LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-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 | 3.169 | 10 | 14 | 27 | rVB | 96387 | 146685 | 6.26% | 1.222% |
| 2 | 5.108 | 338 | 344 | 357 | rBV | 90327 | 142274 | 6.07% | 1.185% |
| 3 | 5.596 | 418 | 427 | 439 | rBV | 426123 | 747811 | 31.91% | 6.229% |
| 4 | 7.194 | 688 | 699 | 715 | rBV | 451492 | 874475 | 37.32% | 7.284% |
| 5 | 7.552 | 751 | 760 | 773 | rBV | 455437 | 852630 | 36.39% | 7.102% |
| 6 | 8.011 | 832 | 838 | 845 | rBV | 96496 | 171876 | 7.33% | 1.432% |
| 7 | 8.334 | 885 | 893 | 900 | rBV | 360869 | 655729 | 27.98% | 5.462% |
| 8 | 9.174 | 1026 | 1036 | 1051 | rBV | 233823 | 502958 | 21.46% | 4.190% |
| 9 | 10.813 | 1307 | 1315 | 1325 | rBV | 100945 | 215768 | 9.21% | 1.797% |
| 10 | 13.263 | 1724 | 1732 | 1757 | rBV | 751611 | 1306302 | 55.75% | 10.882% |
| 11 | 14.092 | 1866 | 1873 | 1885 | rBV | 72972 | 141044 | 6.02% | 1.175% |
| 12 | 14.638 | 1960 | 1966 | 1978 | rBV2 | 207514 | 357451 | 15.25% | 2.978% |
| 13 | 16.131 | 2213 | 2220 | 2240 | rBV2 | 654931 | 1222808 | 52.18% | 10.186% |
| 14 | 17.388 | 2426 | 2434 | 2449 | rBV | 261799 | 479155 | 20.45% | 3.991% |
| 15 | 18.275 | 2580 | 2585 | 2593 | rBV4 | 29268 | 51430 | 2.19% | 0.428% |
| 16 | 19.997 | 2871 | 2878 | 2891 | rBV | 1735752 | 2343309 | 100.00% | 19.520% |
| 17 | 21.295 | 3095 | 3099 | 3111 | rBV3 | 63278 | 168609 | 7.20% | 1.405% |
| 18 | 21.654 | 3152 | 3160 | 3172 | rBV2 | 312154 | 608432 | 25.96% | 5.068% |
| 19 | 21.836 | 3186 | 3191 | 3195 | rBV2 | 23184 | 35924 | 1.53% | 0.299% |
| 20 | 22.435 | 3289 | 3293 | 3298 | rVB | 26852 | 42876 | 1.83% | 0.357% |
| 21 | 23.122 | 3404 | 3410 | 3416 | rVB3 | 33555 | 71401 | 3.05% | 0.595% |
| 22 | 23.310 | 3436 | 3442 | 3452 | rVB3 | 44335 | 98400 | 4.20% | 0.820% |
| 23 | 23.910 | 3539 | 3544 | 3556 | rVB3 | 29195 | 68579 | 2.93% | 0.571% |
| 24 | 24.850 | 3694 | 3704 | 3720 | rBV2 | 223833 | 675095 | 28.81% | 5.624% |
| 25 | 27.282 | 4110 | 4118 | 4120 | rBV9 | 11534 | 23755 | 1.01% | 0.198% |

Sum of corrected areas: 12004776

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
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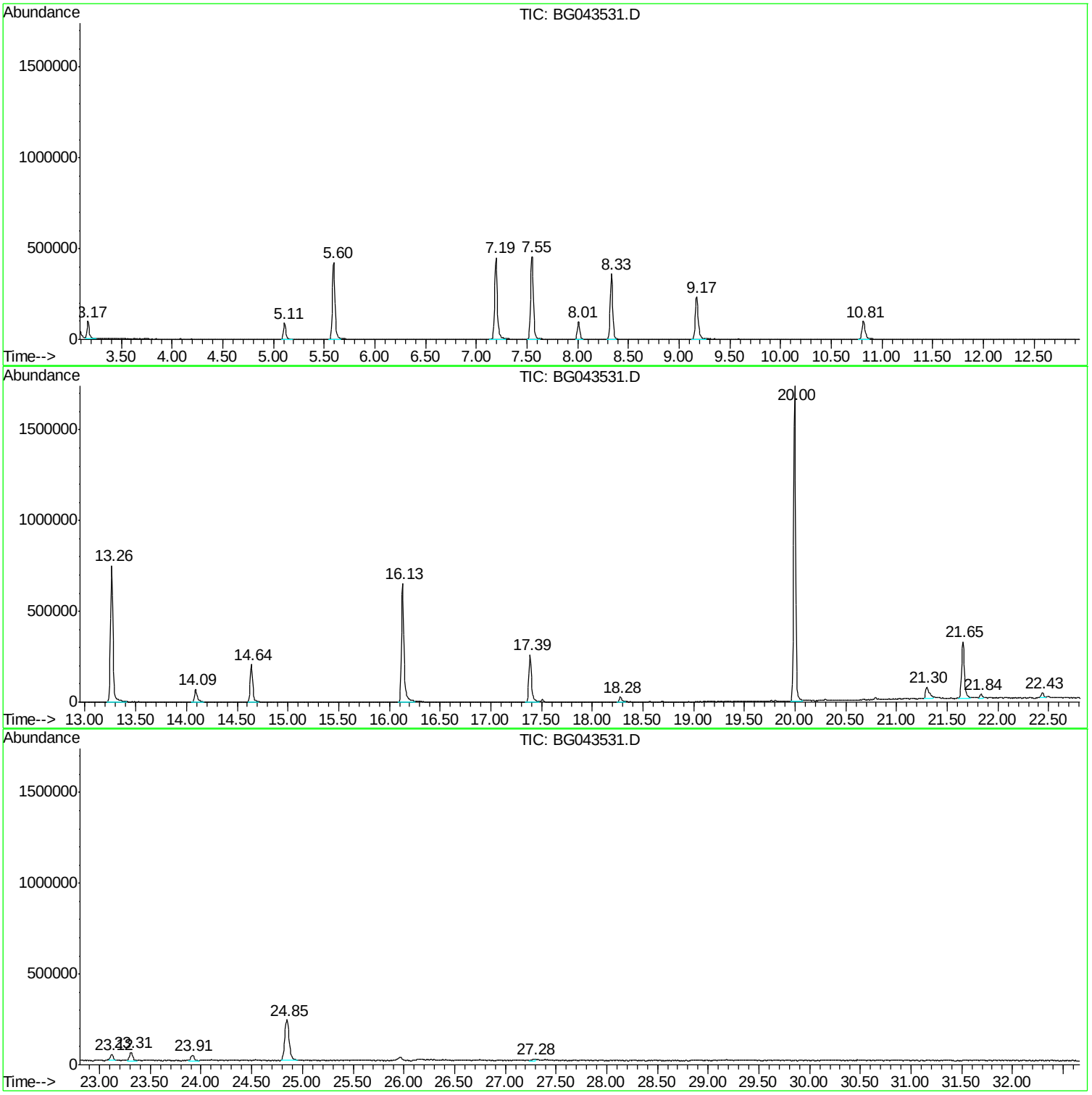
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-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\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

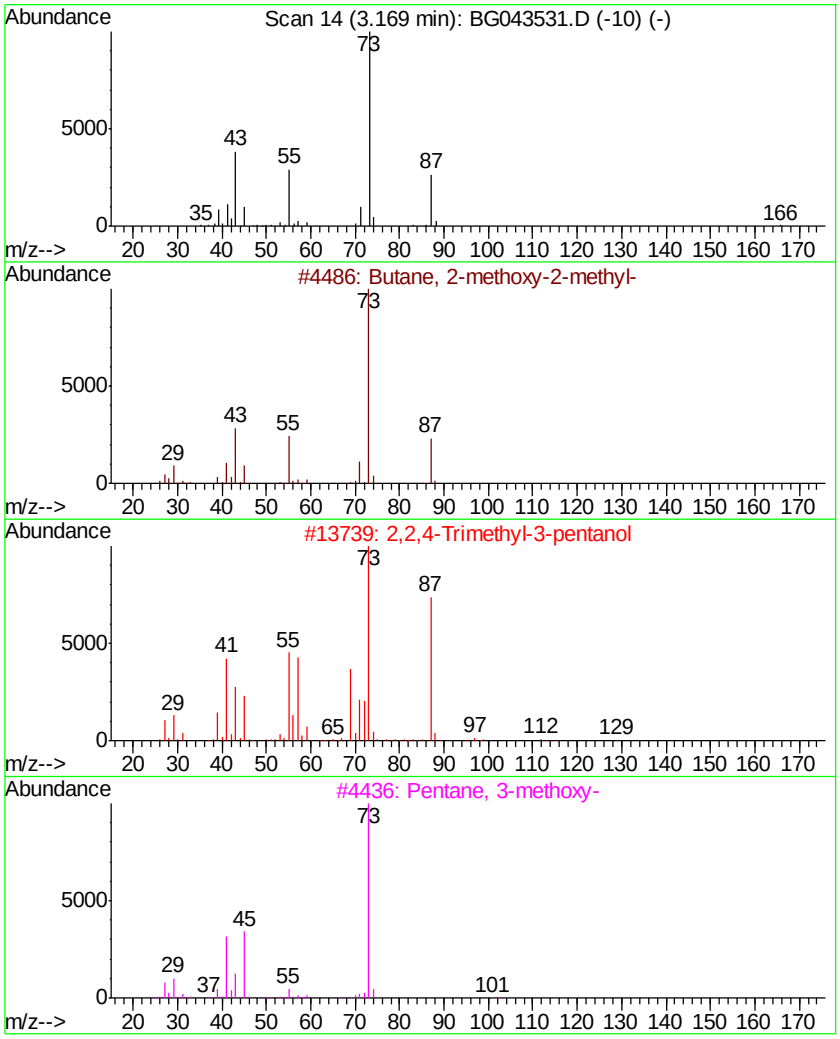
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

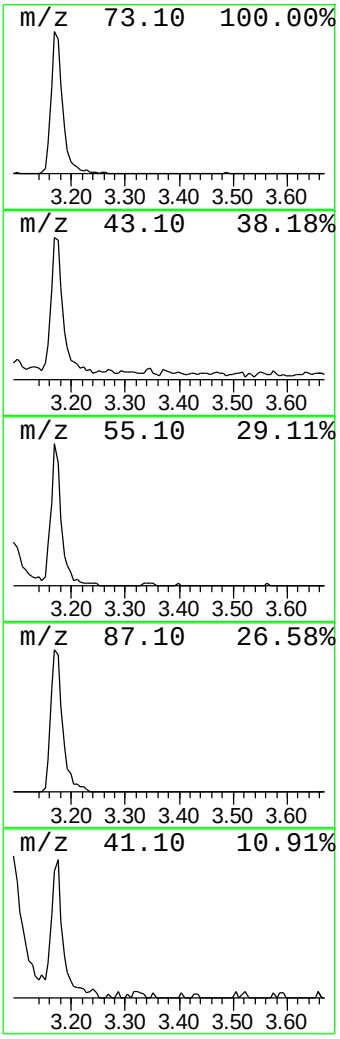
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.17 | 17.07 ng | 146685 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

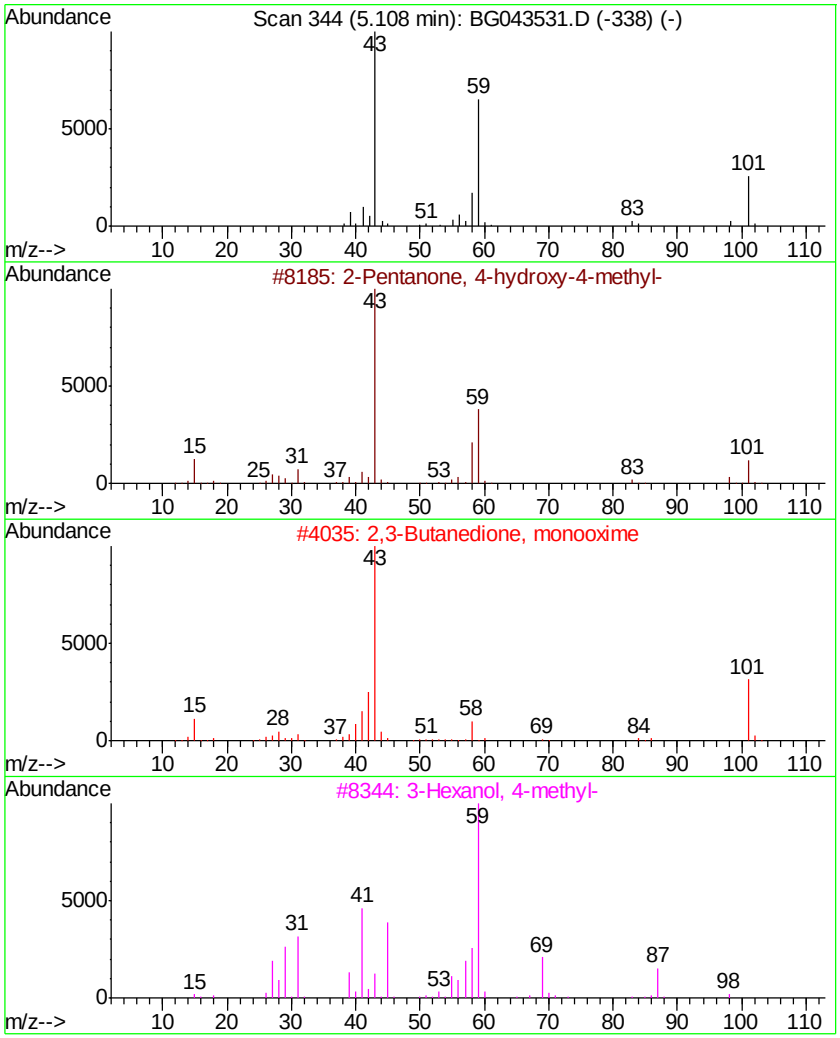
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

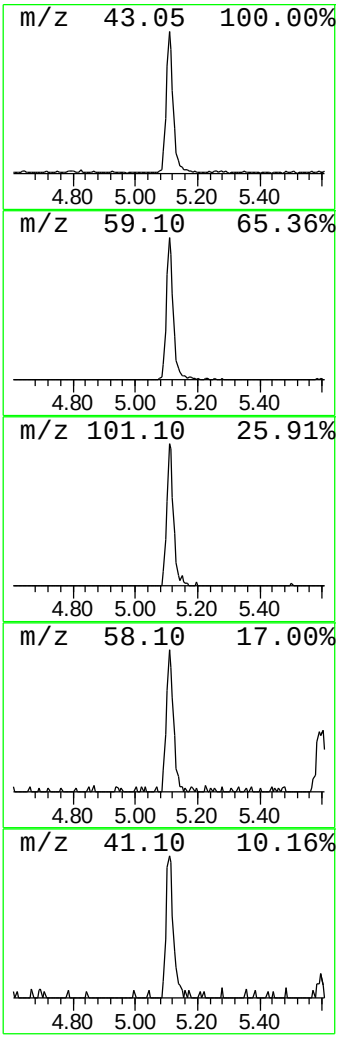
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 16.56 ng | 142274 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 38 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 25 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

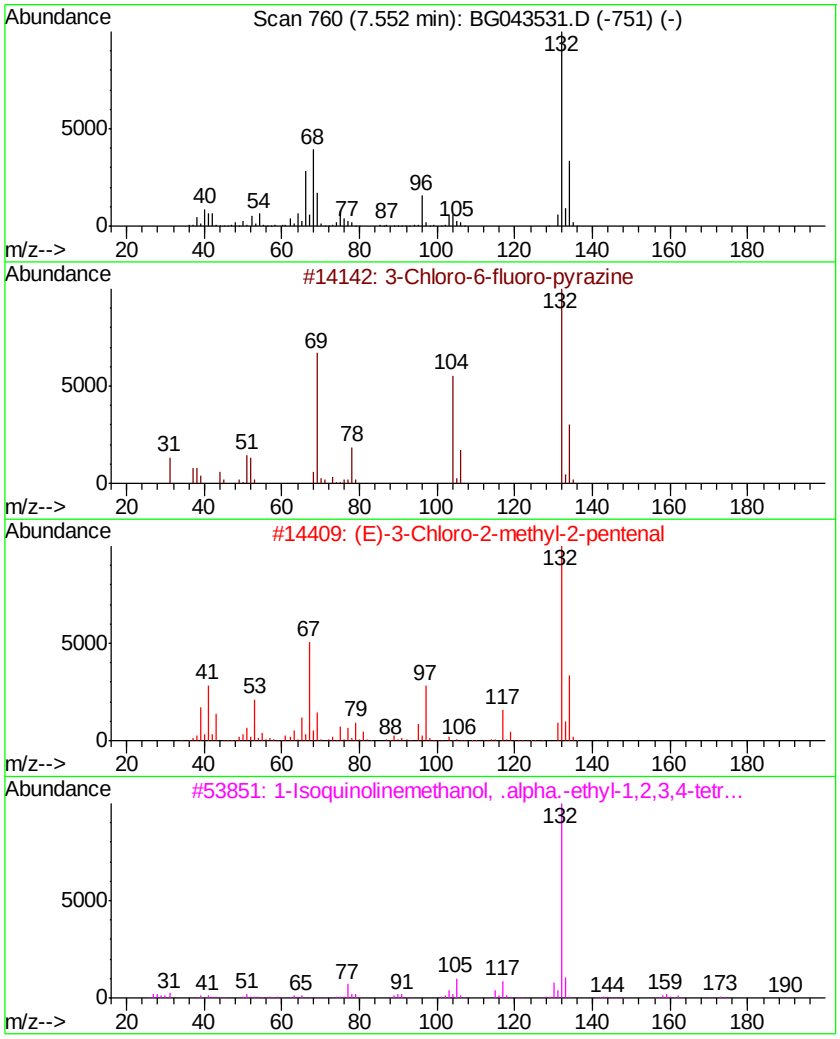
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

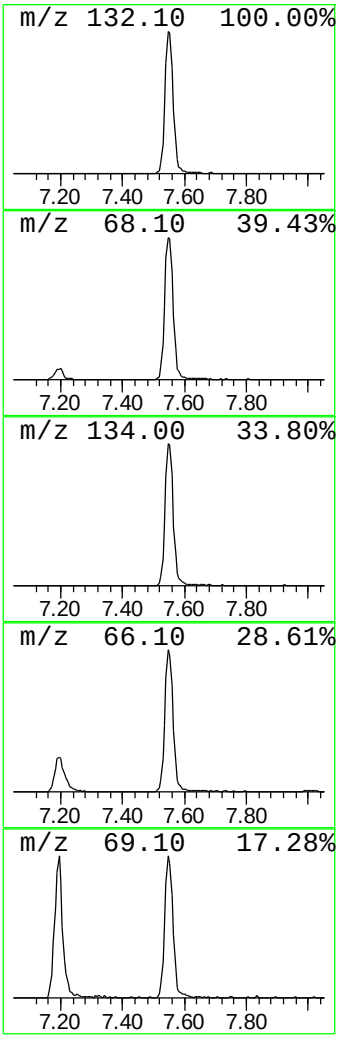
**********

Peak Number 3 unknown7.55 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.55 | 99.21 ng | 852630 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 1-Isoquinolinemethanol, .alpha.-... | 191 | C12H17NO | 114608-92-3 | 12 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

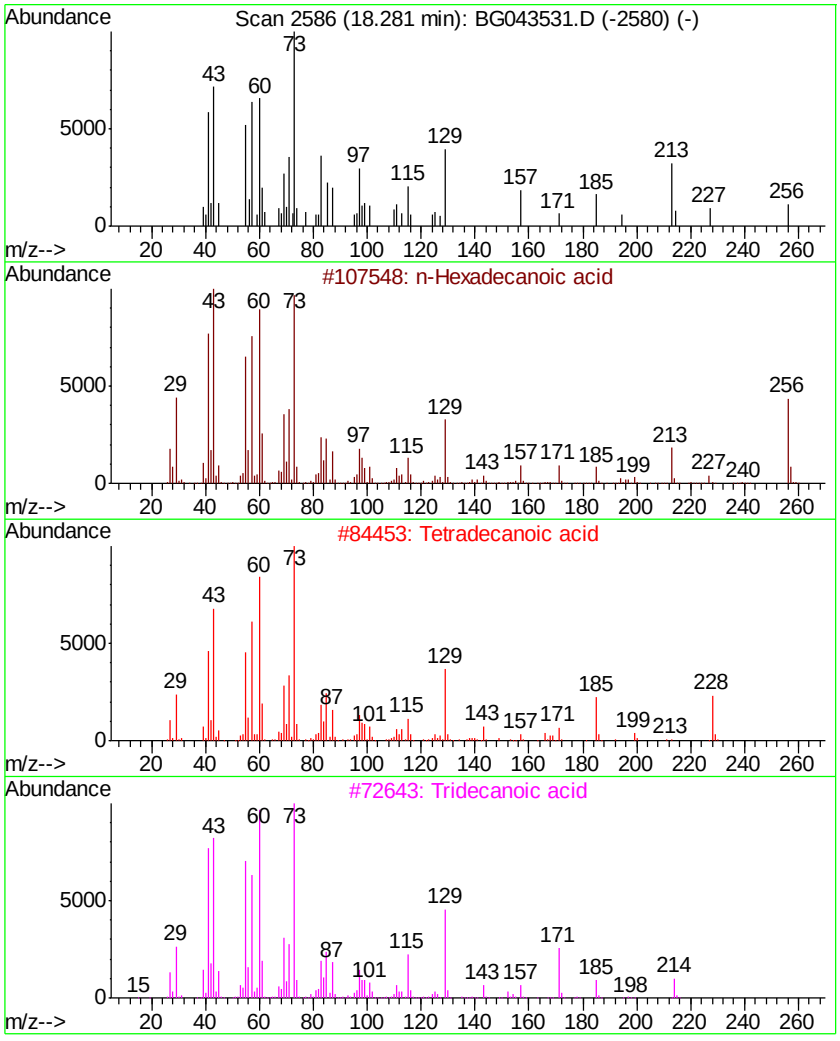
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

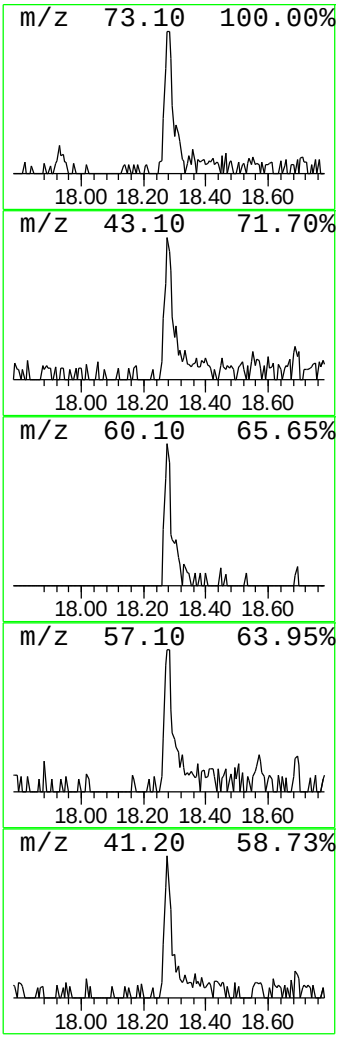
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.28 | 2.15 ng | 51430 | Phenanthrene-d10 | 17.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 52 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 47 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 43 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

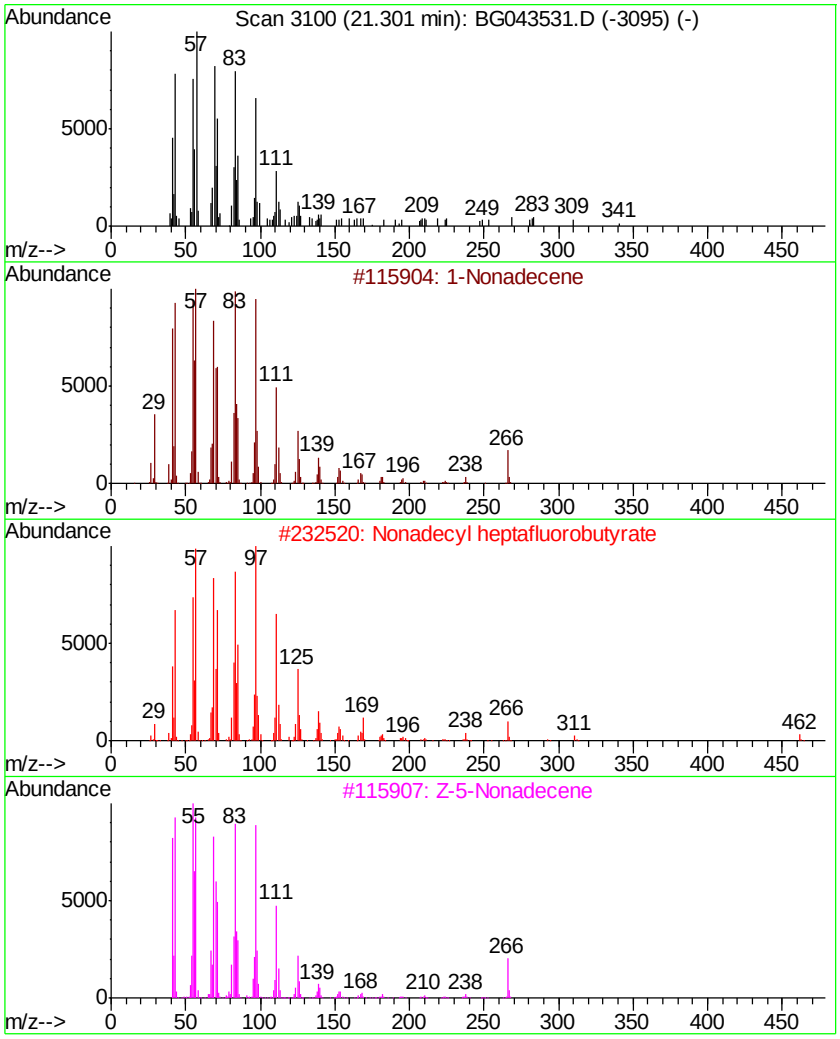
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

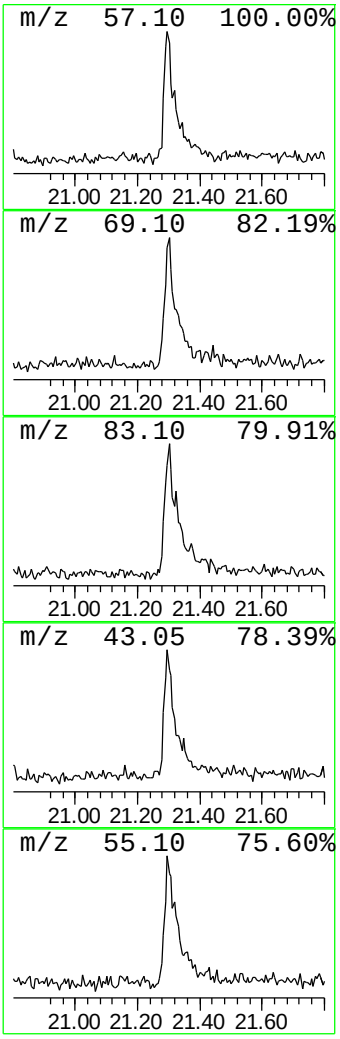
**********

Peak Number 6 1-Nonadecene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.30 | 5.54 ng | 168609 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 93 |
| 2 | Nonadecyl heptafluorobutyrate | 480 | C23H39F7O2 | 1000351-83-9 | 91 |
| 3 | Z-5-Nonadecene | 266 | C19H38 | 1000131-11-8 | 89 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 87 |
| 5 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

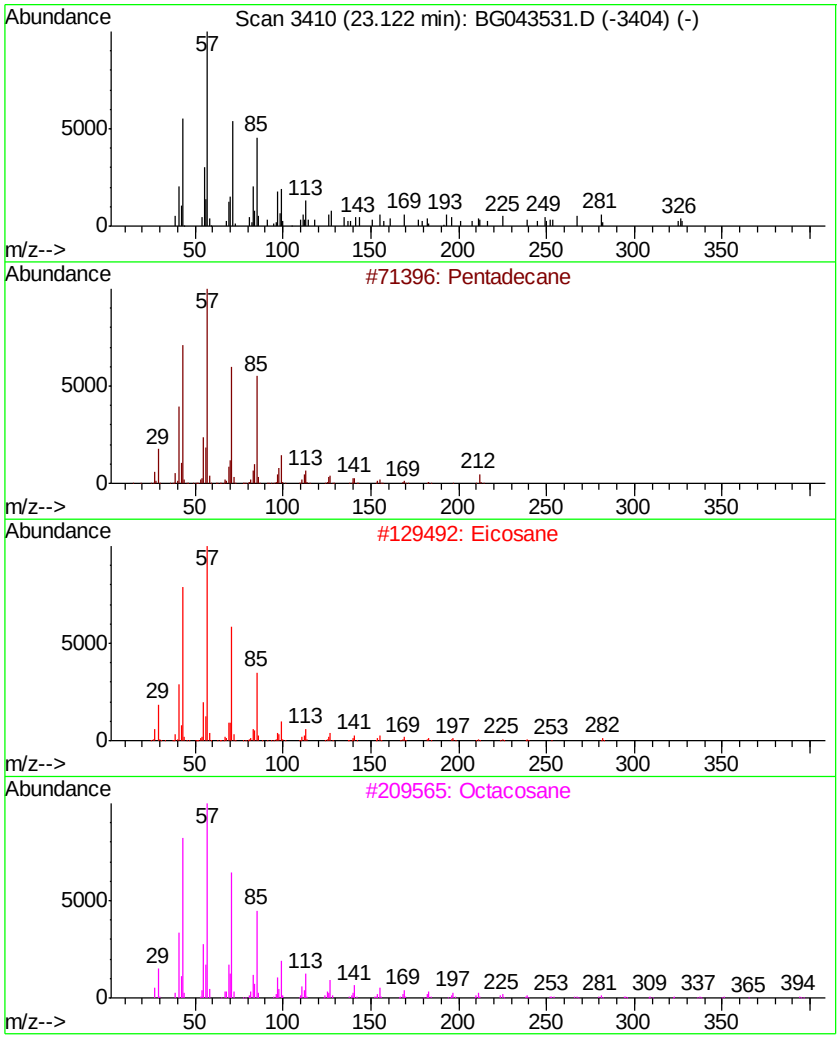
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

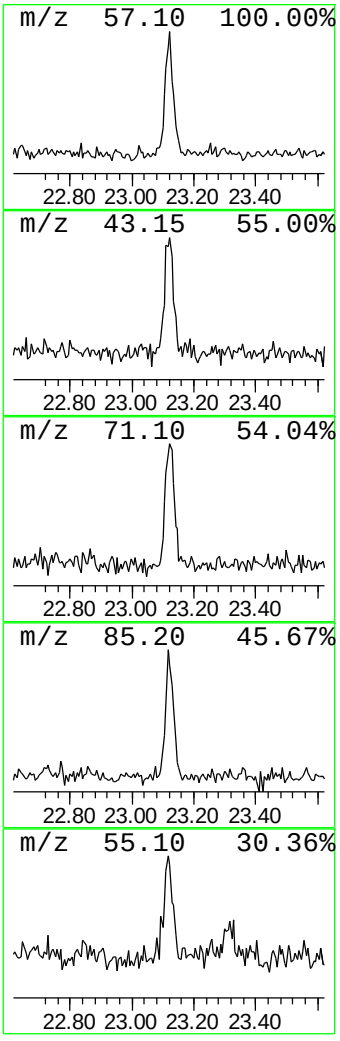
**********

Peak Number 7 Pentadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.12 | 2.35 ng | 71401 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 76 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 76 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 74 |
| 4 | Tetradecane, 2-methyl- | 212 | C15H32 | 001560-95-8 | 72 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 72 |



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Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

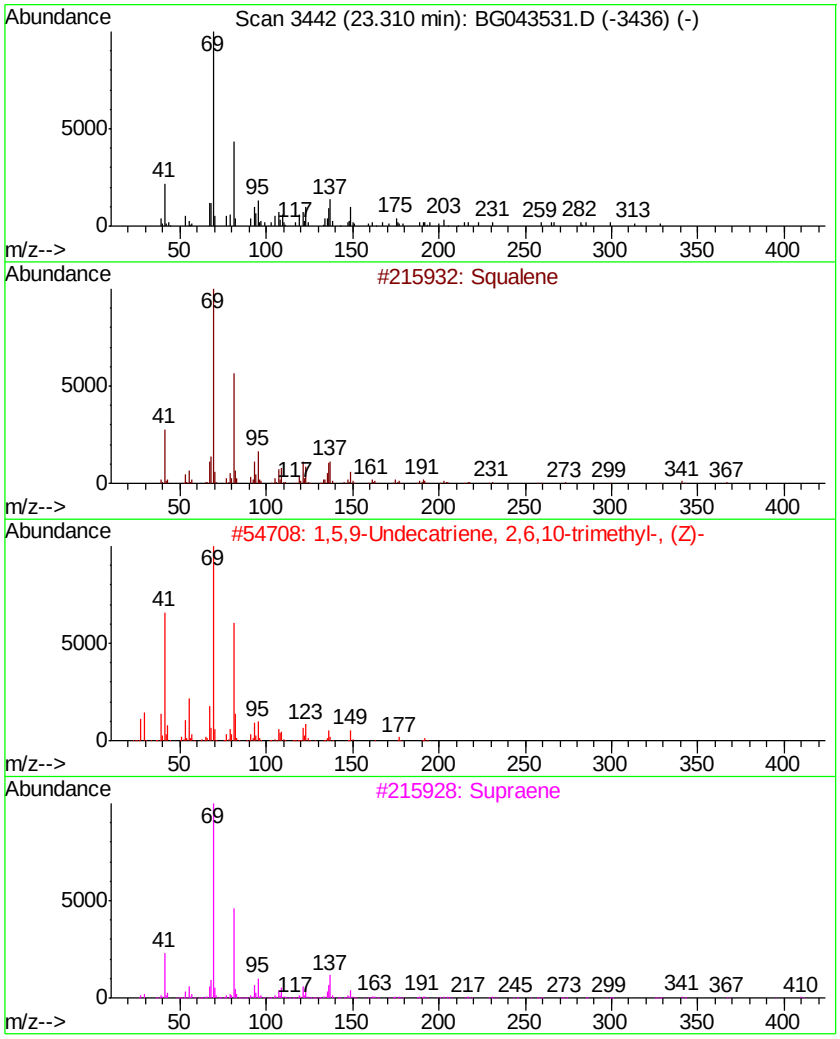
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

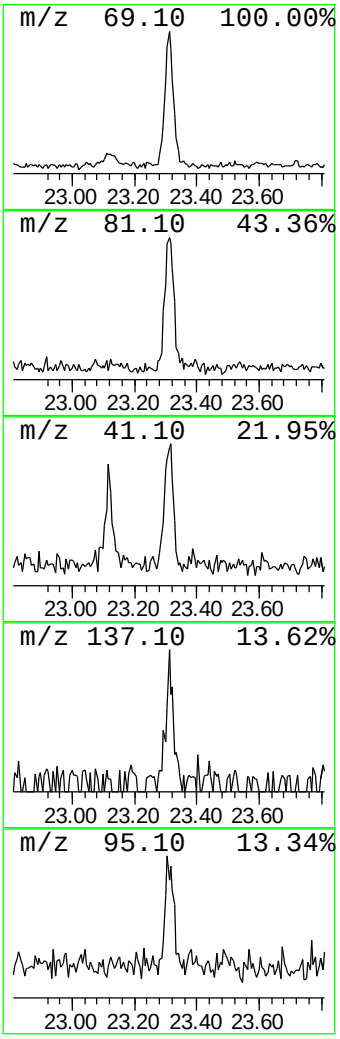
**********

Peak Number 8 Squalene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.31 | 2.92 ng | 98400 | Perylene-d12 | 24.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 90 |
| 2 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 87 |
| 3 | Supraene | 410 | C30H50 | 007683-64-9 | 86 |
| 4 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 64 |
| 5 | 1-(3,5-Dinitrophenoxy)-3,7,11-tr... | 388 | C21H28N2O5 | 1000187-44-2 | 64 |



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Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-1

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

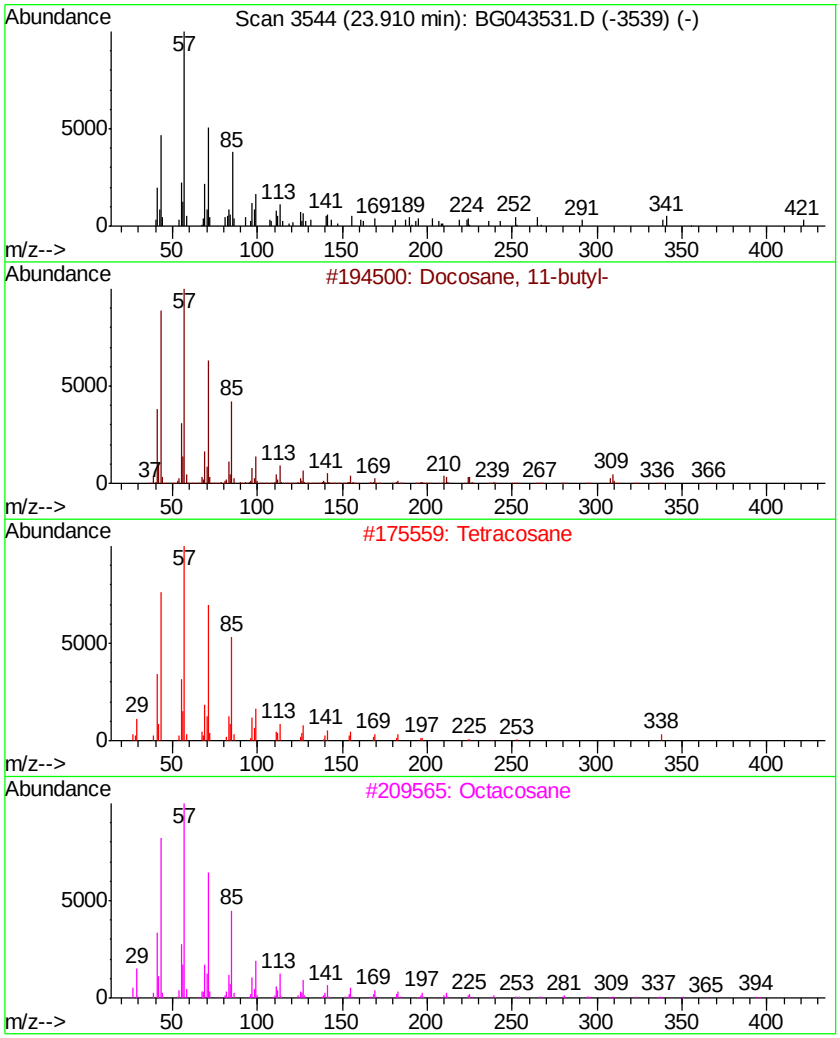
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

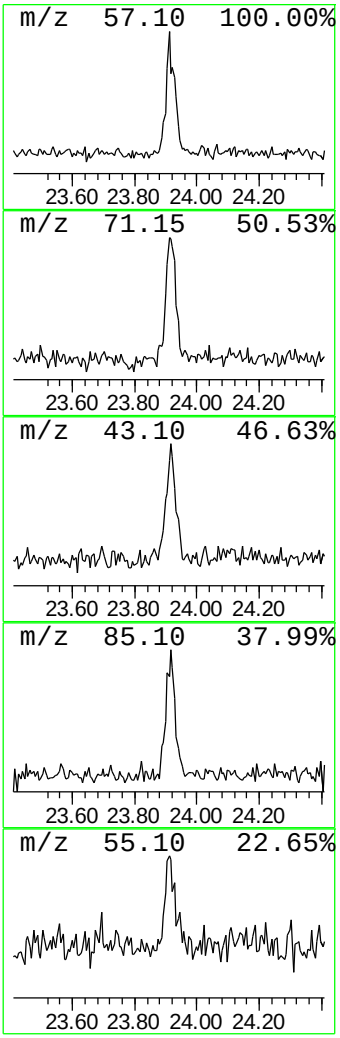
**********

Peak Number 9 Docosane, 11-butyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.91 | 2.03 ng | 68579 | Perylene-d12 | 24.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 83 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 81 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 81 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 74 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 74 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110619\
Data File : BG043531.D
Acq On : 6 Nov 2019 22:05
Operator : JU
Sample : K5701-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** J-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... | 3.17 | 17.1 | ng | 146685 | 1 | 8.01 | 171876 | 20.0 |
| 2-Pentanone, 4-hy... | 5.11 | 16.6 | ng | 142274 | 1 | 8.01 | 171876 | 20.0 |
| unknown7.55 | 7.55 | 99.2 | ng | 852630 | 1 | 8.01 | 171876 | 20.0 |
| n-Hexadecanoic acid | 18.28 | 2.1 | ng | 51430 | 4 | 17.39 | 479155 | 20.0 |
| 1-Nonadecene | 21.30 | 5.5 | ng | 168609 | 5 | 21.65 | 608432 | 20.0 |
| Pentadecane | 23.12 | 2.4 | ng | 71401 | 5 | 21.65 | 608432 | 20.0 |
| Squalene | 23.31 | 2.9 | ng | 98400 | 6 | 24.85 | 675095 | 20.0 |
| Docosane, 11-butyl- | 23.91 | 2.0 | ng | 68579 | 6 | 24.85 | 675095 | 20.0 |