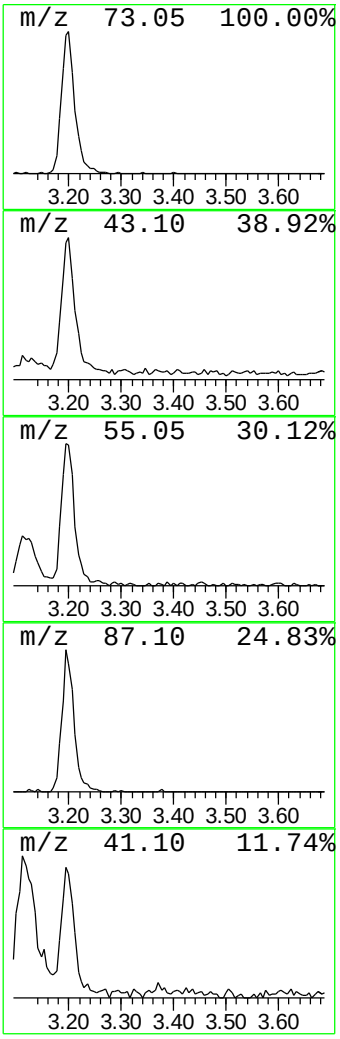
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.19 | 15.46 ng | 240814 | 1,4-Dichlorobenzene-d4 | 8.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 42 |
| 3 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 38 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | 3-Pentanol, 3-methyl- | 102 | C6H14O | 000077-74-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

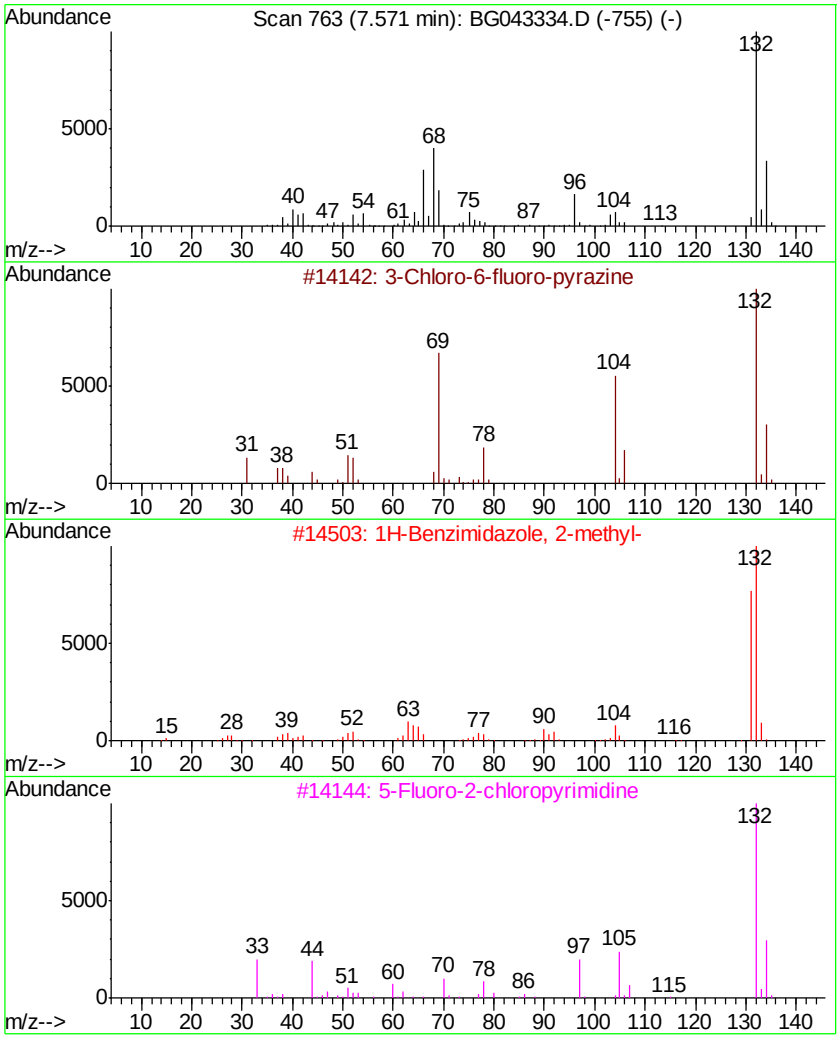
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

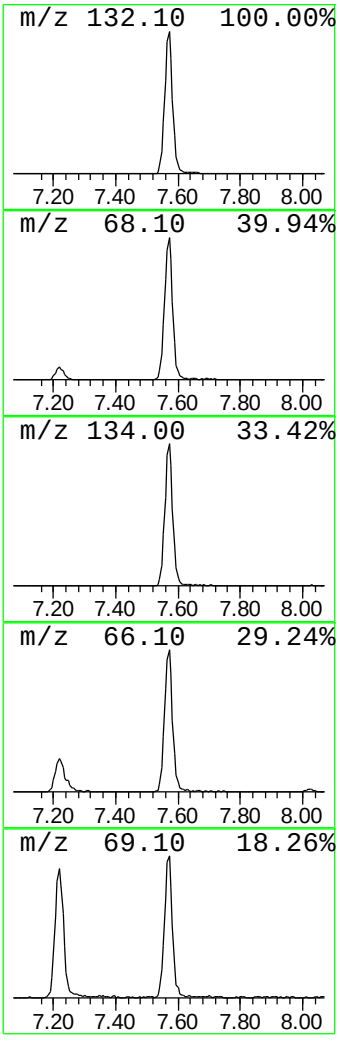
**********

Peak Number 2 unknown7.57 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.57 | 70.44 ng | 1097160 | 1,4-Dichlorobenzene-d4 | 8.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

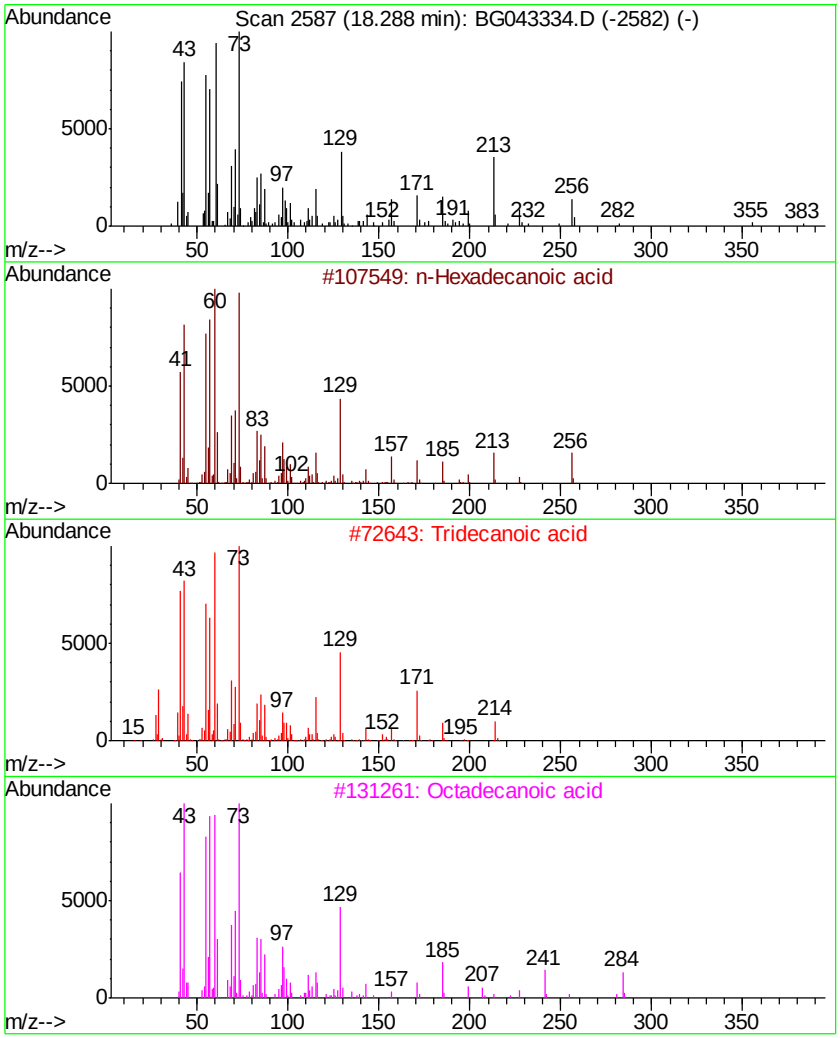
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

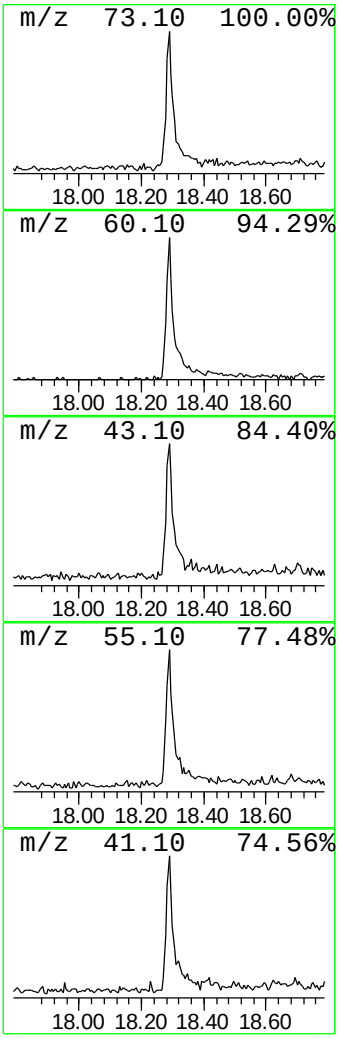
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.29 | 6.89 ng | 265004 | Phenanthrene-d10 | 17.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 95 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 93 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

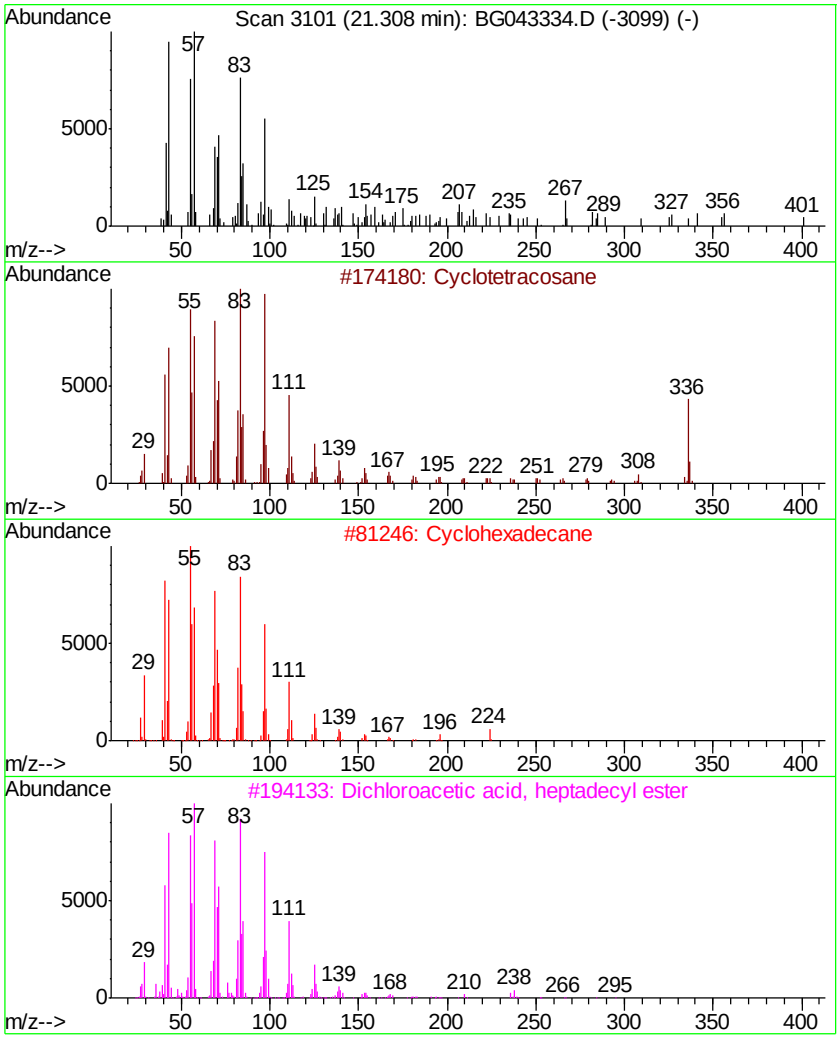
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

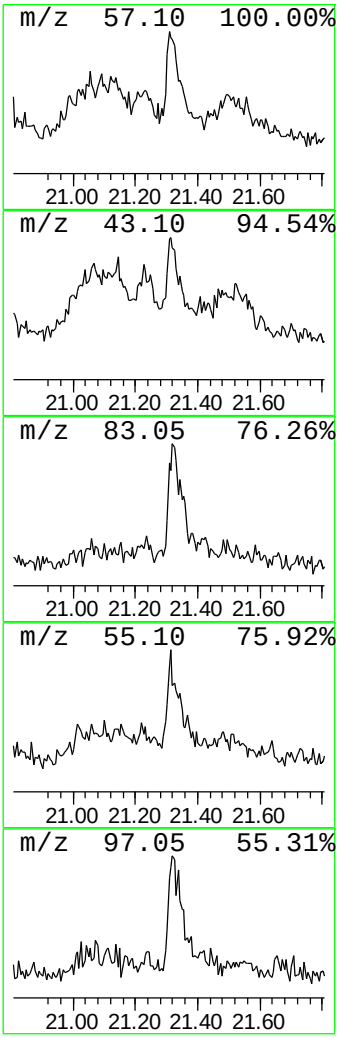
**********

Peak Number 5 Cyclotetracosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.31 | 2.67 ng | 138872 | Chrysene-d12 | 21.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 91 |
| 2 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 87 |
| 3 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 87 |
| 4 | Cetene | 224 | C16H32 | 000629-73-2 | 78 |
| 5 | 1-Tetradecene | 196 | C14H28 | 001120-36-1 | 60 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

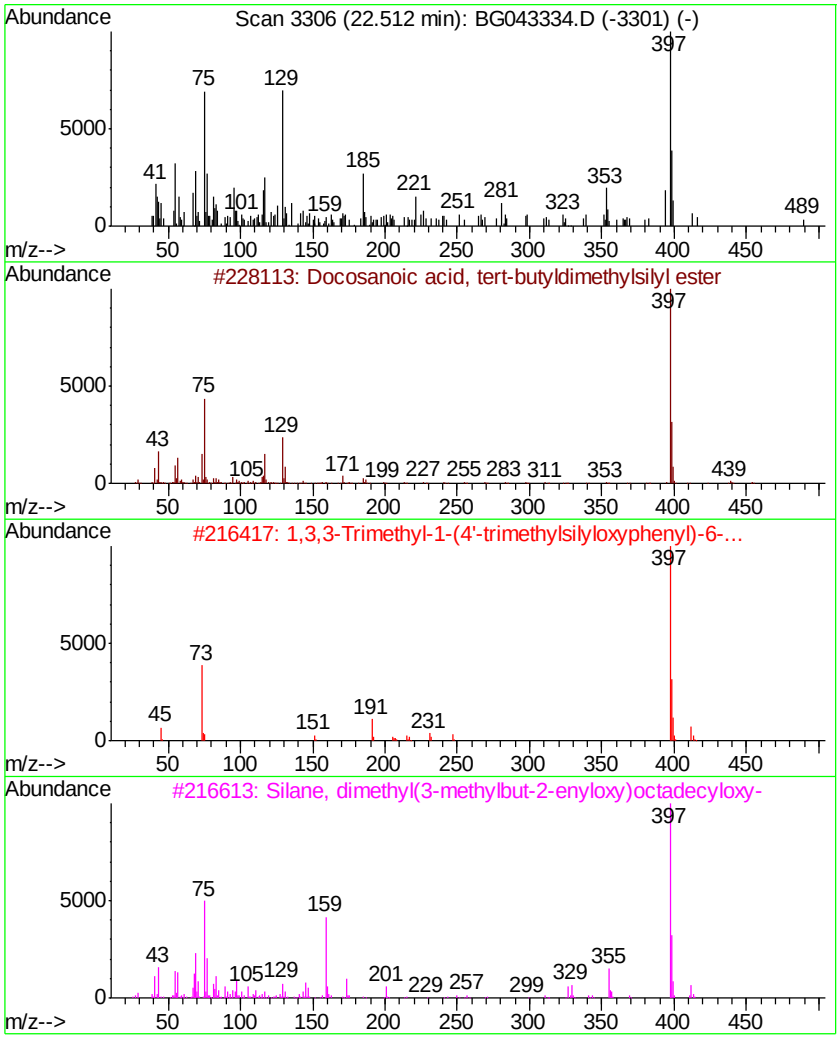
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

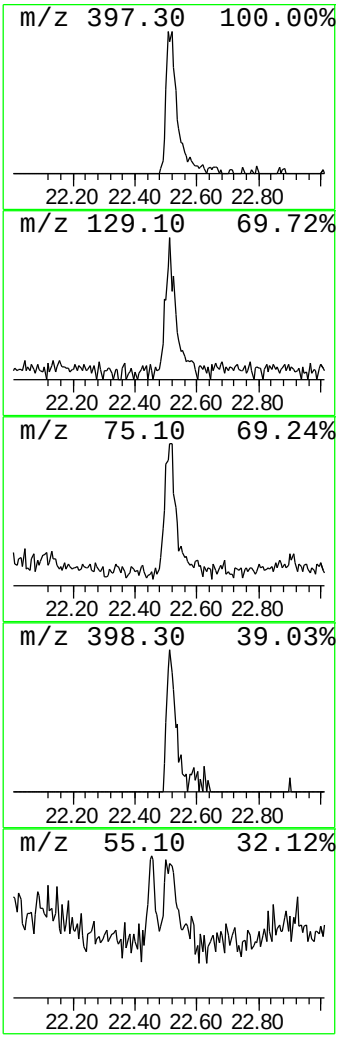
**********

Peak Number 6 Docosanoic acid, tert-butyl... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.51 | 3.12 ng | 161848 | Chrysene-d12 | 21.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosanoic acid, tert-butyldimet... | 454 | C28H58O2Si | 104255-84-7 | 50 |
| 2 | 1,3,3-Trimethyl-1-(4'-trimethyls... | 412 | C24H36O2Si2 | 155726-90-2 | 47 |
| 3 | Silane, dimethyl(3-methylbut-2-e... | 412 | C25H52O2Si | 1000347-97-7 | 46 |
| 4 | Tritriaconta-2-one, 24,25-bis(th... | 570 | C35H70OS2 | 1000111-39-8 | 38 |
| 5 | 1-(Trihexylsilyloxy)tridecane | 482 | C31H66OSi | 1000308-32-8 | 38 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

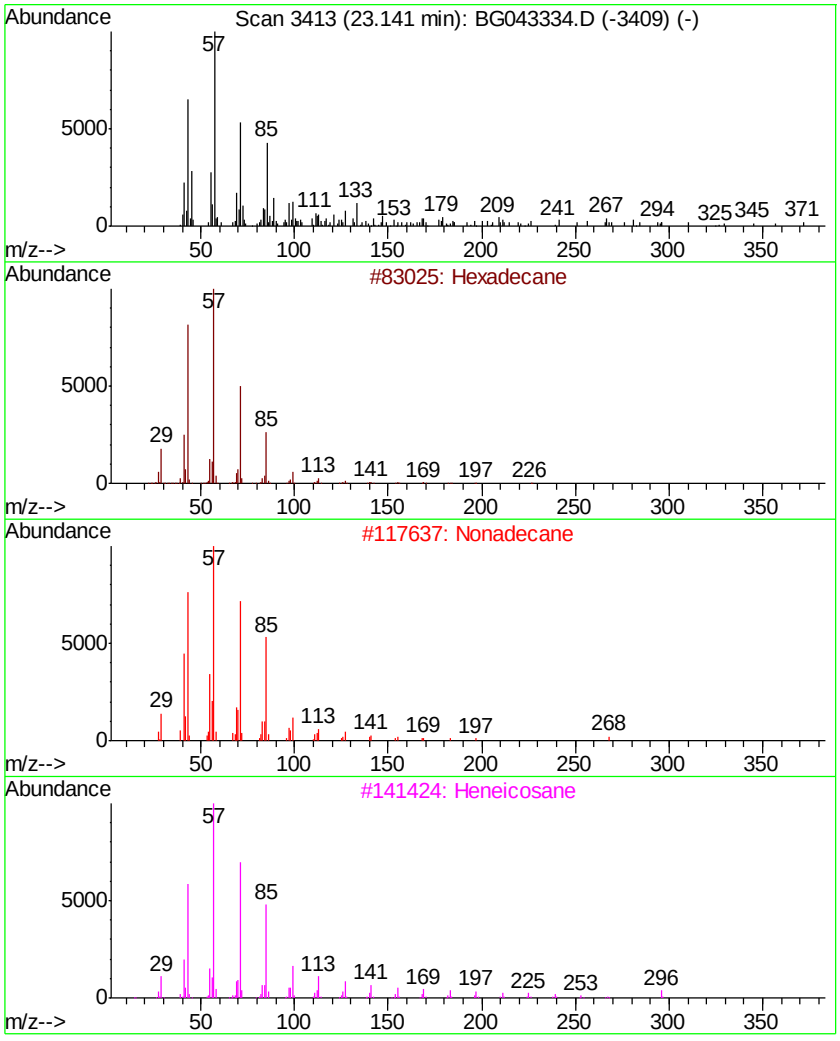
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

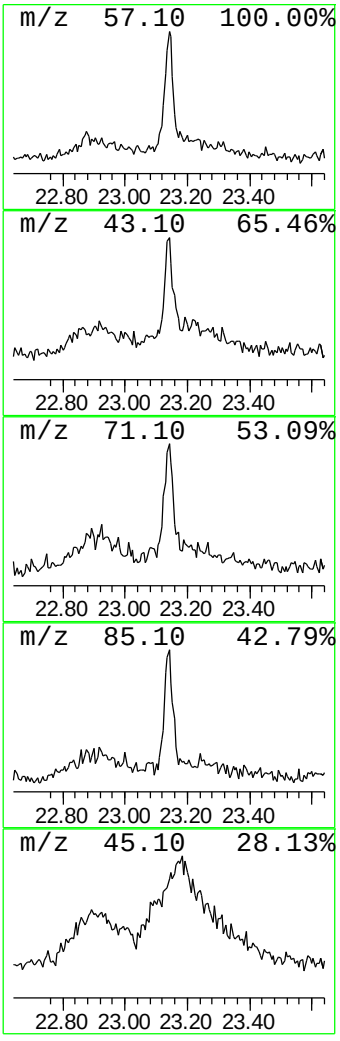
**********

Peak Number 7 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.14 | 2.33 ng | 121007 | Chrysene-d12 | 21.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 93 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 76 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 70 |
| 5 | Heneicosane, 11-decyl- | 437 | C31H64 | 055320-06-4 | 68 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

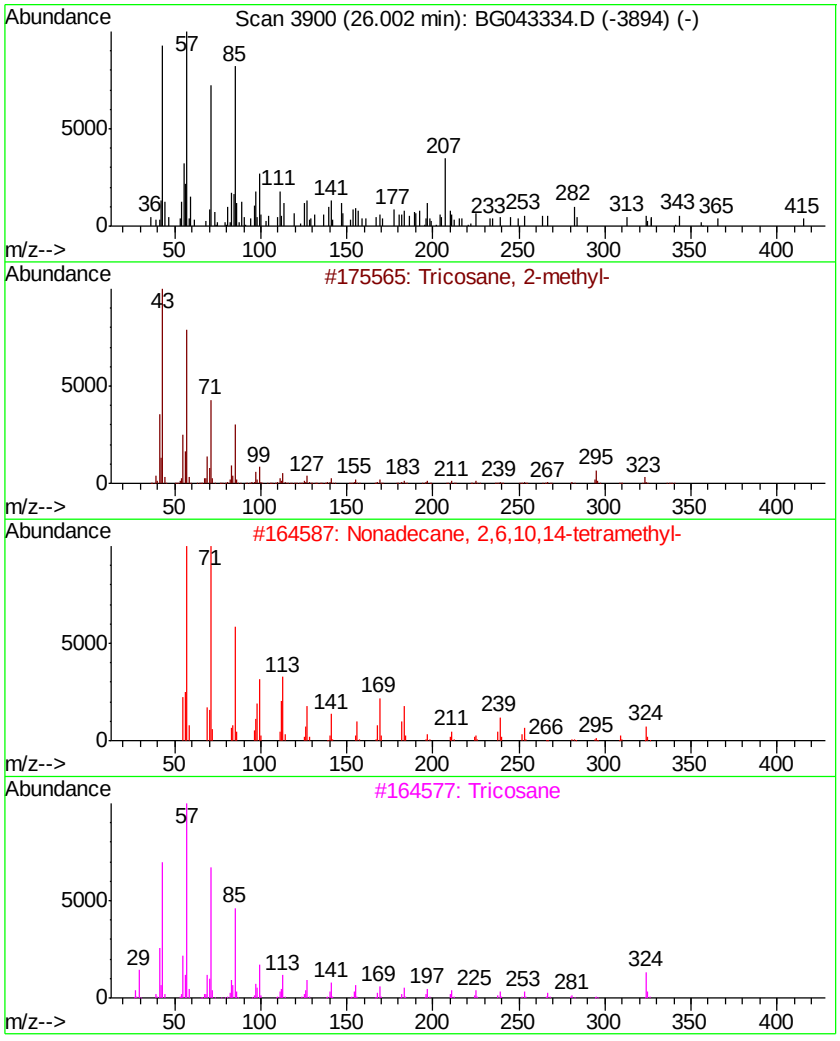
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

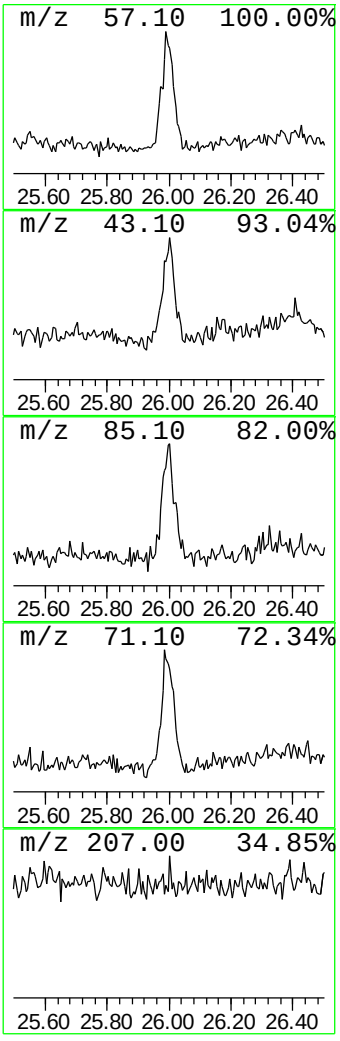
**********

Peak Number 8 Tricosane, 2-methyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.00 | 2.01 ng | 114234 | Perylene-d12 | 24.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricosane, 2-methyl- | 338 | C24H50 | 001928-30-9 | 53 |
| 2 | Nonadecane, 2,6,10,14-tetramethyl- | 324 | C23H48 | 055124-80-6 | 50 |
| 3 | Tricosane | 324 | C23H48 | 000638-67-5 | 50 |
| 4 | Sulfurous acid, hexyl nonyl ester | 292 | C15H32O3S | 1000309-13-1 | 47 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 46 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102419\
Data File : BG043334.D
Acq On : 24 Oct 2019 16:53
Operator : JU
Sample : K5497-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 168-16-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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 |
| Butane, 2-methoxy... | 3.19 | 15.5 | ng | 240814 | 1 | 8.02 | 311539 | 20.0 |
| unknown7.57 | 7.57 | 70.4 | ng | 1097160 | 1 | 8.02 | 311539 | 20.0 |
| n-Hexadecanoic acid | 18.29 | 6.9 | ng | 265004 | 4 | 17.39 | 769125 | 20.0 |
| Cyclotetracosane | 21.31 | 2.7 | ng | 138872 | 5 | 21.66 | 1039070 | 20.0 |
| Docosanoic acid, ... | 22.51 | 3.1 | ng | 161848 | 5 | 21.66 | 1039070 | 20.0 |
| Hexadecane | 23.14 | 2.3 | ng | 121007 | 5 | 21.66 | 1039070 | 20.0 |
| Tricosane, 2-methyl- | 26.00 | 2.0 | ng | 114234 | 6 | 24.86 | 1137860 | 20.0 |