LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

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-BG061520.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 | 3.367 | 41 | 47 | 58 | rBV | 66573 | 122352 | 3.16% | 0.737% |
| 2 | 4.524 | 237 | 244 | 257 | rBV | 270987 | 515053 | 13.31% | 3.104% |
| 3 | 5.223 | 355 | 363 | 369 | rBV | 30048 | 55179 | 1.43% | 0.333% |
| 4 | 5.529 | 409 | 415 | 426 | rBV | 247278 | 446445 | 11.53% | 2.691% |
| 5 | 7.144 | 684 | 690 | 702 | rBV2 | 163315 | 323679 | 8.36% | 1.951% |
| 6 | 7.914 | 814 | 821 | 833 | rBV | 161021 | 306249 | 7.91% | 1.846% |
| 7 | 8.237 | 867 | 876 | 891 | rBV | 529871 | 988758 | 25.54% | 5.959% |
| 8 | 9.077 | 1012 | 1019 | 1028 | rBV | 468196 | 857123 | 22.14% | 5.166% |
| 9 | 10.722 | 1292 | 1299 | 1308 | rBV | 211907 | 385204 | 9.95% | 2.322% |
| 10 | 13.183 | 1707 | 1718 | 1728 | rBV | 1432490 | 2222688 | 57.42% | 13.396% |
| 11 | 14.017 | 1853 | 1860 | 1867 | rBV | 113640 | 174448 | 4.51% | 1.051% |
| 12 | 14.563 | 1946 | 1953 | 1961 | rBV2 | 342012 | 557477 | 14.40% | 3.360% |
| 13 | 15.309 | 2073 | 2080 | 2085 | rBV | 160724 | 236960 | 6.12% | 1.428% |
| 14 | 15.474 | 2101 | 2108 | 2119 | rBV | 39788 | 84191 | 2.17% | 0.507% |
| 15 | 16.067 | 2201 | 2209 | 2219 | rBV3 | 1325052 | 2299235 | 59.39% | 13.857% |
| 16 | 16.590 | 2291 | 2298 | 2306 | rBV | 164434 | 253514 | 6.55% | 1.528% |
| 17 | 17.313 | 2415 | 2421 | 2431 | rBV | 463129 | 697461 | 18.02% | 4.204% |
| 18 | 18.223 | 2570 | 2576 | 2583 | rBV | 88495 | 136211 | 3.52% | 0.821% |
| 19 | 19.416 | 2773 | 2779 | 2784 | rBV | 55605 | 71229 | 1.84% | 0.429% |
| 20 | 19.933 | 2861 | 2867 | 2880 | rBV | 2904993 | 3871092 | 100.00% | 23.331% |
| 21 | 21.231 | 3083 | 3088 | 3104 | rBV | 161480 | 366536 | 9.47% | 2.209% |
| 22 | 21.572 | 3140 | 3146 | 3155 | rBV | 463089 | 781418 | 20.19% | 4.710% |
| 23 | 24.697 | 3668 | 3678 | 3694 | rBV | 279634 | 839665 | 21.69% | 5.061% |

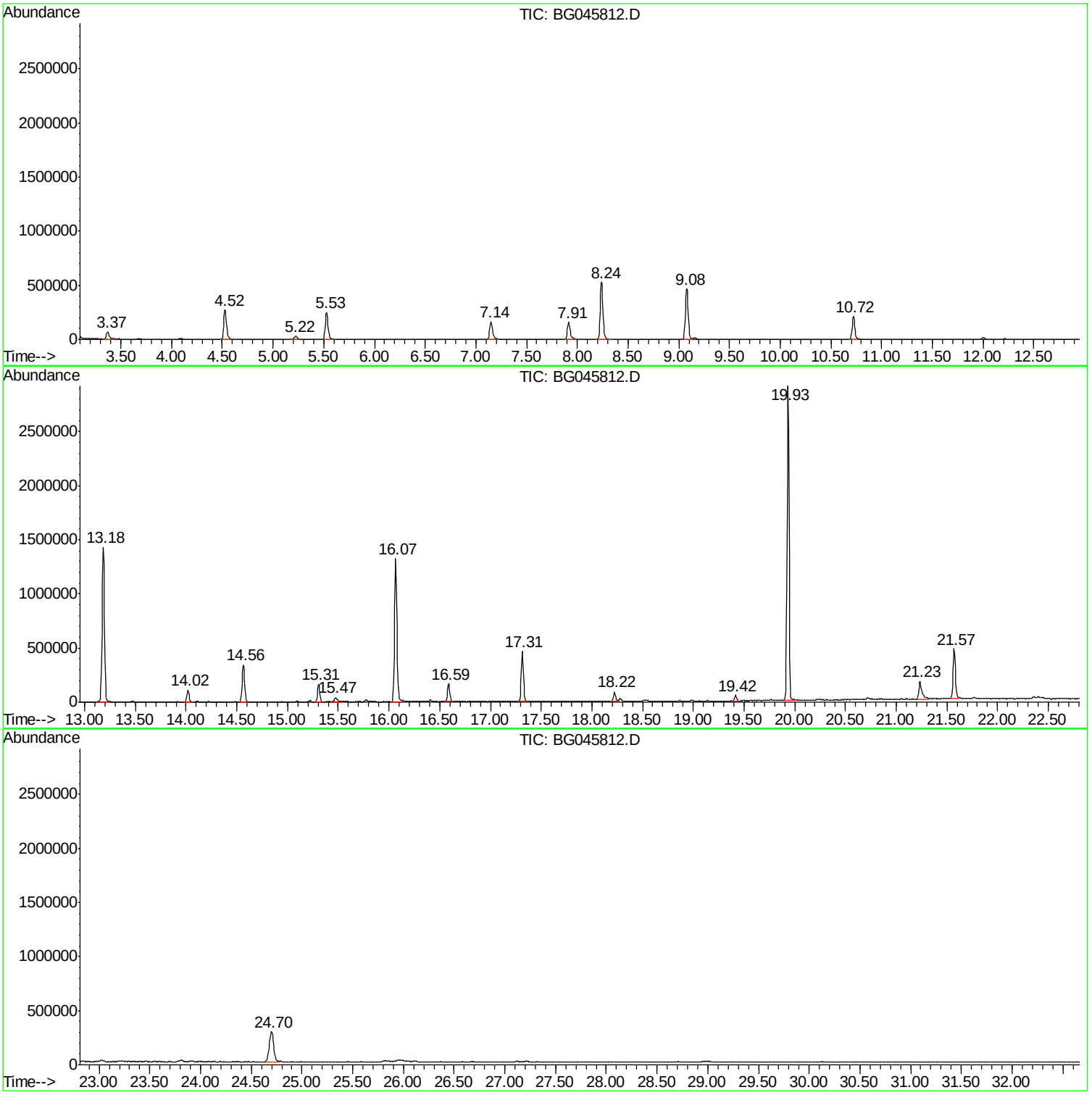
Sum of corrected areas: 16592167

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.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\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

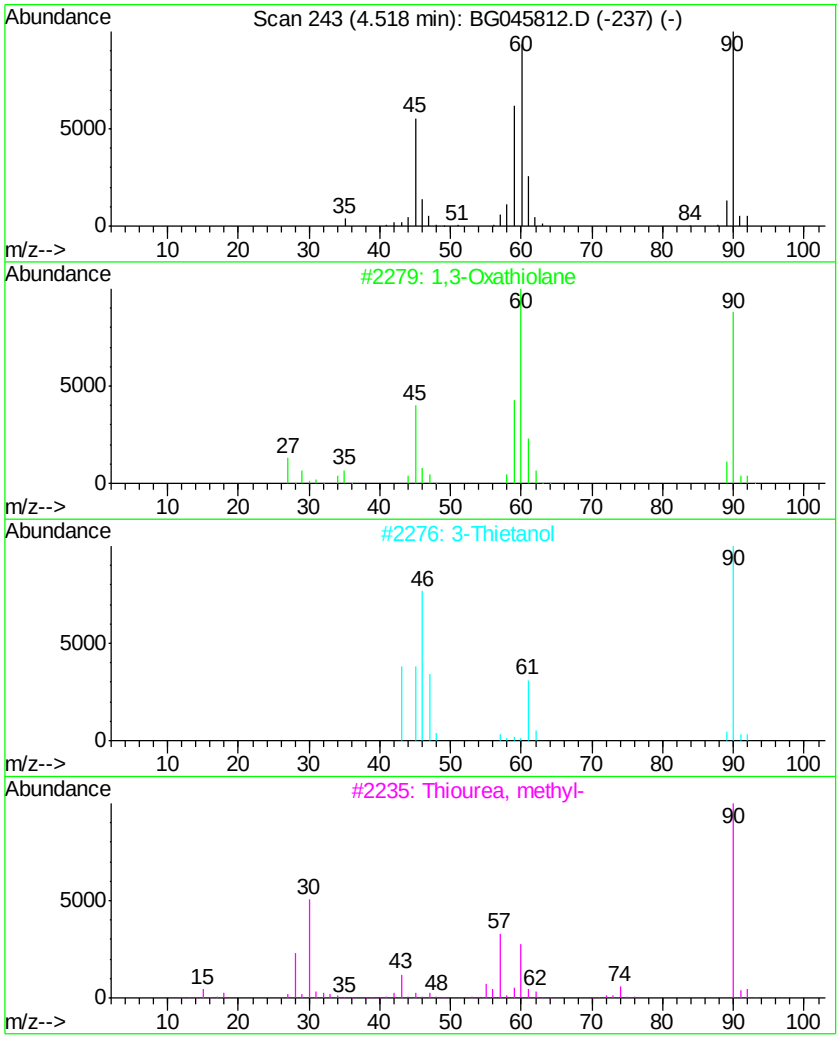
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

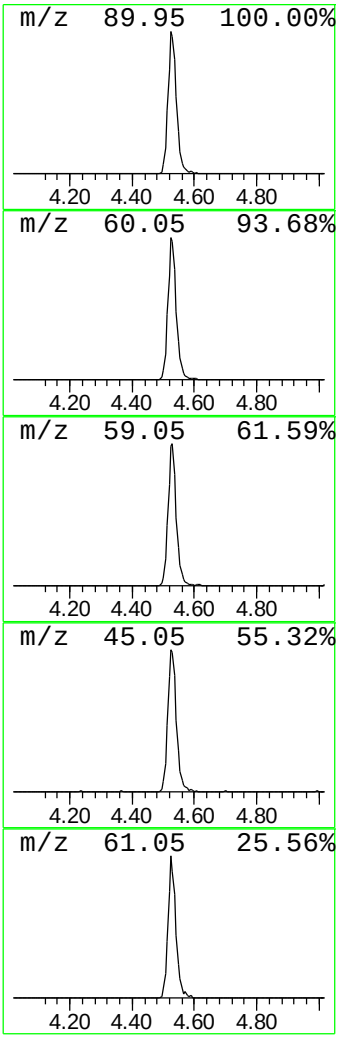
**********

Peak Number 1 1,3-Oxathiolane Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.52 | 33.64 ng | 515053 | 1,4-Dichlorobenzene-d4 | 7.91 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Oxathiolane | 90 | C3H6OS | 002094-97-5 | 90 |
| 2 | 3-Thietanol | 90 | C3H6OS | 010304-16-2 | 53 |
| 3 | Thiourea, methyl- | 90 | C2H6N2S | 000598-52-7 | 50 |
| 4 | Acrolein, 2-chloro- | 90 | C3H3ClO | 000683-51-2 | 36 |
| 5 | Heptanoic acid, 2-hydroxy-, meth... | 160 | C8H16O3 | 054340-91-9 | 36 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

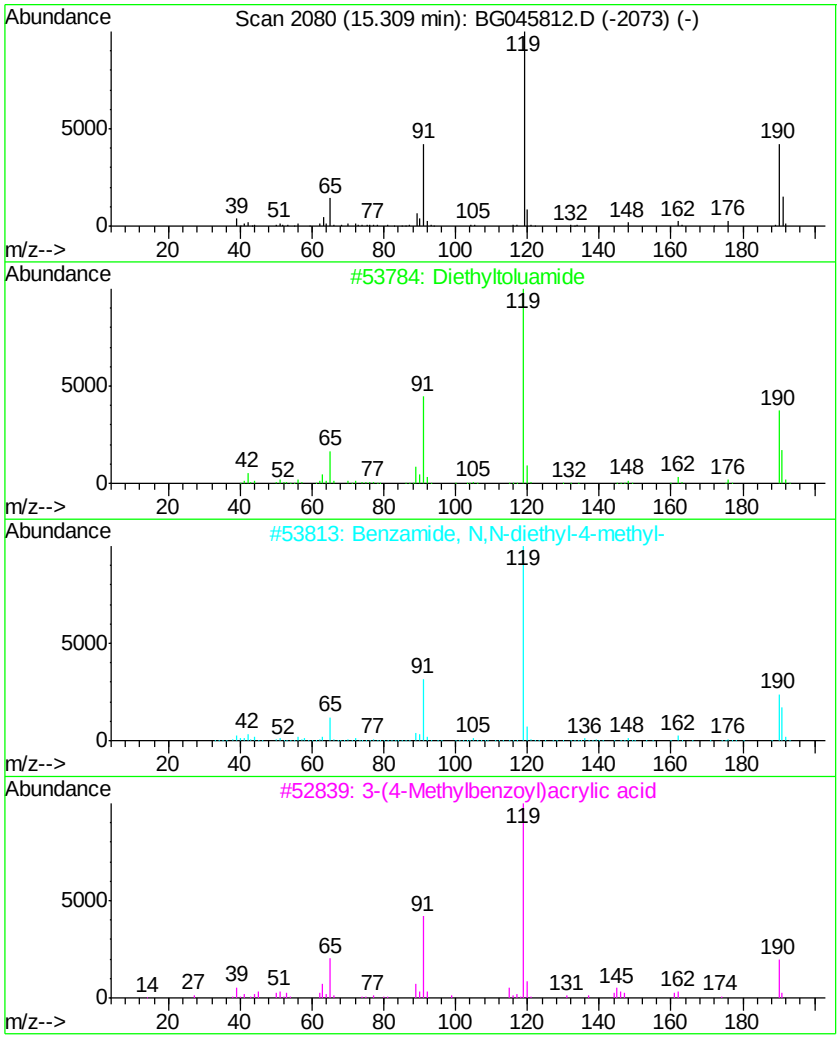
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

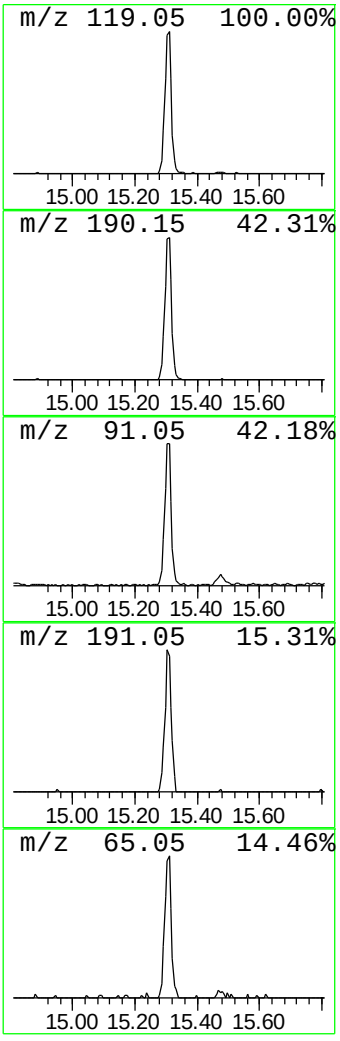
**********

Peak Number 4 Diethyltoluamide Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.31 | 8.50 ng | 236960 | Acenaphthene-d10 | 14.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diethyltoluamide | 191 | C12H17NO | 000134-62-3 | 94 |
| 2 | Benzamide, N,N-diethyl-4-methyl- | 191 | C12H17NO | 002728-05-4 | 81 |
| 3 | 3-(4-Methylbenzoyl)acrylic acid | 190 | C11H10O3 | 020972-36-5 | 72 |
| 4 | Benzamide, N-(1,1-dimethylethyl)... | 191 | C12H17NO | 042498-32-8 | 59 |
| 5 | m-Toluic acid, 2-butyl ester | 192 | C12H16O2 | 005448-57-7 | 53 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

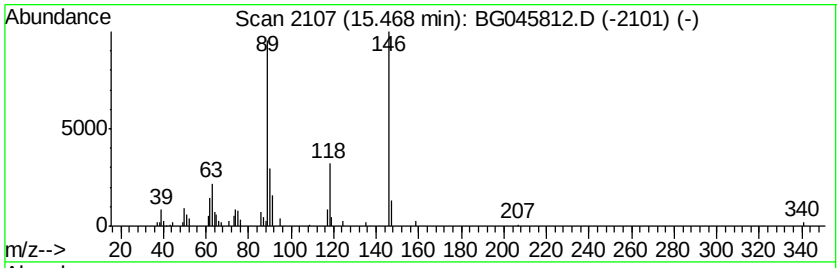
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

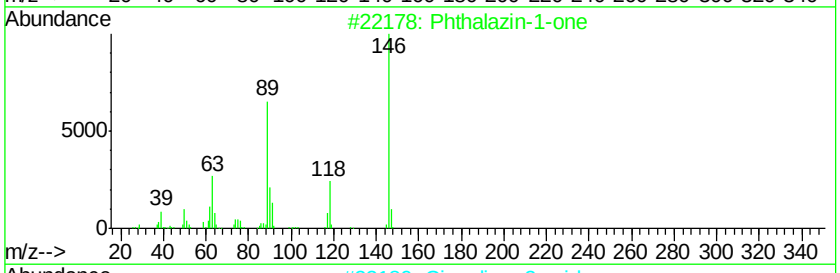
**********

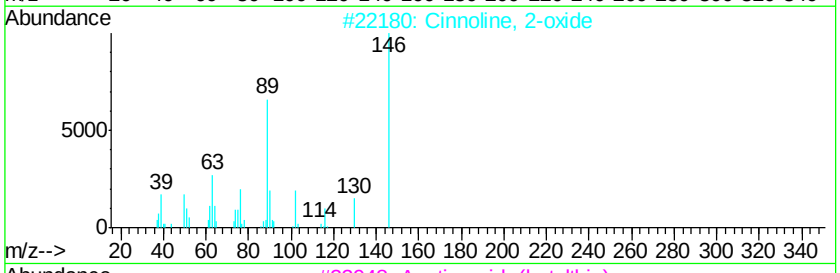
Peak Number 5 Phthalazin-1-one Concentration Rank 8

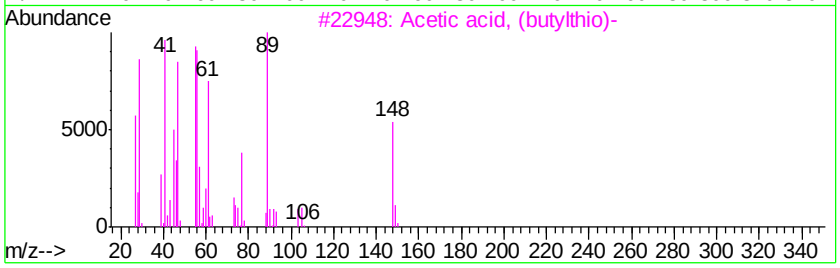
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.47 | 3.02 ng | 84191 | Acenaphthene-d10 | 14.56 |

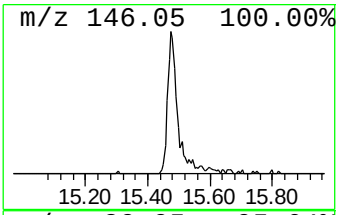
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phthalazin-1-one | 146 | C8H6N2O | 000119-39-1 | 95 |
| 2 | Cinnoline, 2-oxide | 146 | C8H6N2O | 004215-44-5 | 86 |
| 3 | Acetic acid, (butylthio)- | 148 | C6H12O2S | 020600-61-7 | 47 |
| 4 | 3-Chloroisocoumarin | 180 | C9H5ClO2 | 051050-54-5 | 45 |
| 5 | Cinnoline, 1-oxide | 146 | C8H6N2O | 001125-61-7 | 45 |

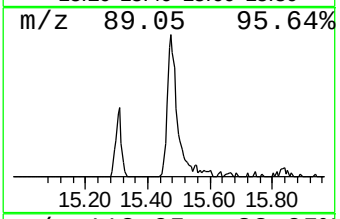


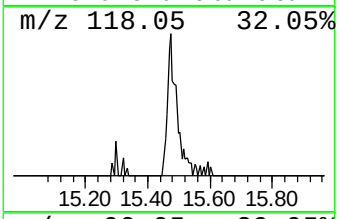



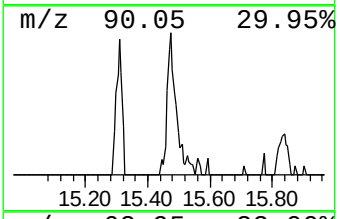



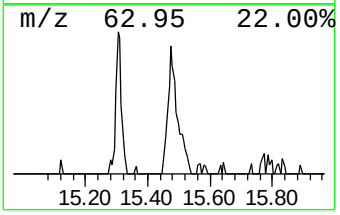



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

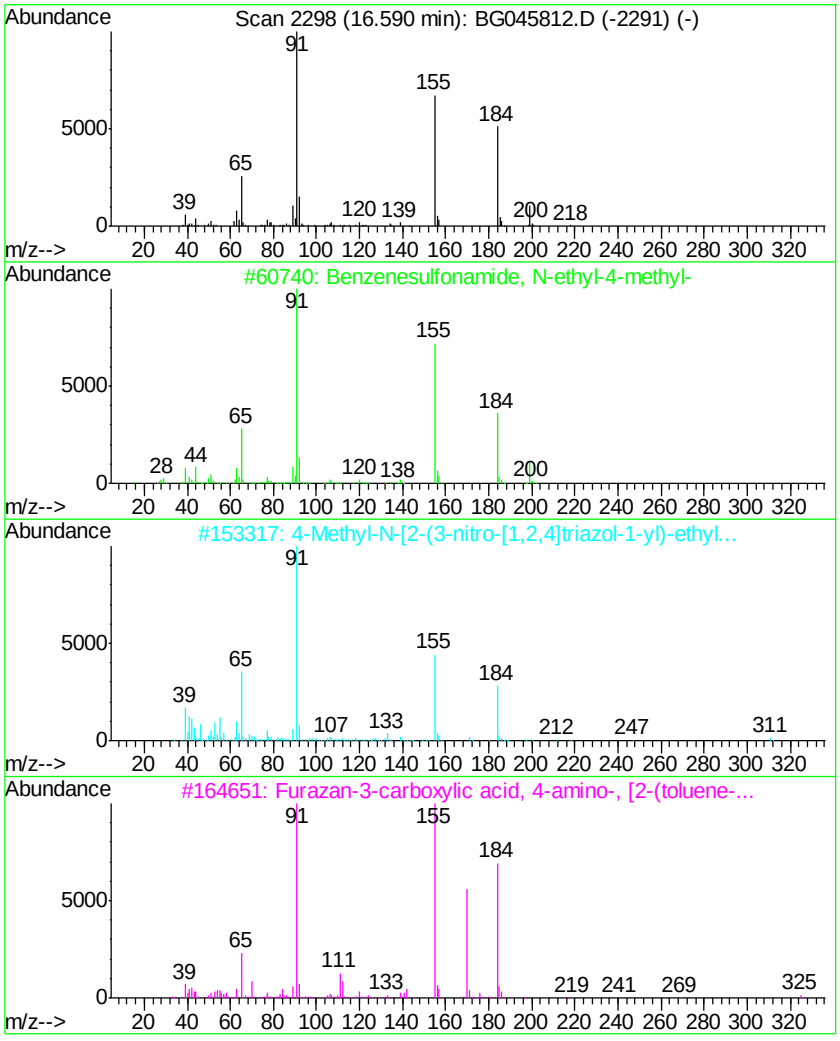
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

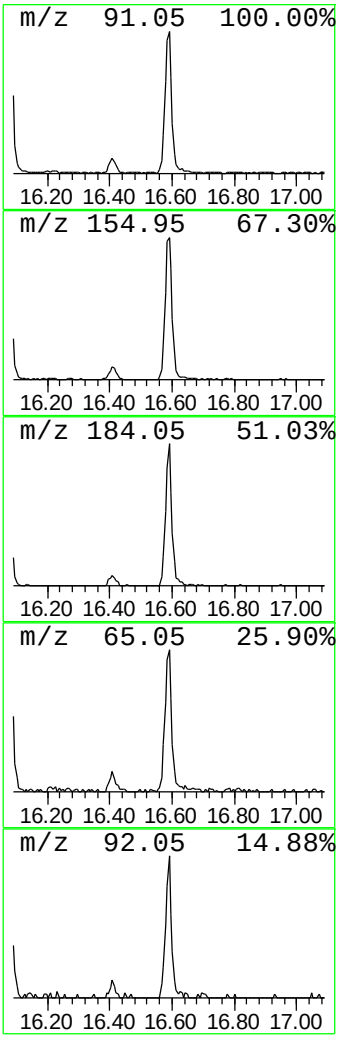
**********

Peak Number 6 Benzenesulfonamide, N-ethyl... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.59 | 7.27 ng | 253514 | Phenanthrene-d10 | 17.31 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfonamide, N-ethyl-4-me... | 199 | C9H13NO2S | 000080-39-7 | 97 |
| 2 | 4-Methyl-N-[2-(3-nitro-[1,2,4]tr... | 311 | C11H13N5O4S | 1000301-03-5 | 72 |
| 3 | Furazan-3-carboxylic acid, 4-ami... | 325 | C12H15N5O4S | 1000304-69-4 | 59 |
| 4 | 4-Methyl-N-(2-oxobutyl)benzenesu... | 241 | C11H15NO3S | 1000192-14-5 | 53 |
| 5 | N-Sulfinyl-p-toluenesulfonamide | 217 | C7H7NO3S2 | 004104-47-6 | 50 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

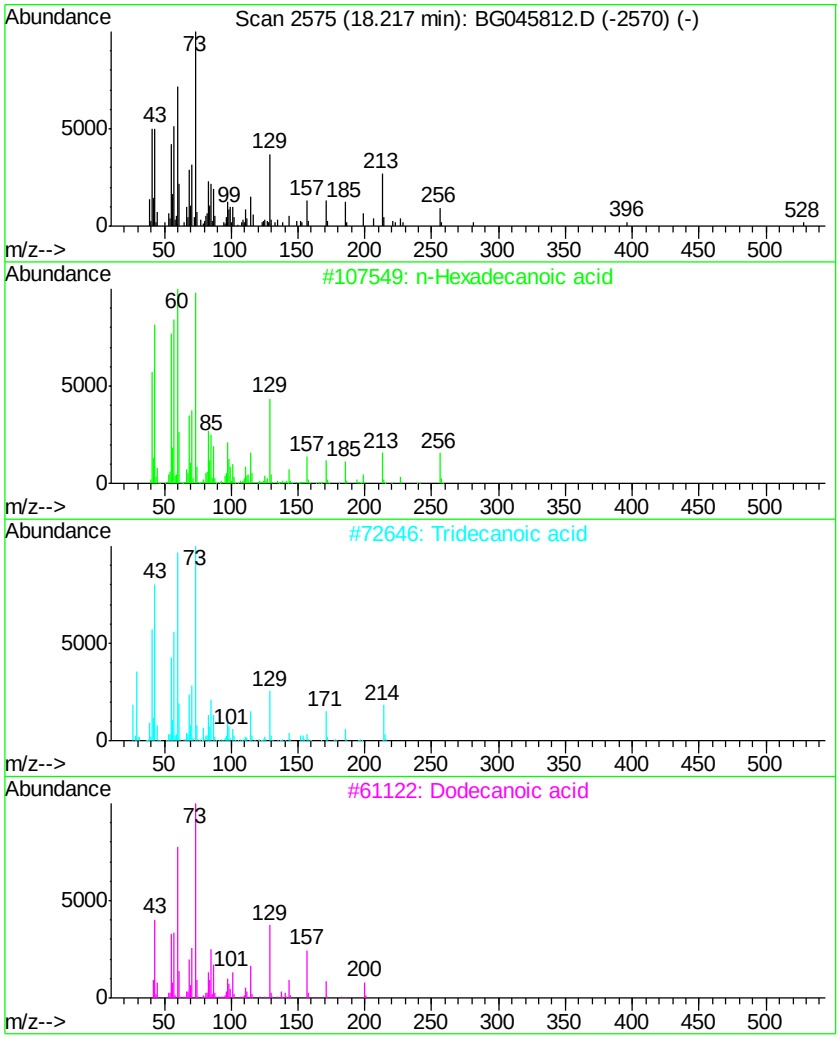
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

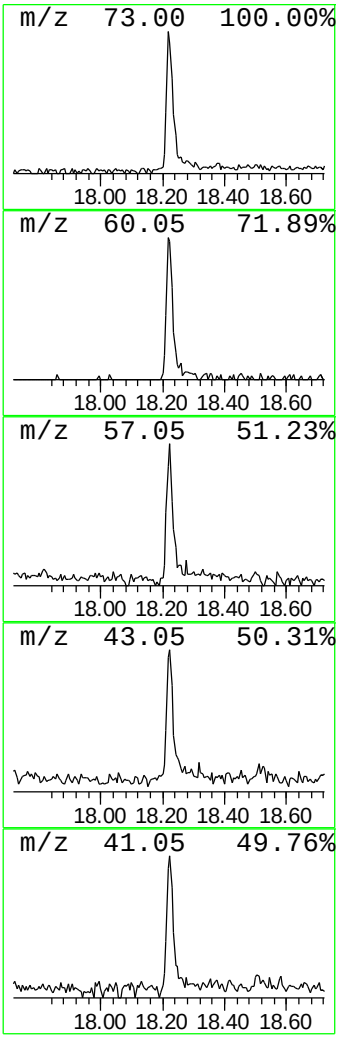
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.22 | 3.91 ng | 136211 | Phenanthrene-d10 | 17.31 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 89 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

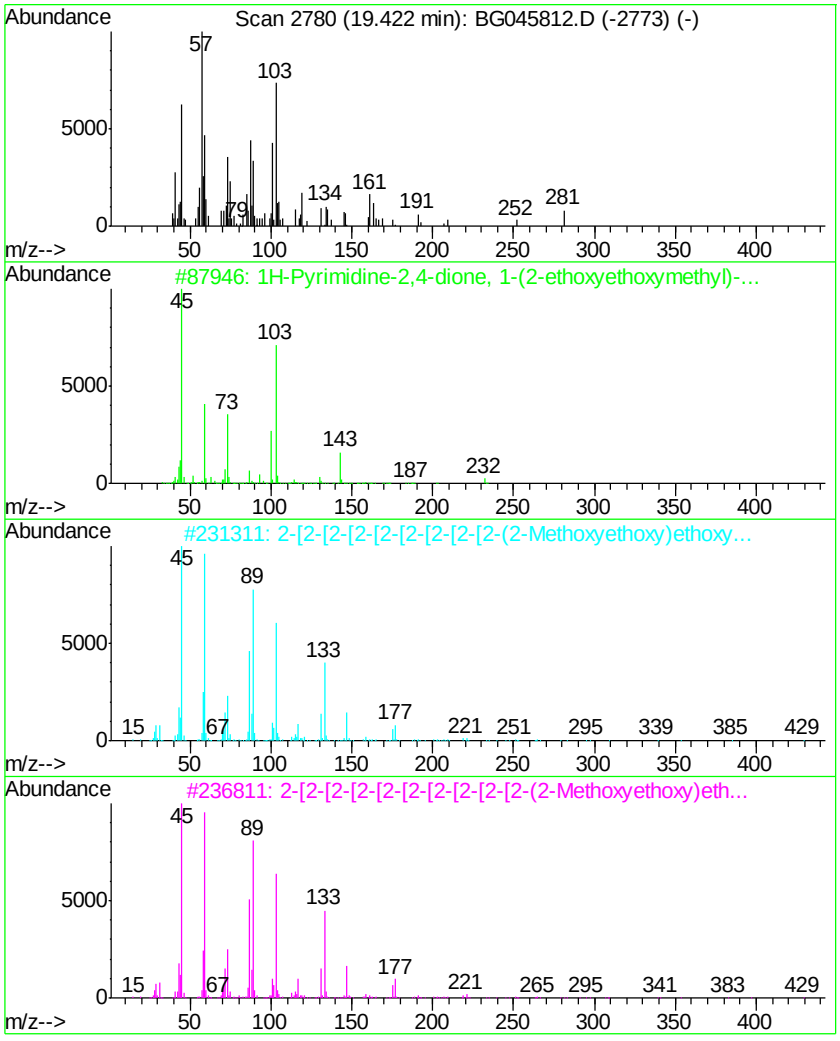
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

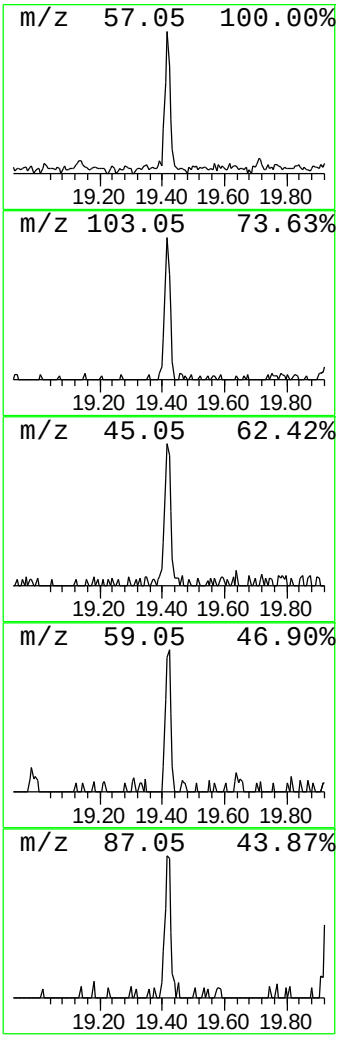
**********

Peak Number 8 unknown19.42 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.42 | 2.04 ng | 71229 | Phenanthrene-d10 | 17.31 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Pyrimidine-2,4-dione, 1-(2-et... | 232 | C9H13FN2O4 | 1000310-13-7 | 38 |
| 2 | 2-[2-[2-[2-[2-[2-[2-[2-(2-Met... | 472 | C21H44O11 | 1000352-11-2 | 38 |
| 3 | 2-[2-[2-[2-[2-[2-[2-[2-[2-(2-... | 516 | C23H48O12 | 1000352-04-4 | 38 |
| 4 | 1-tert-Butoxy-2-ethoxyethane | 146 | C8H18O2 | 051422-54-9 | 35 |
| 5 | Methane, diethoxy- | 104 | C5H12O2 | 000462-95-3 | 35 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG061920\
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Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

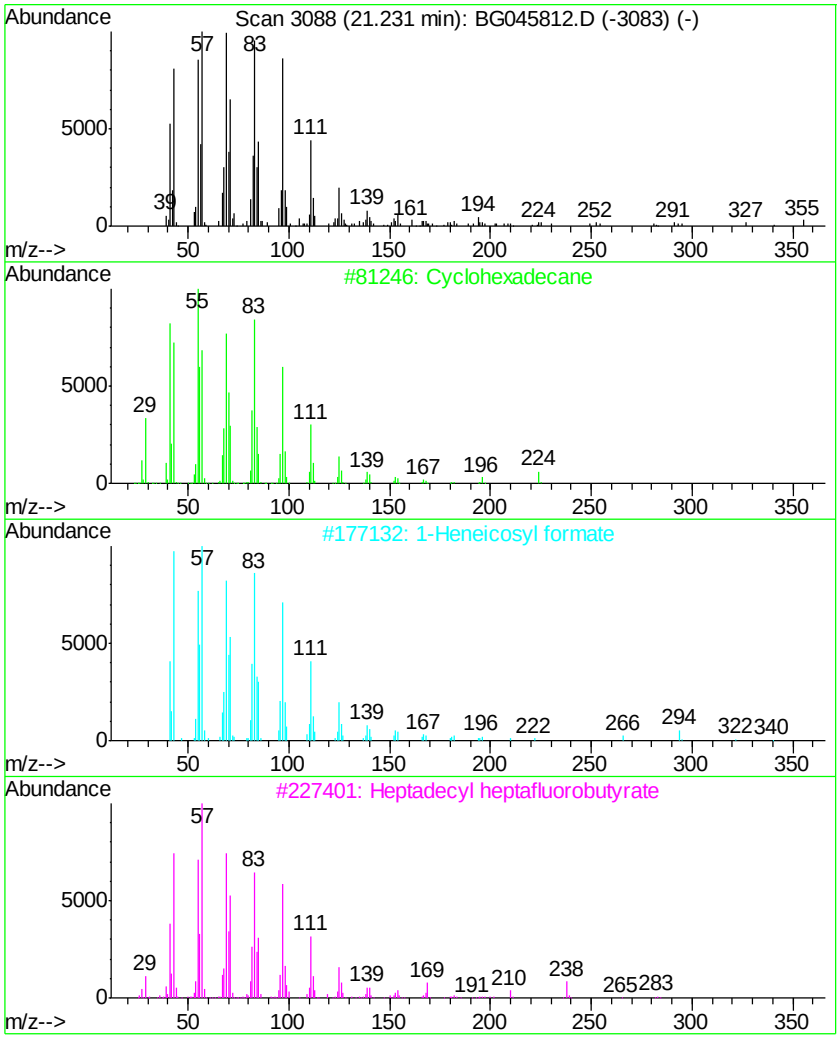
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

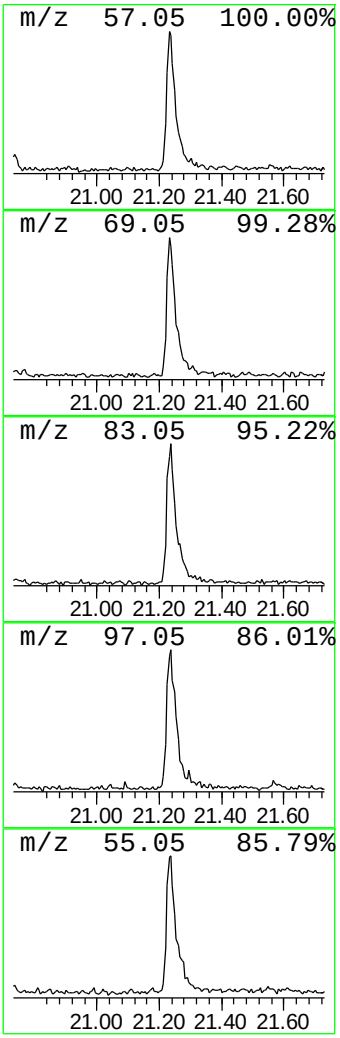
**********

Peak Number 9 Cyclohexadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.23 | 9.38 ng | 366536 | Chrysene-d12 | 21.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 97 |
| 2 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 95 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 4 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 5 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG061920\
Data File : BG045812.D
Acq On : 19 Jun 2020 12:45
Operator : CG/JU
Sample : L3033-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** LF001MW003-200616

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061520.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 |
| 1,3-Oxathiolane | 4.52 | 33.6 | ng | 515053 | 1 | 7.91 | 306249 | 20.0 |
| Diethyltoluamide | 15.31 | 8.5 | ng | 236960 | 3 | 14.56 | 557477 | 20.0 |
| Phthalazin-1-one | 15.47 | 3.0 | ng | 84191 | 3 | 14.56 | 557477 | 20.0 |
| Benzenesulfonamid... | 16.59 | 7.3 | ng | 253514 | 4 | 17.31 | 697461 | 20.0 |
| n-Hexadecanoic acid | 18.22 | 3.9 | ng | 136211 | 4 | 17.31 | 697461 | 20.0 |
| unknown19.42 | 19.42 | 2.0 | ng | 71229 | 4 | 17.31 | 697461 | 20.0 |
| Cyclohexadecane | 21.23 | 9.4 | ng | 366536 | 5 | 21.57 | 781418 | 20.0 |