LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

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-BG052919.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 | 3.135 | 3 | 8 | 16 | rVV | 107159 | 217062 | 5.12% | 0.751% |
| 2 | 3.212 | 16 | 21 | 32 | rVB | 335332 | 518095 | 12.23% | 1.792% |
| 3 | 5.662 | 430 | 438 | 449 | rBV | 1109148 | 1769860 | 41.78% | 6.123% |
| 4 | 7.272 | 703 | 712 | 725 | rBV | 1211051 | 2148192 | 50.71% | 7.432% |
| 5 | 7.654 | 769 | 777 | 792 | rBV | 1141734 | 2003222 | 47.29% | 6.930% |
| 6 | 8.124 | 850 | 857 | 865 | rBV | 265480 | 453932 | 10.71% | 1.570% |
| 7 | 8.447 | 905 | 912 | 921 | rBV | 809621 | 1426646 | 33.68% | 4.936% |
| 8 | 9.305 | 1049 | 1058 | 1066 | rBV | 730722 | 1324809 | 31.27% | 4.583% |
| 9 | 10.950 | 1330 | 1338 | 1345 | rBV | 370361 | 650283 | 15.35% | 2.250% |
| 10 | 13.376 | 1743 | 1751 | 1762 | rBV | 2065979 | 3158439 | 74.55% | 10.927% |
| 11 | 14.193 | 1881 | 1890 | 1896 | rBV | 215837 | 325710 | 7.69% | 1.127% |
| 12 | 14.757 | 1979 | 1986 | 1995 | rVB2 | 620573 | 1001468 | 23.64% | 3.465% |
| 13 | 16.238 | 2231 | 2238 | 2254 | rBV | 1759601 | 2675355 | 63.15% | 9.255% |
| 14 | 17.501 | 2446 | 2453 | 2464 | rBV2 | 811493 | 1245068 | 29.39% | 4.307% |
| 15 | 18.353 | 2592 | 2598 | 2607 | rBV | 251237 | 388976 | 9.18% | 1.346% |
| 16 | 19.616 | 2809 | 2813 | 2822 | rBV2 | 117406 | 167630 | 3.96% | 0.580% |
| 17 | 20.092 | 2888 | 2894 | 2900 | rBV | 3294180 | 4236462 | 100.00% | 14.656% |
| 18 | 21.373 | 3108 | 3112 | 3121 | rVB2 | 91222 | 154592 | 3.65% | 0.535% |
| 19 | 21.778 | 3174 | 3181 | 3188 | rBV | 791990 | 1305161 | 30.81% | 4.515% |
| 20 | 21.925 | 3201 | 3206 | 3215 | rVB | 117931 | 189218 | 4.47% | 0.655% |
| 21 | 22.548 | 3307 | 3312 | 3318 | rBV | 191118 | 305289 | 7.21% | 1.056% |
| 22 | 23.259 | 3426 | 3433 | 3441 | rBV2 | 264361 | 534731 | 12.62% | 1.850% |
| 23 | 24.093 | 3568 | 3575 | 3582 | rVB2 | 267604 | 542499 | 12.81% | 1.877% |
| 24 | 25.115 | 3734 | 3749 | 3759 | rVB2 | 437092 | 1764890 | 41.66% | 6.106% |
| 25 | 26.244 | 3934 | 3941 | 3949 | rVB4 | 142298 | 398003 | 9.39% | 1.377% |

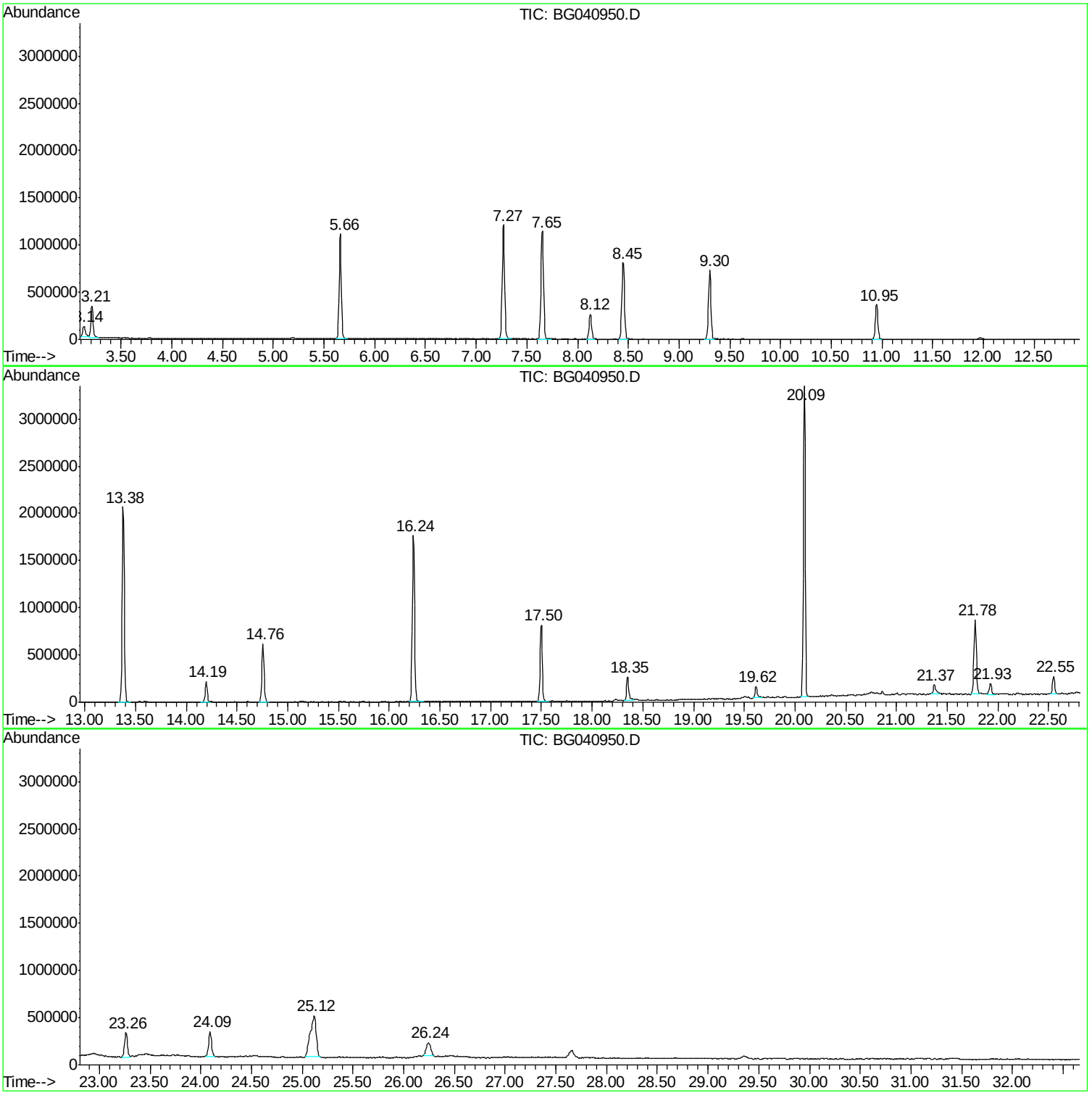
Sum of corrected areas: 28905592

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

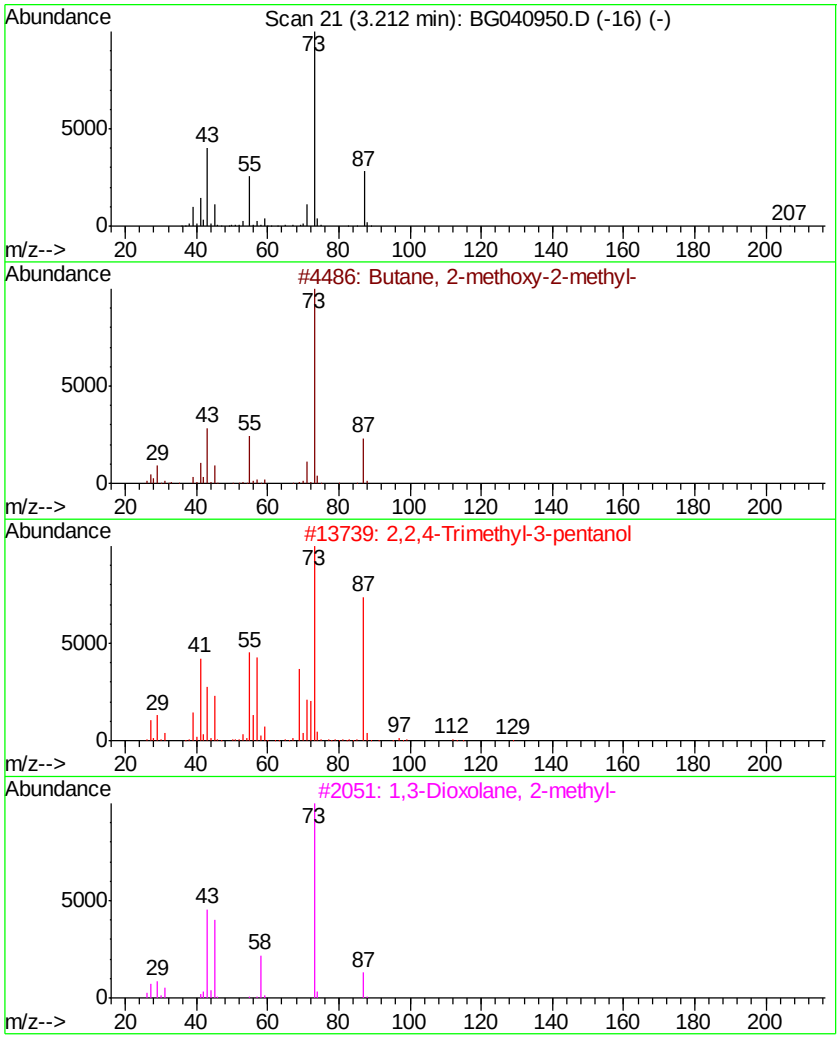
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

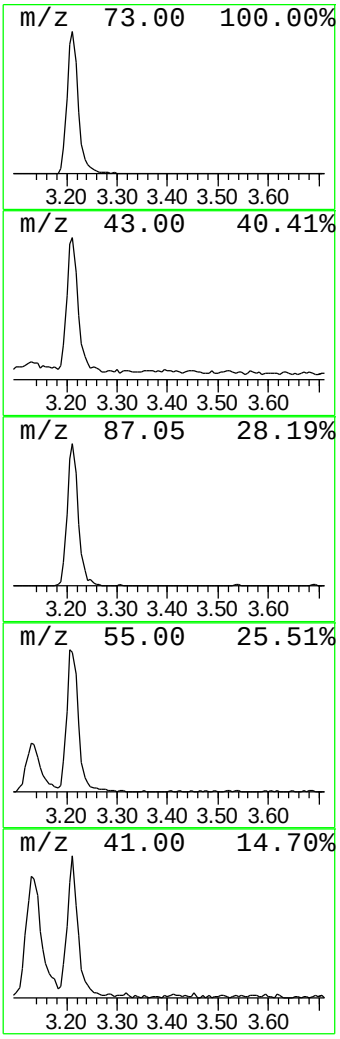
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.21 | 22.83 ng | 518095 | 1,4-Dichlorobenzene-d4 | 8.12 |

| 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 | 25 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

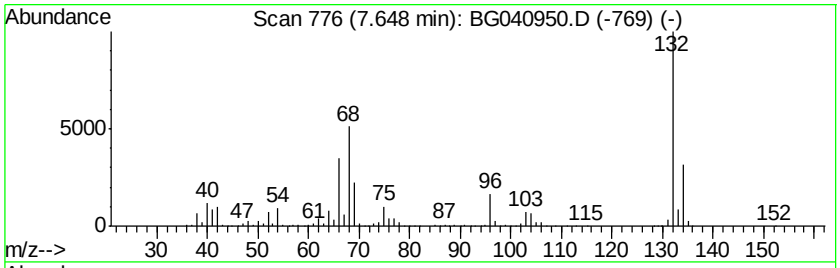
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

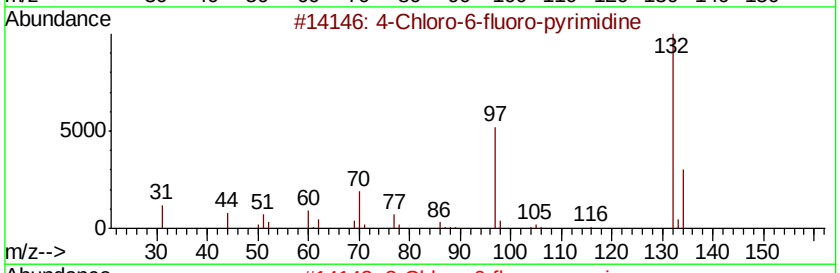
**********

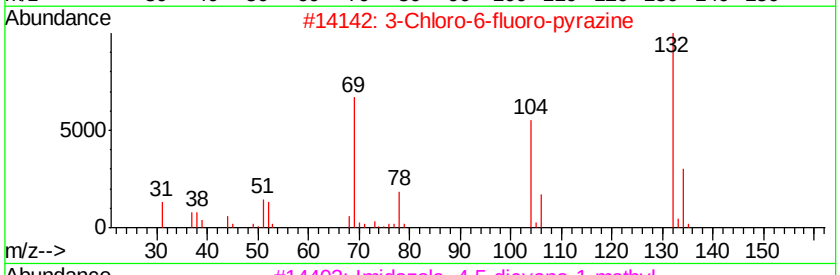
Peak Number 3 unknown7.65 Concentration Rank 1

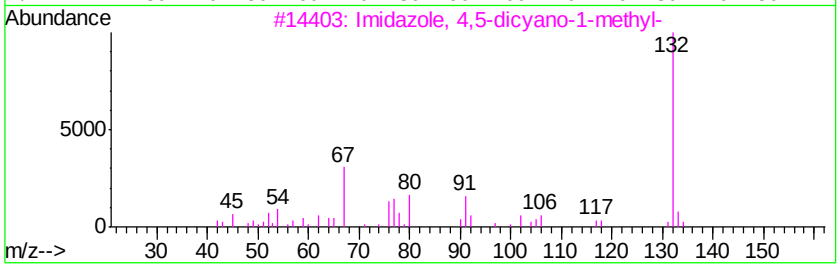
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.65 | 88.26 ng | 2003220 | 1,4-Dichlorobenzene-d4 | 8.12 |

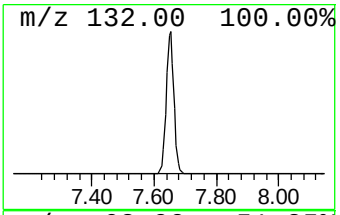
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 3 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 25 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 22 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |

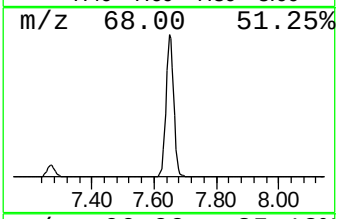


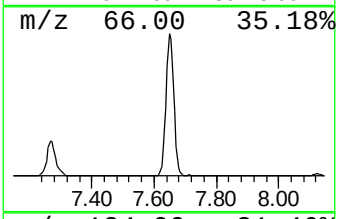



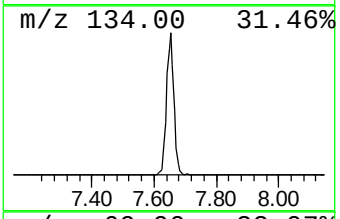



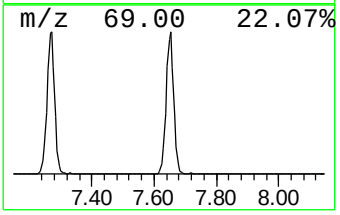



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

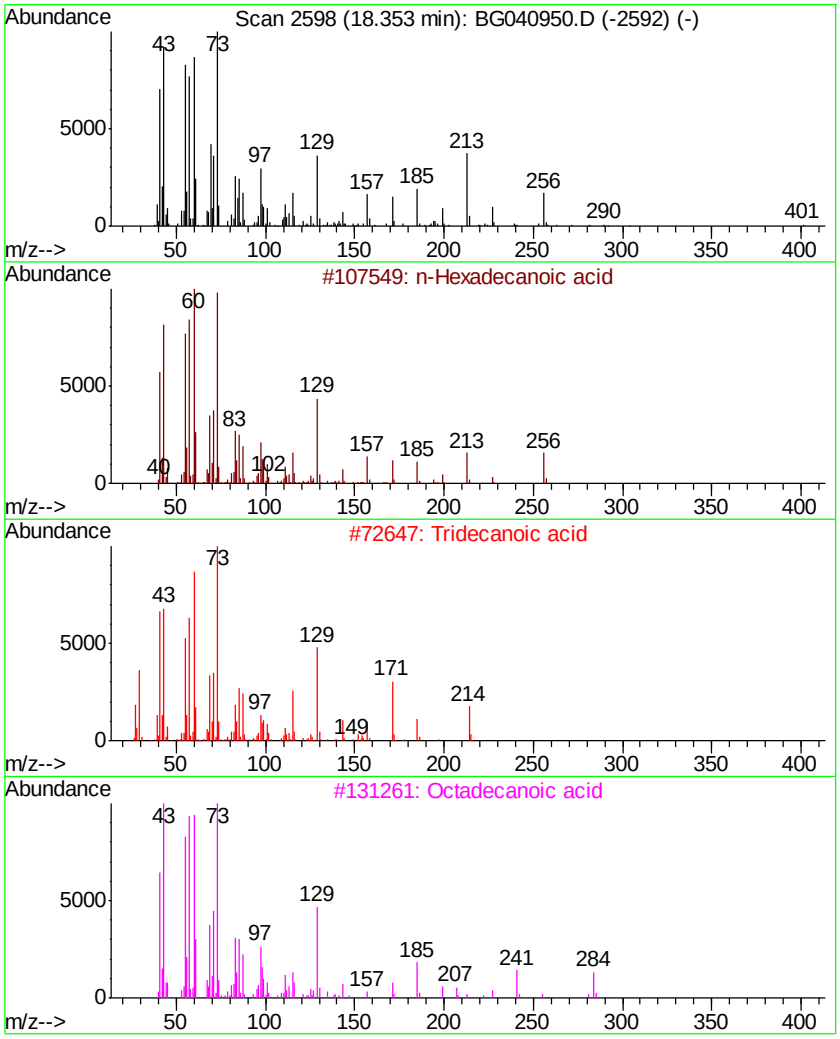
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

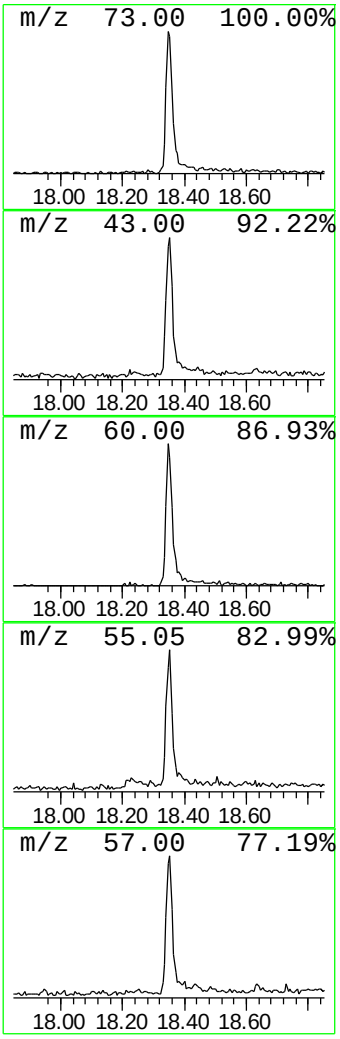
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.35 | 6.25 ng | 388976 | Phenanthrene-d10 | 17.50 |

| 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 | 96 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

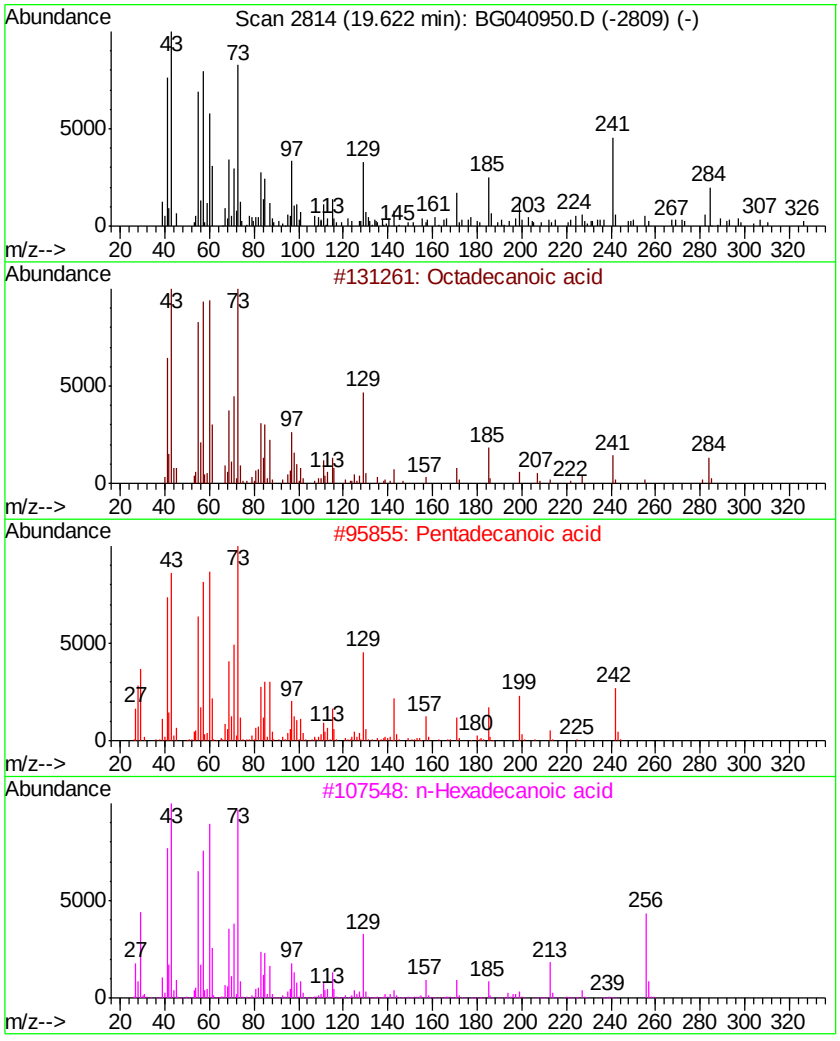
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

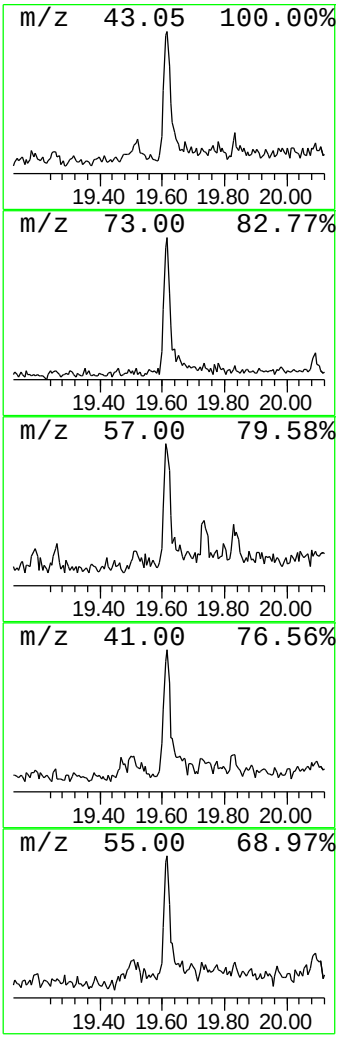
**********

Peak Number 6 Octadecanoic acid Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.62 | 2.69 ng | 167630 | Phenanthrene-d10 | 17.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 89 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

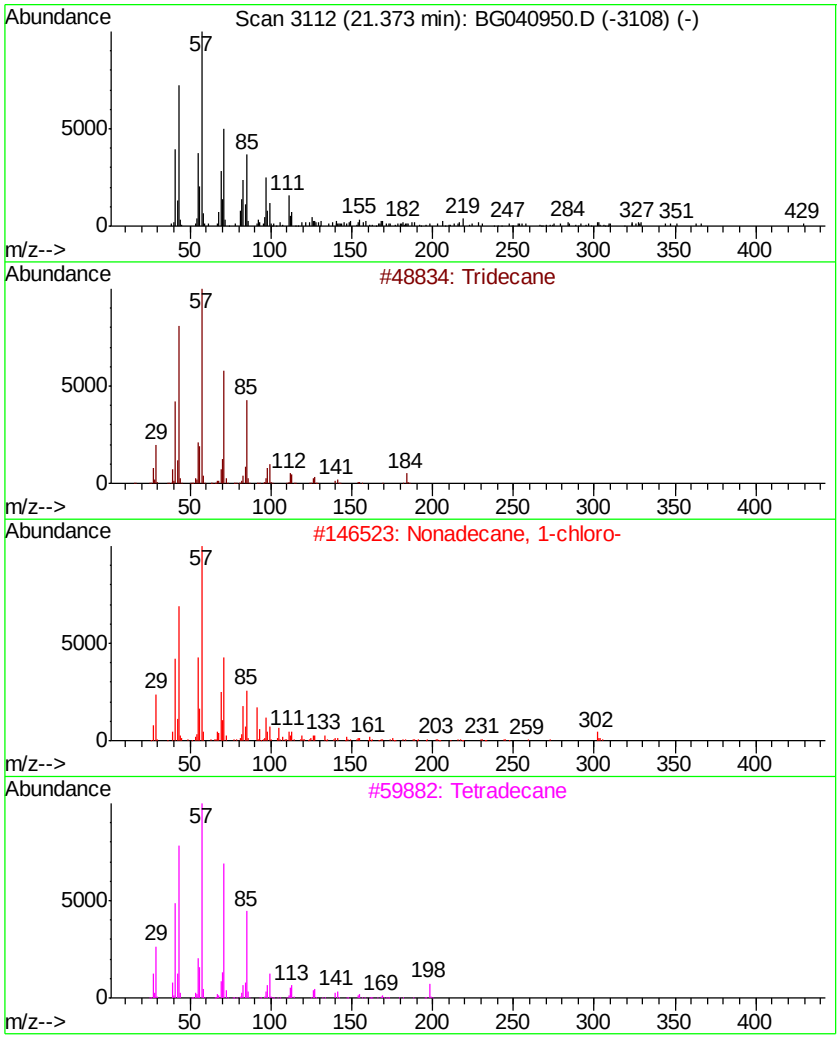
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

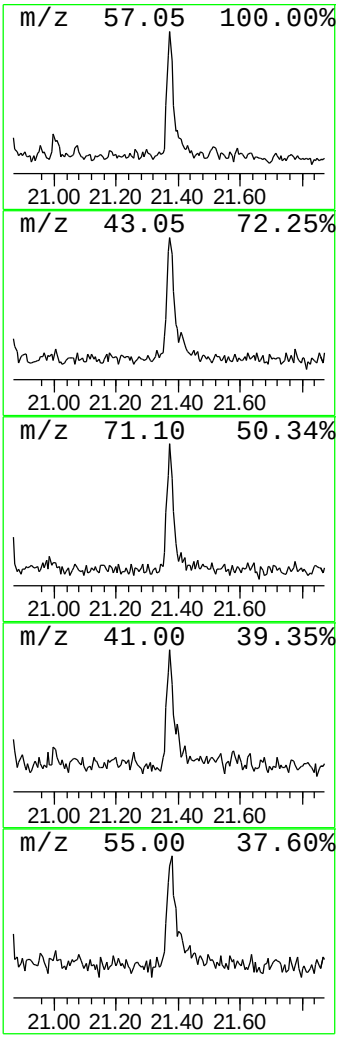
**********

Peak Number 7 Tridecane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.37 | 2.37 ng | 154592 | Chrysene-d12 | 21.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane | 184 | C13H28 | 000629-50-5 | 93 |
| 2 | Nonadecane, 1-chloro- | 302 | C19H39Cl | 062016-76-6 | 93 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 92 |
| 4 | Sulfurous acid, butyl octadecyl ... | 390 | C22H46O3S | 1000309-18-5 | 91 |
| 5 | 1-Octadecanesulphonyl chloride | 352 | C18H37ClO2S | 1000342-70-4 | 87 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

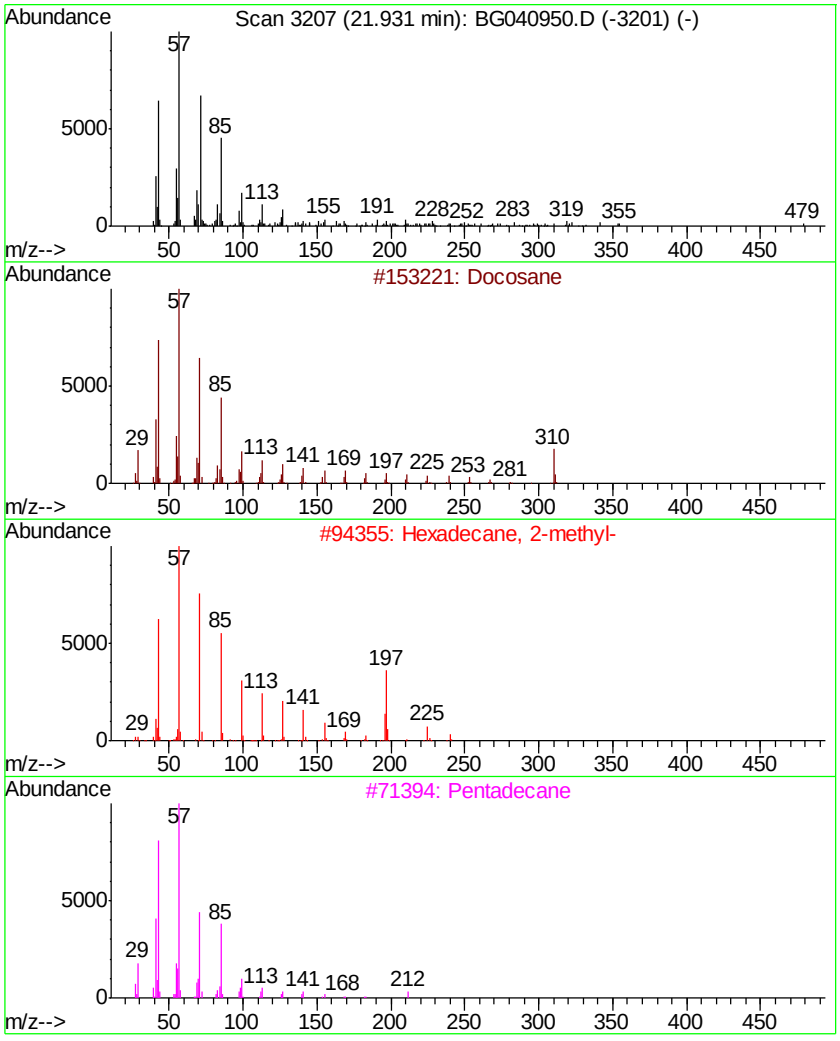
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

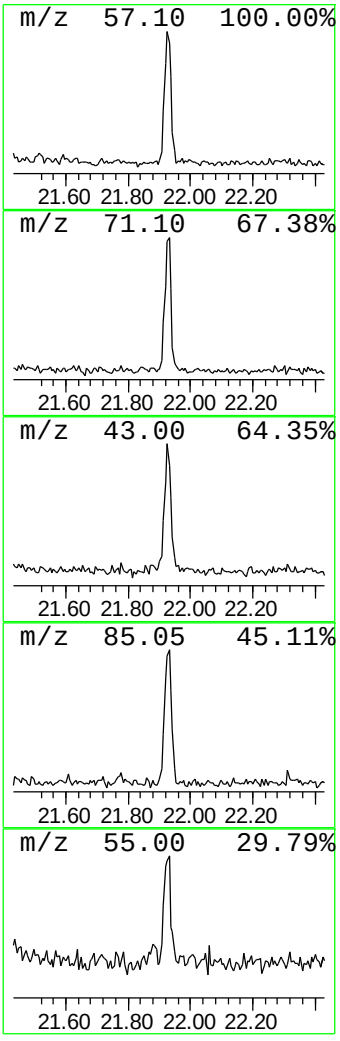
**********

Peak Number 8 Docosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.93 | 2.90 ng | 189218 | Chrysene-d12 | 21.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane | 310 | C22H46 | 000629-97-0 | 93 |
| 2 | Hexadecane, 2-methyl- | 240 | C17H36 | 001560-92-5 | 93 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 93 |
| 4 | Heptadecane, 2-methyl- | 254 | C18H38 | 001560-89-0 | 90 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

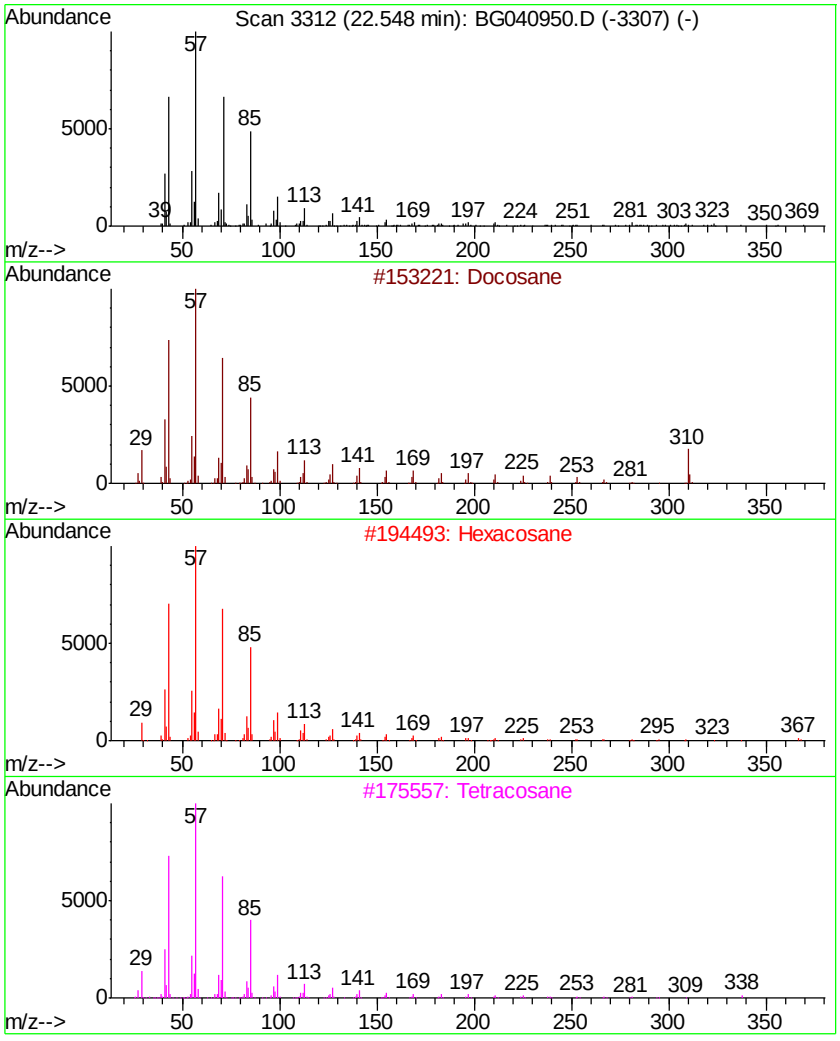
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

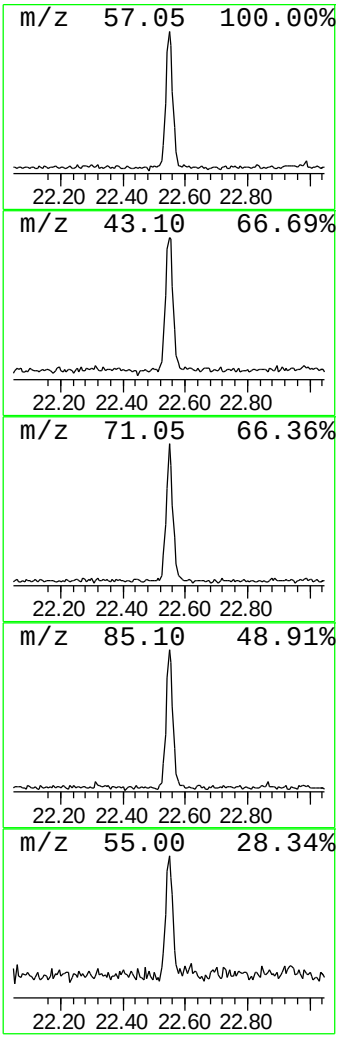
**********

Peak Number 9 Hexacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.55 | 4.68 ng | 305289 | Chrysene-d12 | 21.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane | 310 | C22H46 | 000629-97-0 | 93 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 4 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 86 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

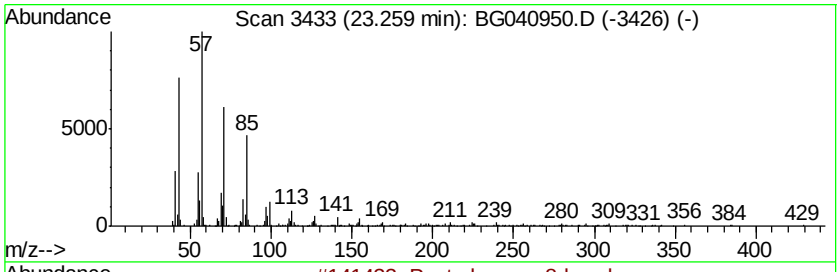
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

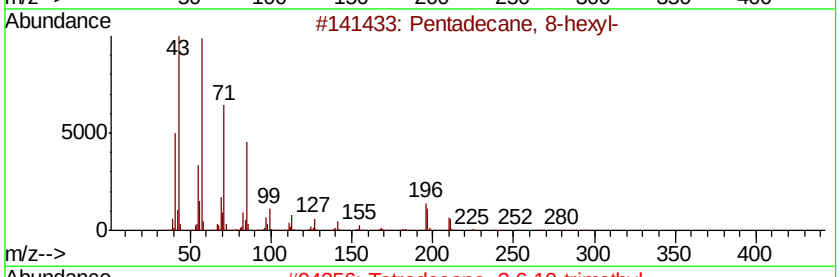
**********

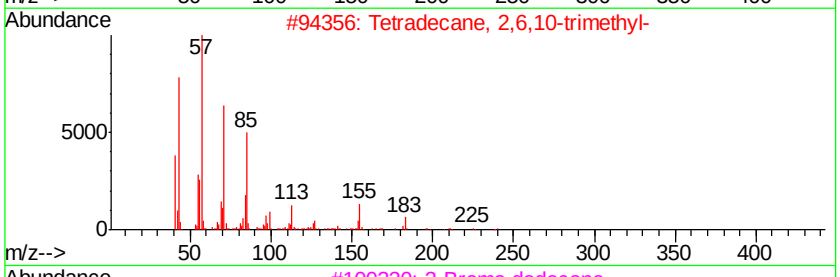
Peak Number 10 Pentadecane, 8-hexyl- Concentration Rank 5

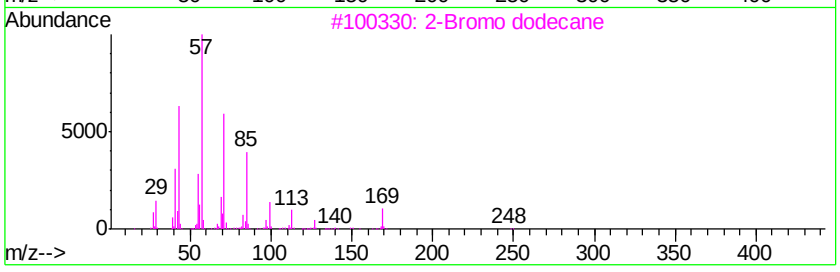
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.26 | 8.19 ng | 534731 | Chrysene-d12 | 21.78 |

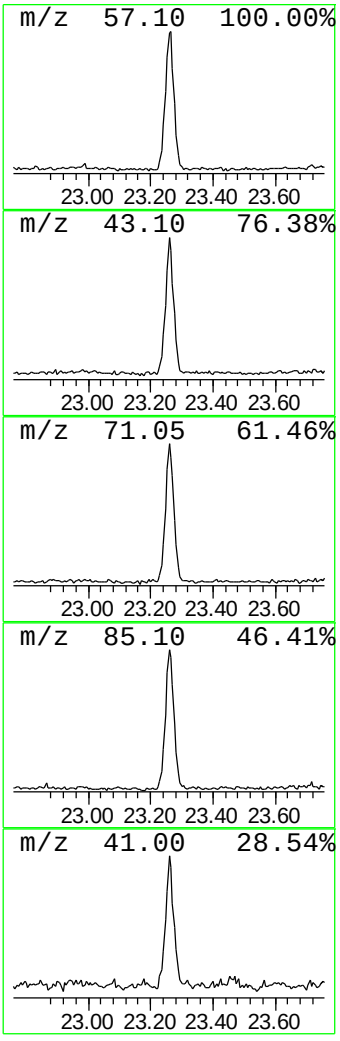
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane, 8-hexyl- | 296 | C21H44 | 013475-75-7 | 93 |
| 2 | Tetradecane, 2,6,10-trimethyl- | 240 | C17H36 | 014905-56-7 | 93 |
| 3 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 91 |
| 4 | Decane, 1-iodo- | 268 | C10H21I | 002050-77-3 | 90 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

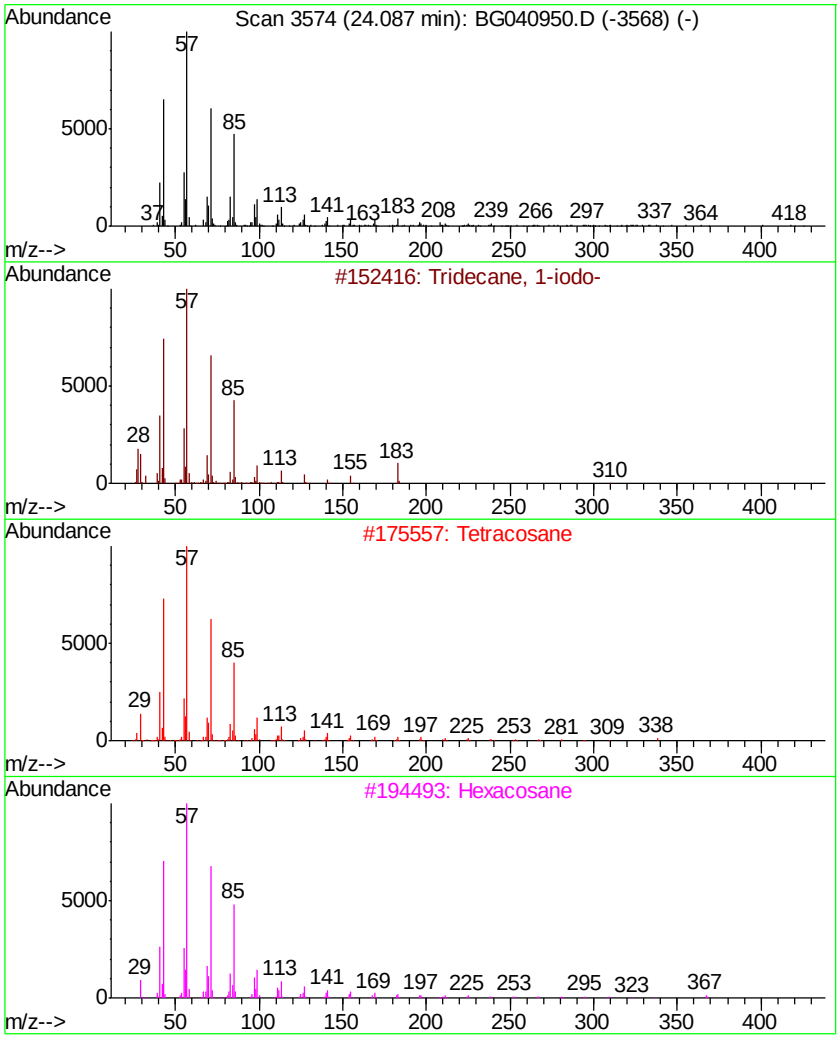
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

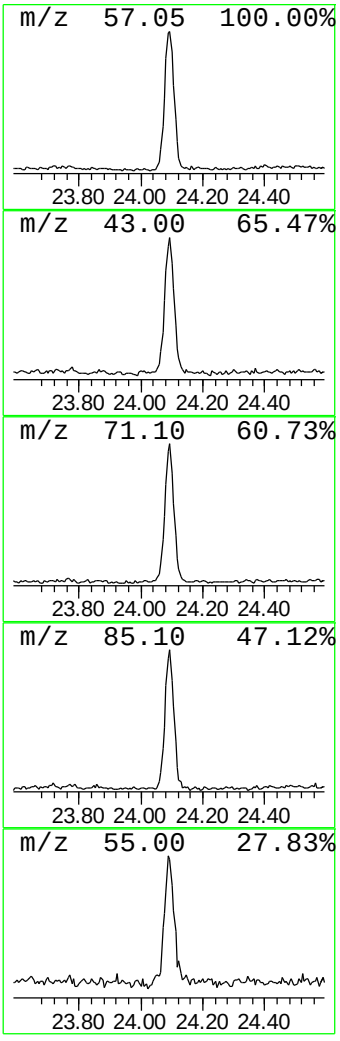
**********

Peak Number 11 Tridecane, 1-iodo- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.09 | 6.15 ng | 542499 | Perylene-d12 | 25.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 93 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Heneicosane, 11-decyl- | 437 | C31H64 | 055320-06-4 | 90 |
| 5 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

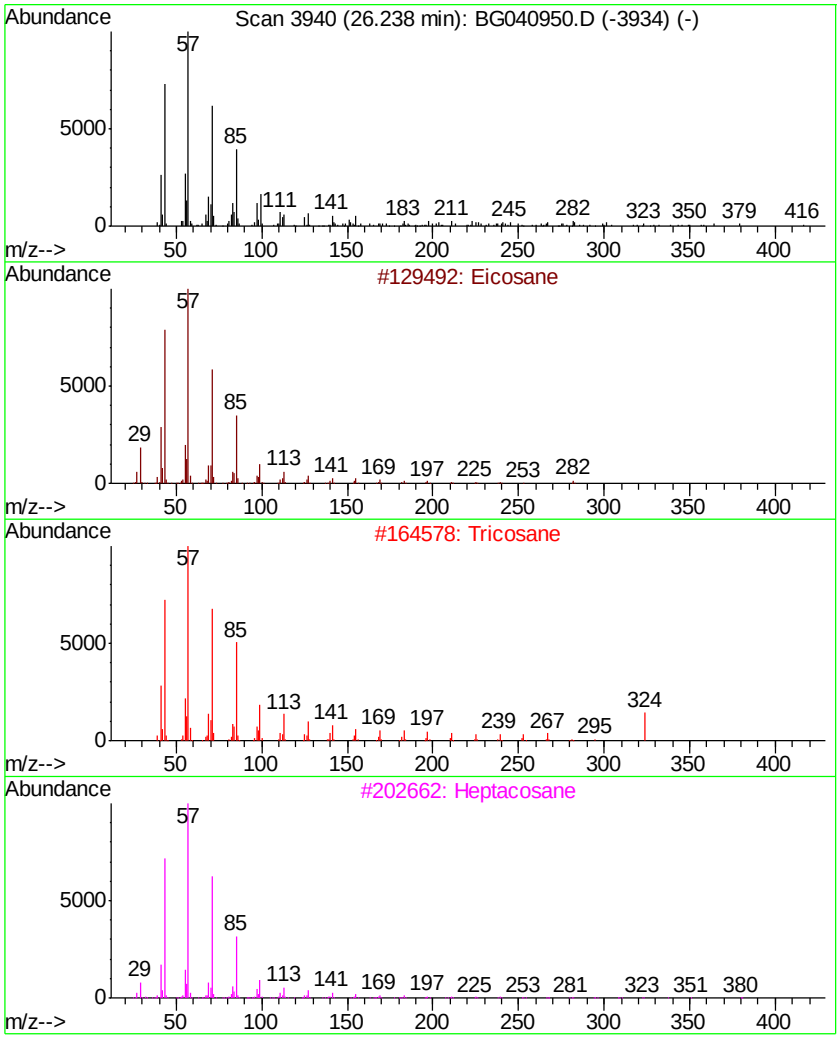
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

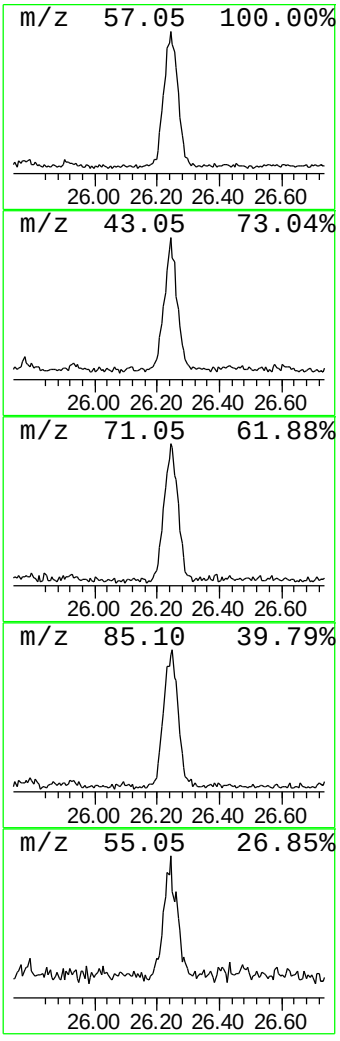
**********

Peak Number 12 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.24 | 4.51 ng | 398003 | Perylene-d12 | 25.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 98 |
| 2 | Tricosane | 324 | C23H48 | 000638-67-5 | 91 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 4 | Tetradecane, 2,6,10-trimethyl- | 240 | C17H36 | 014905-56-7 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG053019\
Data File : BG040950.D
Acq On : 30 May 2019 13:51
Operator : HP/JU
Sample : K3054-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CULVER-CBTC-WC1B-052419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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... | 3.21 | 22.8 | ng | 518095 | 1 | 8.12 | 453932 | 20.0 |
| unknown7.65 | 7.65 | 88.3 | ng | 2003220 | 1 | 8.12 | 453932 | 20.0 |
| n-Hexadecanoic acid | 18.35 | 6.3 | ng | 388976 | 4 | 17.50 | 1245070 | 20.0 |
| Octadecanoic acid | 19.62 | 2.7 | ng | 167630 | 4 | 17.50 | 1245070 | 20.0 |
| Tridecane | 21.37 | 2.4 | ng | 154592 | 5 | 21.78 | 1305160 | 20.0 |
| Docosane | 21.93 | 2.9 | ng | 189218 | 5 | 21.78 | 1305160 | 20.0 |
| Hexacosane | 22.55 | 4.7 | ng | 305289 | 5 | 21.78 | 1305160 | 20.0 |
| Pentadecane, 8-he... | 23.26 | 8.2 | ng | 534731 | 5 | 21.78 | 1305160 | 20.0 |
| Tridecane, 1-iodo- | 24.09 | 6.2 | ng | 542499 | 6 | 25.12 | 1764890 | 20.0 |
| Eicosane | 26.24 | 4.5 | ng | 398003 | 6 | 25.12 | 1764890 | 20.0 |