LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

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-BG092519.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 | 3.152 | 6 | 11 | 20 | rBV3 | 57305 | 128460 | 4.67% | 0.739% |
| 2 | 3.228 | 20 | 24 | 33 | rVB | 134698 | 211281 | 7.68% | 1.215% |
| 3 | 5.631 | 426 | 433 | 449 | rBV | 652028 | 1152702 | 41.89% | 6.631% |
| 4 | 7.223 | 696 | 704 | 716 | rBV | 722965 | 1355999 | 49.27% | 7.801% |
| 5 | 7.588 | 758 | 766 | 780 | rBV | 730318 | 1318425 | 47.91% | 7.585% |
| 6 | 8.052 | 837 | 845 | 856 | rBV2 | 156338 | 279483 | 10.16% | 1.608% |
| 7 | 8.375 | 892 | 900 | 911 | rBV | 534725 | 974426 | 35.41% | 5.606% |
| 8 | 9.209 | 1034 | 1042 | 1061 | rBV | 395715 | 822656 | 29.89% | 4.733% |
| 9 | 10.854 | 1314 | 1322 | 1335 | rBV | 171975 | 369338 | 13.42% | 2.125% |
| 10 | 13.299 | 1731 | 1738 | 1756 | rBV | 1057630 | 1763569 | 64.08% | 10.145% |
| 11 | 14.121 | 1872 | 1878 | 1891 | rBV | 118211 | 206872 | 7.52% | 1.190% |
| 12 | 14.673 | 1966 | 1972 | 1987 | rBV | 341472 | 589505 | 21.42% | 3.391% |
| 13 | 16.160 | 2219 | 2225 | 2247 | rBV | 1007632 | 1770127 | 64.32% | 10.183% |
| 14 | 17.423 | 2433 | 2440 | 2454 | rBV | 426932 | 767207 | 27.88% | 4.414% |
| 15 | 17.535 | 2455 | 2459 | 2468 | rVB5 | 22876 | 49696 | 1.81% | 0.286% |
| 16 | 18.310 | 2586 | 2591 | 2595 | rBV4 | 31415 | 52817 | 1.92% | 0.304% |
| 17 | 20.032 | 2877 | 2884 | 2896 | rBV | 1881140 | 2752060 | 100.00% | 15.832% |
| 18 | 20.331 | 2929 | 2935 | 2940 | rBV3 | 23445 | 35641 | 1.30% | 0.205% |
| 19 | 21.330 | 3100 | 3105 | 3114 | rBV2 | 120052 | 244740 | 8.89% | 1.408% |
| 20 | 21.695 | 3159 | 3167 | 3180 | rBV2 | 471347 | 928898 | 33.75% | 5.344% |
| 21 | 21.883 | 3195 | 3199 | 3203 | rVB3 | 22196 | 30187 | 1.10% | 0.174% |
| 22 | 22.488 | 3298 | 3302 | 3318 | rVB2 | 56521 | 123970 | 4.50% | 0.713% |
| 23 | 23.181 | 3415 | 3420 | 3426 | rVB4 | 39436 | 73988 | 2.69% | 0.426% |
| 24 | 23.375 | 3446 | 3453 | 3462 | rVB2 | 24139 | 61103 | 2.22% | 0.352% |
| 25 | 23.992 | 3551 | 3558 | 3565 | rVB2 | 56607 | 119770 | 4.35% | 0.689% |
| 26 | 24.914 | 3705 | 3715 | 3733 | rBV2 | 328164 | 1056685 | 38.40% | 6.079% |
| 27 | 26.066 | 3904 | 3911 | 3921 | rVB6 | 35341 | 103148 | 3.75% | 0.593% |
| 28 | 27.417 | 4139 | 4141 | 4152 | rVB8 | 17527 | 40299 | 1.46% | 0.232% |

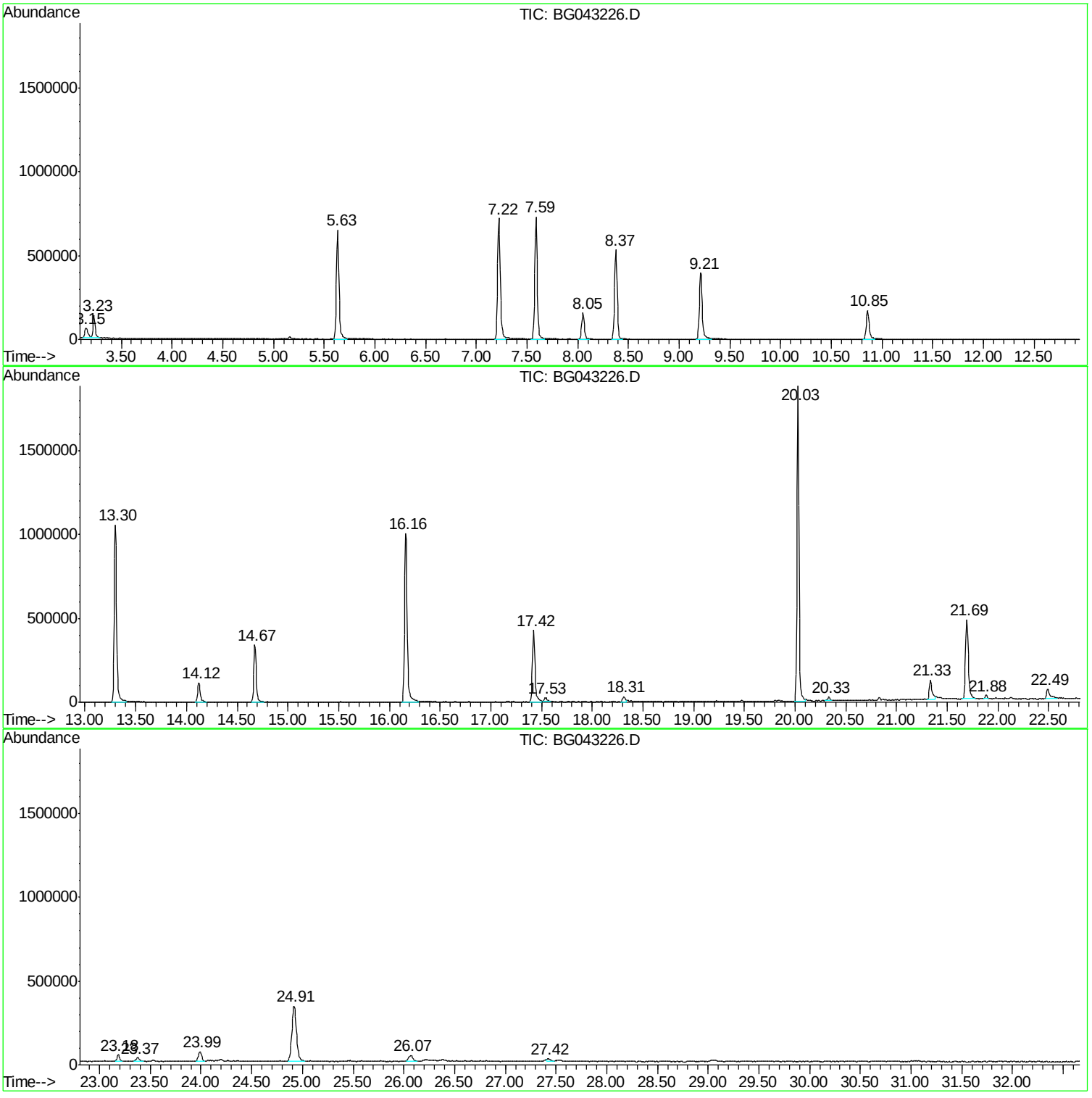
Sum of corrected areas: 17383052

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

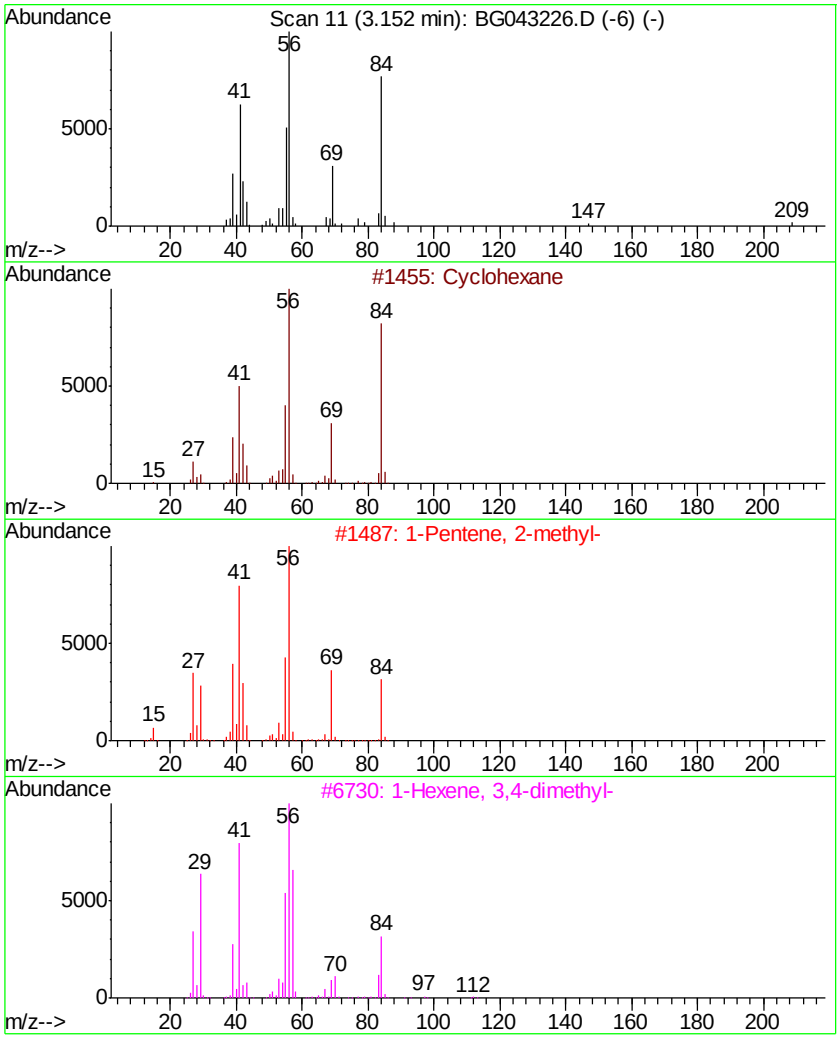
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

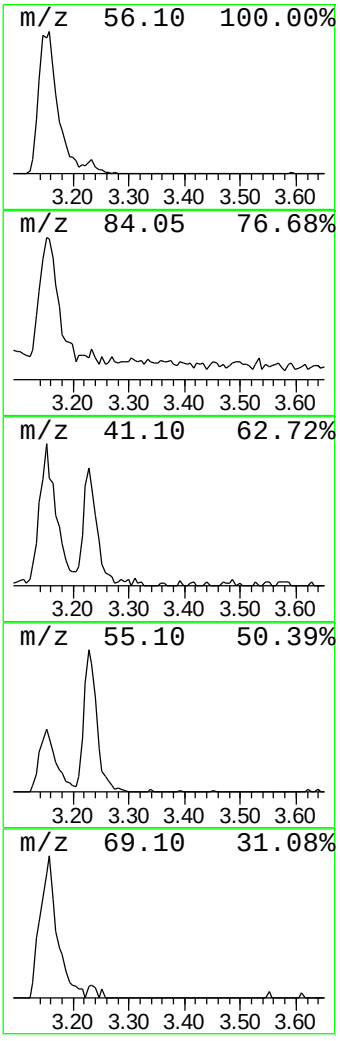
**********

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.15 | 9.19 ng | 128460 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane | 84 | C6H12 | 000110-82-7 | 91 |
| 2 | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 86 |
| 3 | 1-Hexene, 3,4-dimethyl- | 112 | C8H16 | 016745-94-1 | 72 |
| 4 | Pyridine-D5- | 84 | C5D5N | 007291-22-7 | 64 |
| 5 | Cyclopentanone | 84 | C5H8O | 000120-92-3 | 53 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

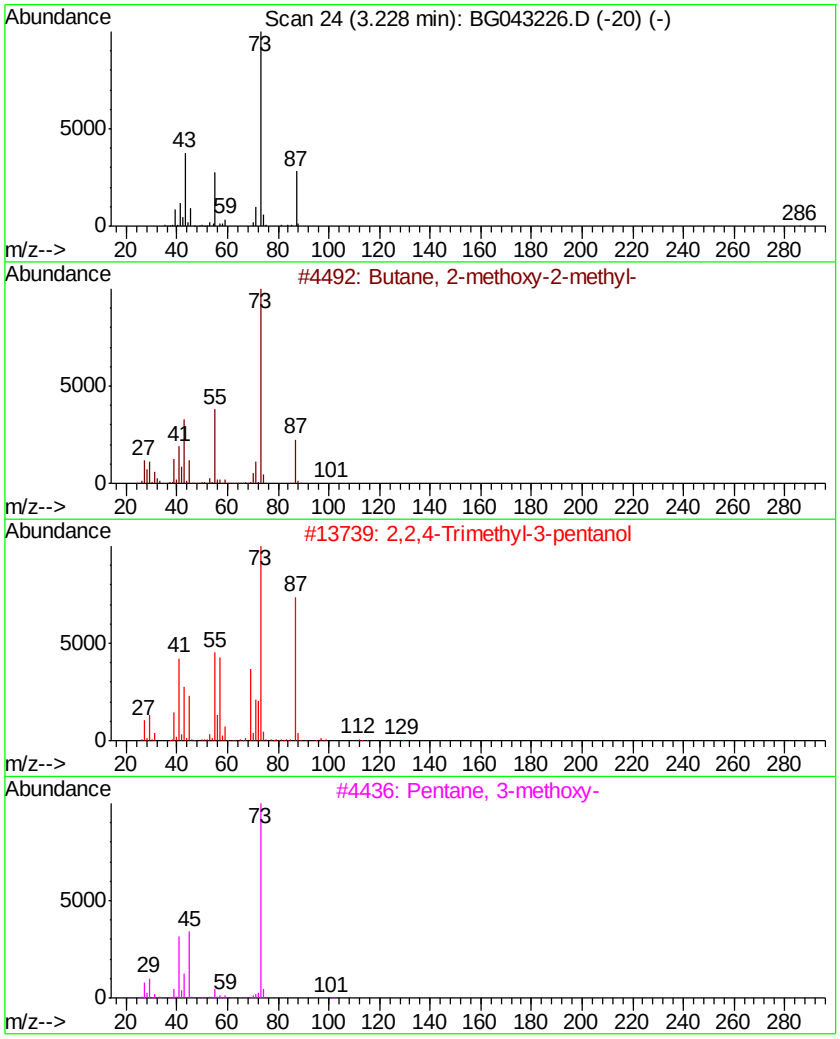
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

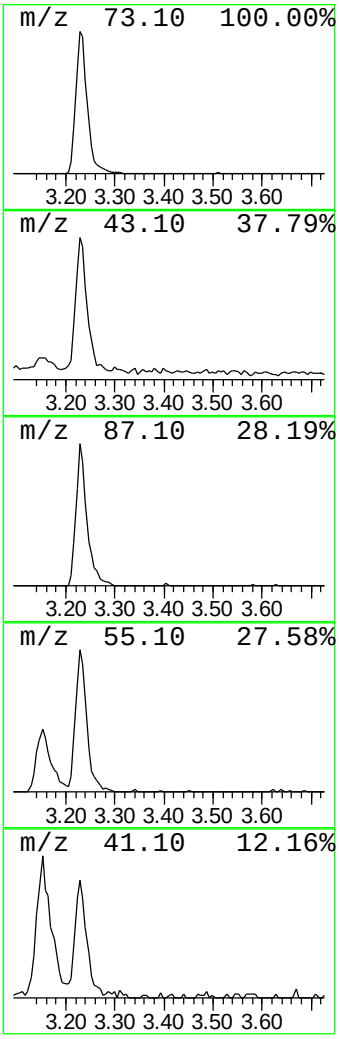
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.23 | 15.12 ng | 211281 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 64 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 10 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

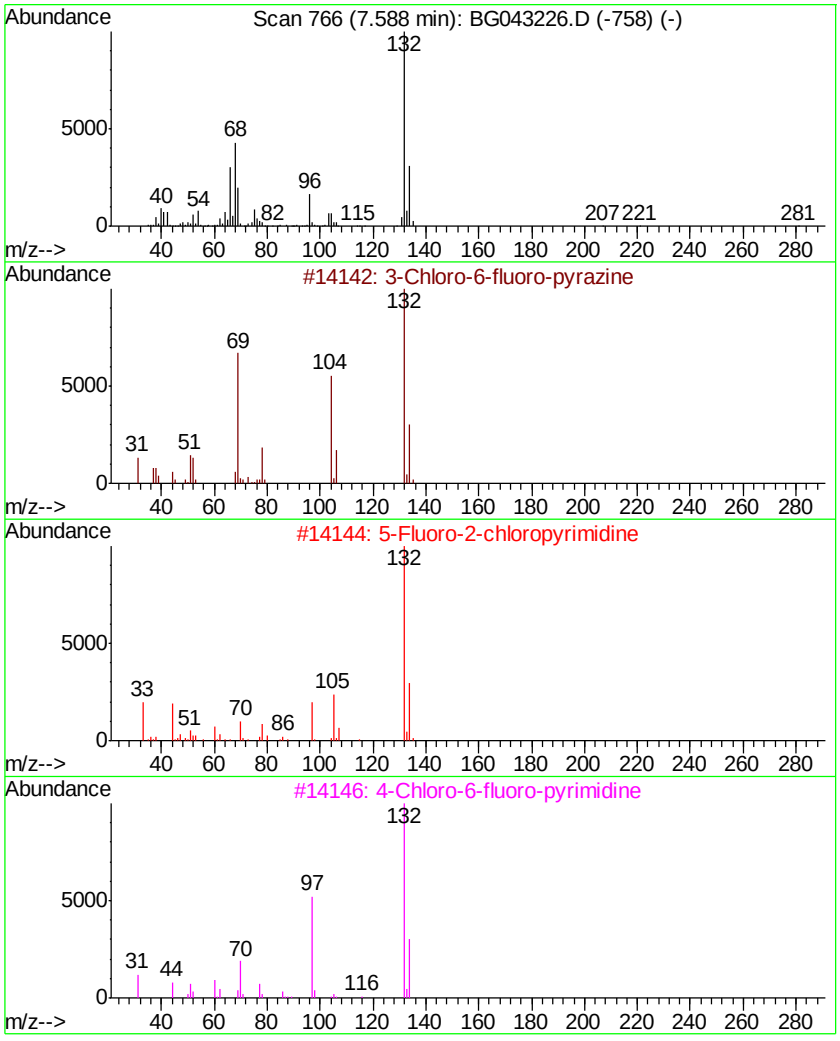
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

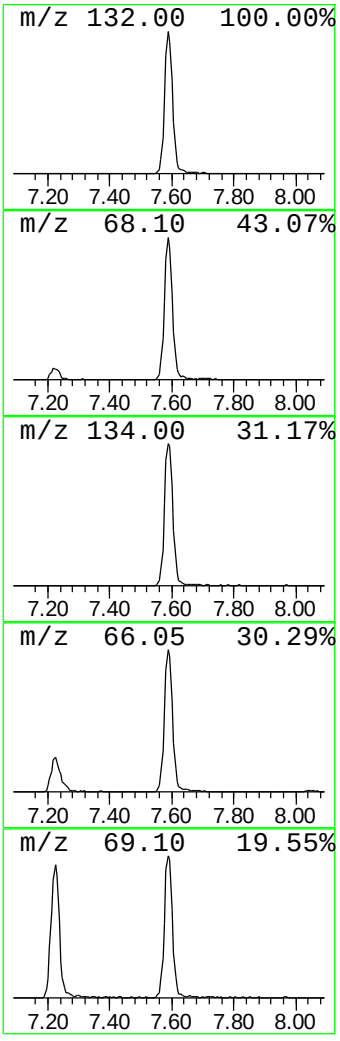
**********

Peak Number 3 unknown7.59 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.59 | 94.35 ng | 1318430 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 27 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 5 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 13 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

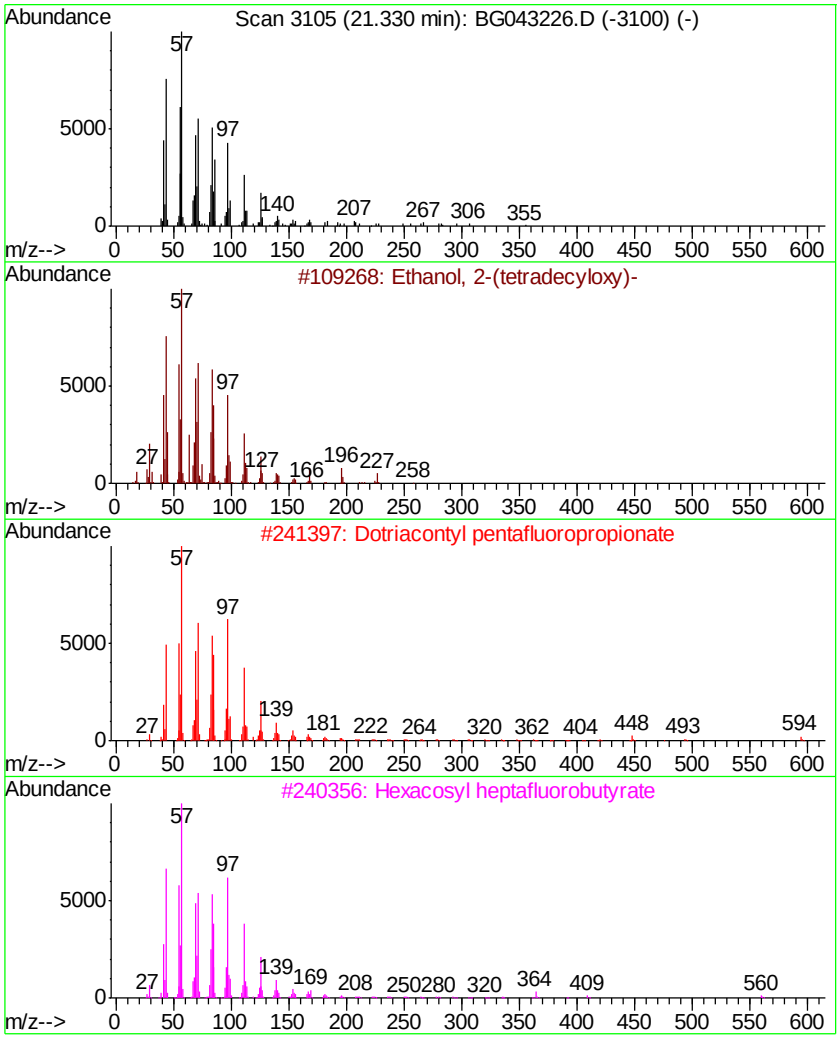
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

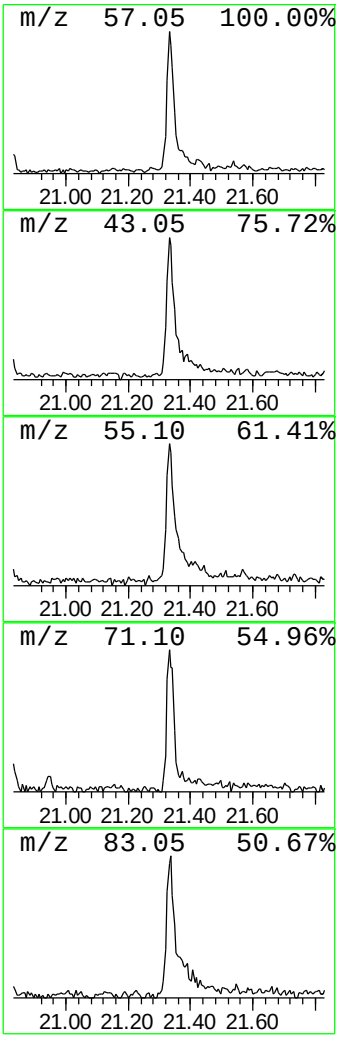
**********

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.33 | 5.27 ng | 244740 | Chrysene-d12 | 21.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 91 |
| 2 | Dotriacontyl pentafluoropropionate | 612 | C35H65F5O2 | 1000351-81-4 | 91 |
| 3 | Hexacosyl heptafluorobutyrate | 578 | C30H53F7O2 | 1000351-83-3 | 91 |
| 4 | Dotriacontyl heptafluorobutyrate | 662 | C36H65F7O2 | 1000351-84-2 | 91 |
| 5 | Dotriacontyl trifluoroacetate | 562 | C34H65F3O2 | 1000351-75-4 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

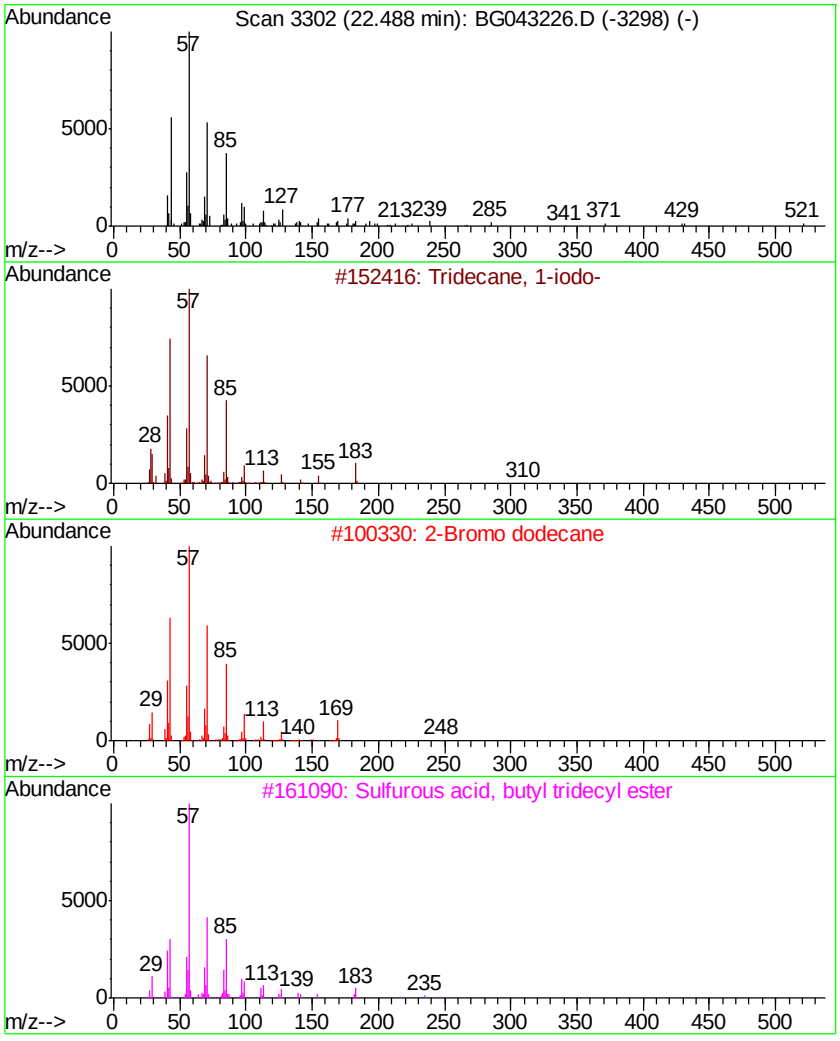
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

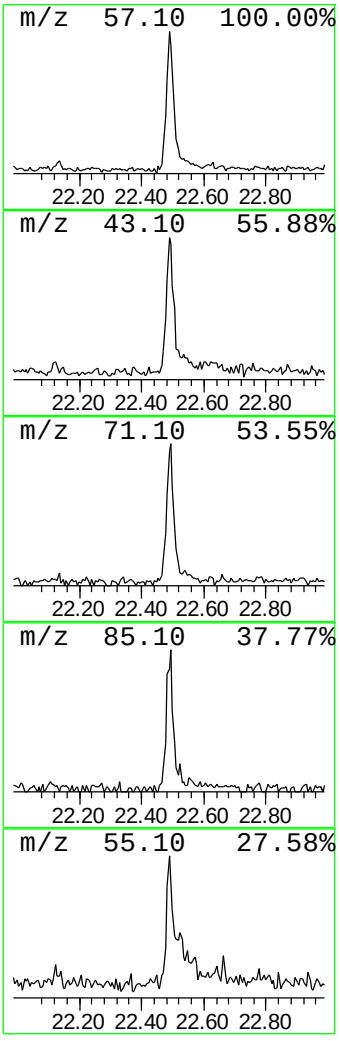
**********

Peak Number 6 Tridecane, 1-iodo- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.49 | 2.67 ng | 123970 | Chrysene-d12 | 21.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 74 |
| 2 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 72 |
| 3 | Sulfurous acid, butyl tridecyl e... | 320 | C17H36O3S | 1000309-18-0 | 72 |
| 4 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 64 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 64 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

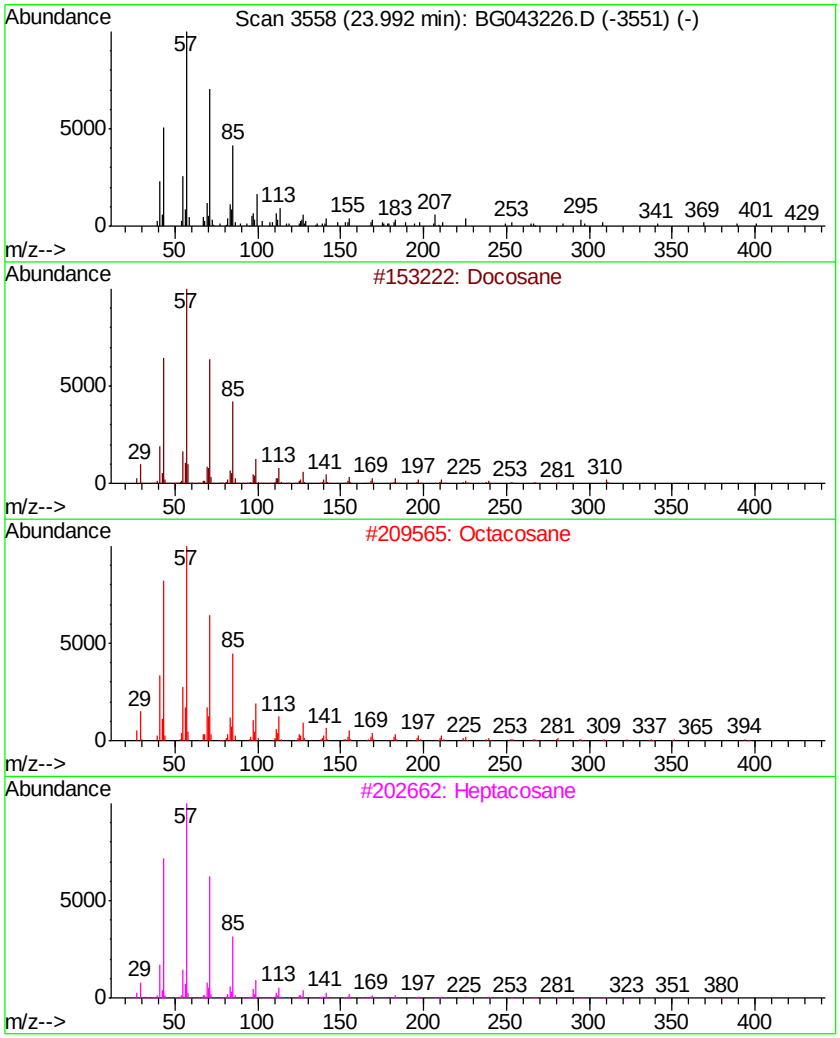
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

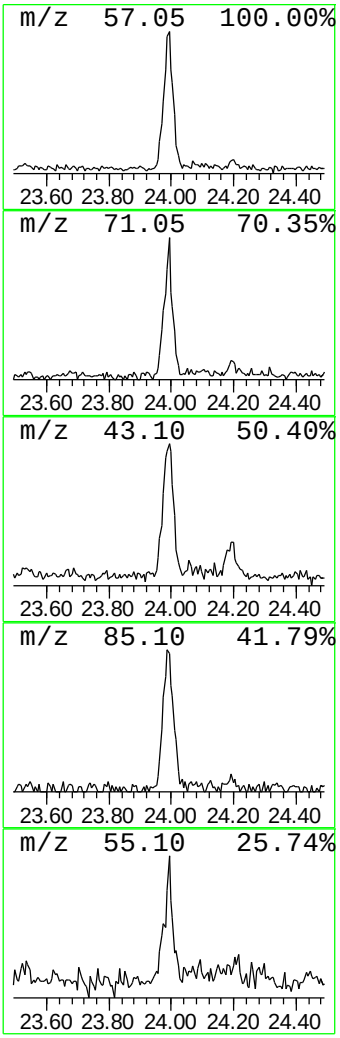
**********

Peak Number 7 Docosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.99 | 2.27 ng | 119770 | Perylene-d12 | 24.91 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane | 310 | C22H46 | 000629-97-0 | 83 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 80 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 80 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |
| 5 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101519\
Data File : BG043226.D
Acq On : 15 Oct 2019 19:49
Operator : JU
Sample : K5350-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** VNJ-11935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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 |
| 1-Pentene, 2-methyl- | 3.15 | 9.2 | ng | 128460 | 1 | 8.05 | 279483 | 20.0 |
| Butane, 2-methoxy... | 3.23 | 15.1 | ng | 211281 | 1 | 8.05 | 279483 | 20.0 |
| unknown7.59 | 7.59 | 94.3 | ng | 1318430 | 1 | 8.05 | 279483 | 20.0 |
| Ethanol, 2-(tetra... | 21.33 | 5.3 | ng | 244740 | 5 | 21.69 | 928898 | 20.0 |
| Tridecane, 1-iodo- | 22.49 | 2.7 | ng | 123970 | 5 | 21.69 | 928898 | 20.0 |
| Docosane | 23.99 | 2.3 | ng | 119770 | 6 | 24.91 | 1056690 | 20.0 |