LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

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-BG123019.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 | 5.034 | 324 | 331 | 344 | rBV | 328499 | 533304 | 9.30% | 1.602% |
| 2 | 5.510 | 404 | 412 | 428 | rBV | 1500216 | 2466997 | 43.02% | 7.411% |
| 3 | 7.102 | 674 | 683 | 701 | rBV | 1650438 | 2971774 | 51.82% | 8.927% |
| 4 | 7.467 | 737 | 745 | 760 | rBV | 1593295 | 2786039 | 48.58% | 8.369% |
| 5 | 7.931 | 816 | 824 | 833 | rBV | 266945 | 455711 | 7.95% | 1.369% |
| 6 | 8.254 | 870 | 879 | 887 | rBV | 1179583 | 2072508 | 36.14% | 6.226% |
| 7 | 9.082 | 1012 | 1020 | 1034 | rBV | 916549 | 1713623 | 29.88% | 5.148% |
| 8 | 10.733 | 1290 | 1301 | 1314 | rBV | 357200 | 679247 | 11.84% | 2.040% |
| 9 | 13.189 | 1712 | 1719 | 1732 | rBV | 2563556 | 4112940 | 71.72% | 12.355% |
| 10 | 13.407 | 1749 | 1756 | 1764 | rBV2 | 56273 | 90465 | 1.58% | 0.272% |
| 11 | 14.018 | 1854 | 1860 | 1865 | rBV | 101322 | 167380 | 2.92% | 0.503% |
| 12 | 14.564 | 1946 | 1953 | 1969 | rVB | 629588 | 1034732 | 18.04% | 3.108% |
| 13 | 16.051 | 2199 | 2206 | 2226 | rBV | 2077520 | 3427740 | 59.77% | 10.297% |
| 14 | 17.308 | 2414 | 2420 | 2433 | rBV | 763340 | 1216987 | 21.22% | 3.656% |
| 15 | 19.923 | 2859 | 2865 | 2875 | rBV | 4241343 | 5734862 | 100.00% | 17.227% |
| 16 | 21.227 | 3082 | 3087 | 3102 | rBV | 221553 | 523990 | 9.14% | 1.574% |
| 17 | 21.556 | 3136 | 3143 | 3153 | rBV | 725207 | 1229547 | 21.44% | 3.693% |
| 18 | 21.767 | 3175 | 3179 | 3189 | rVB3 | 46456 | 74080 | 1.29% | 0.223% |
| 19 | 22.355 | 3275 | 3279 | 3285 | rBV | 68547 | 115000 | 2.01% | 0.345% |
| 20 | 23.031 | 3386 | 3394 | 3400 | rBV2 | 83174 | 164089 | 2.86% | 0.493% |
| 21 | 23.812 | 3520 | 3527 | 3535 | rBV2 | 80529 | 178550 | 3.11% | 0.536% |
| 22 | 24.664 | 3661 | 3672 | 3680 | rBV | 465737 | 1307400 | 22.80% | 3.927% |
| 23 | 25.822 | 3857 | 3869 | 3878 | rBV4 | 52468 | 163030 | 2.84% | 0.490% |
| 24 | 27.126 | 4083 | 4091 | 4099 | rVB6 | 21808 | 69869 | 1.22% | 0.210% |

Sum of corrected areas: 33289864

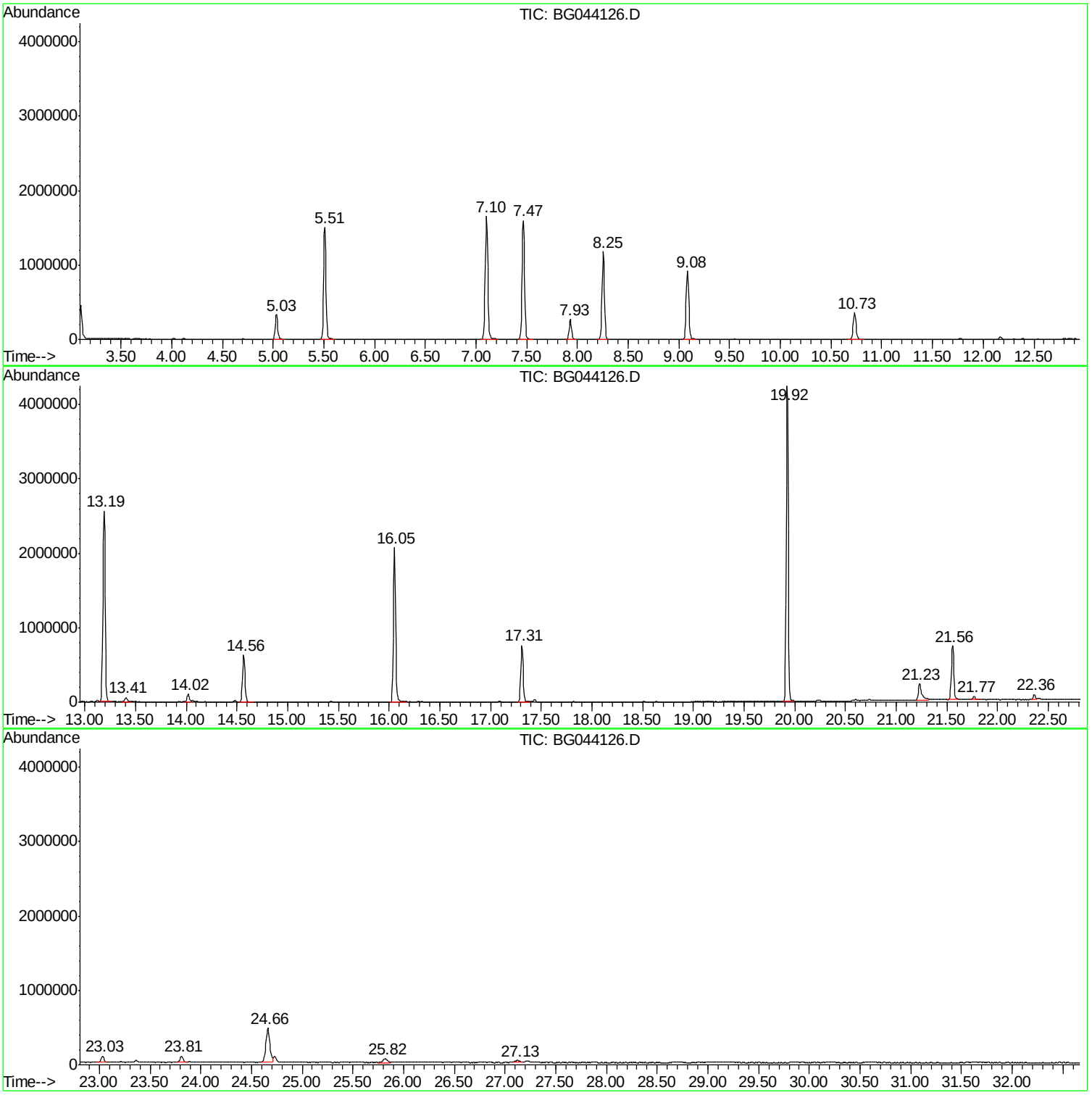
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

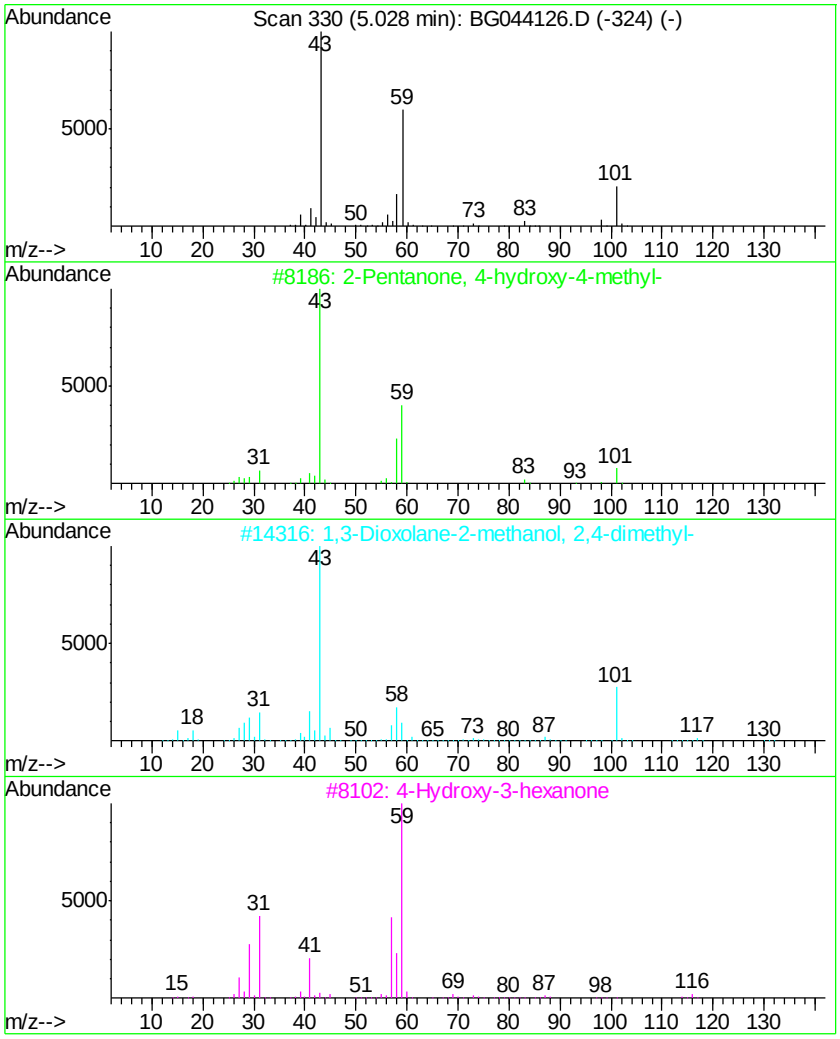
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

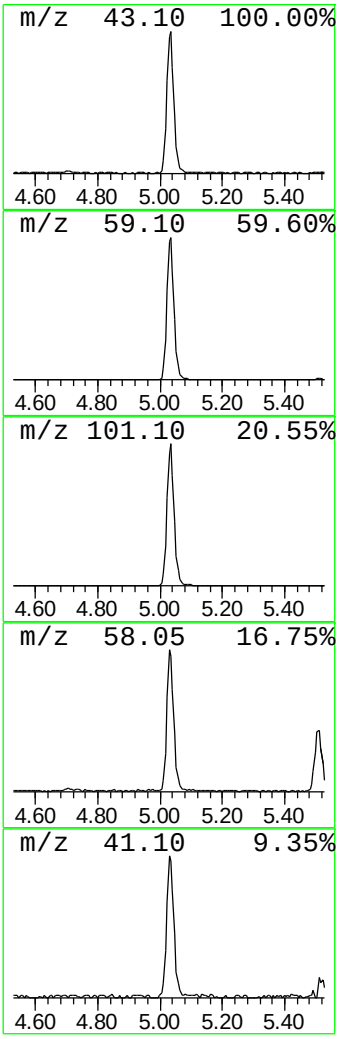
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.03 | 23.41 ng | 533304 | 1,4-Dichlorobenzene-d4 | 7.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 1,3-Dioxolane-2-methanol, 2,4-di... | 132 | C6H12O3 | 053951-43-2 | 28 |
| 3 | 4-Hydroxy-3-hexanone | 116 | C6H12O2 | 004984-85-4 | 23 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

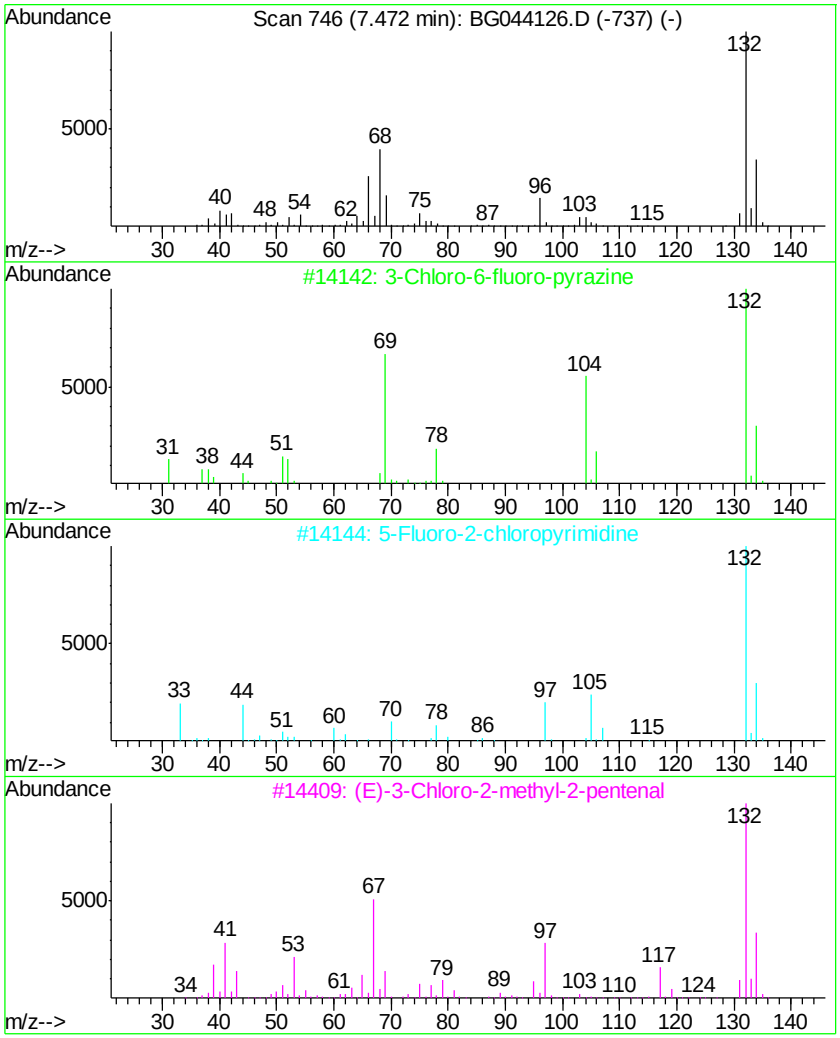
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

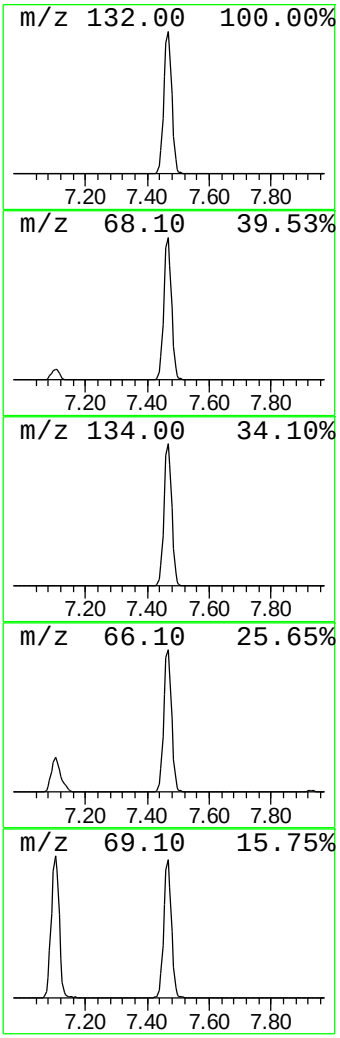
**********

Peak Number 2 unknown7.47 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.47 | 122.27 ng | 2786040 | 1,4-Dichlorobenzene-d4 | 7.93 |

| 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 | 16 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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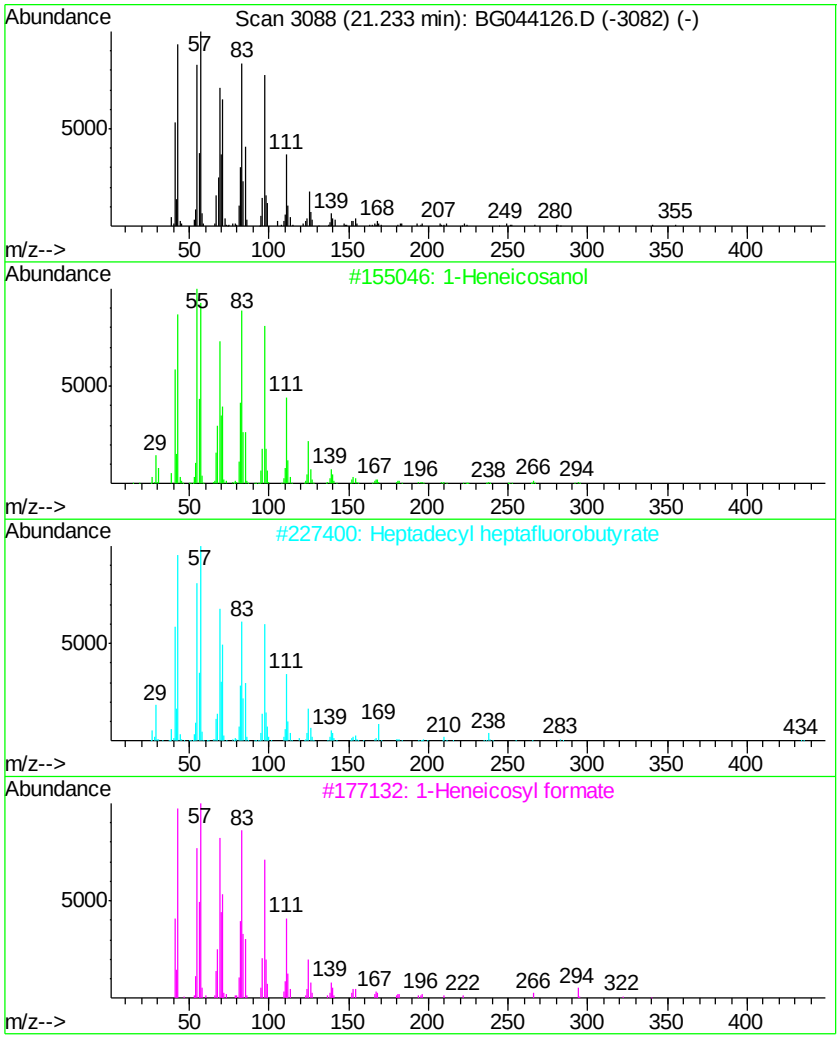
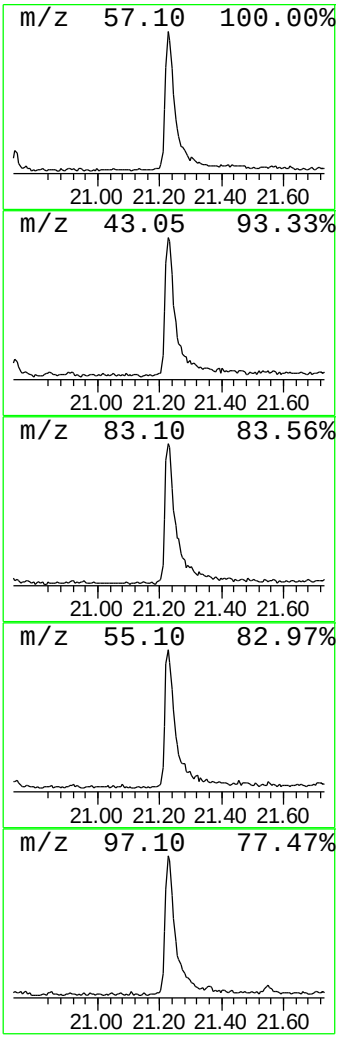
Peak Number 4 1-Heneicosanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.23 | 8.52 ng | 523990 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 3 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 94 |
| 4 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 5 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 93 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

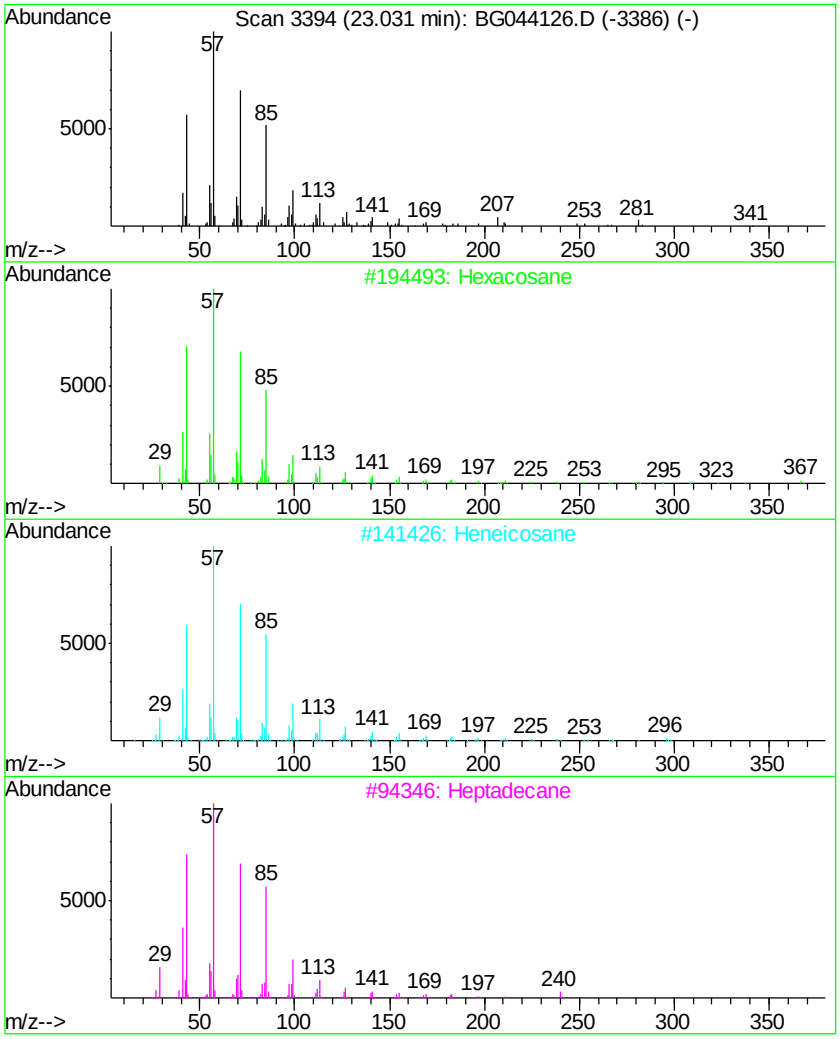
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

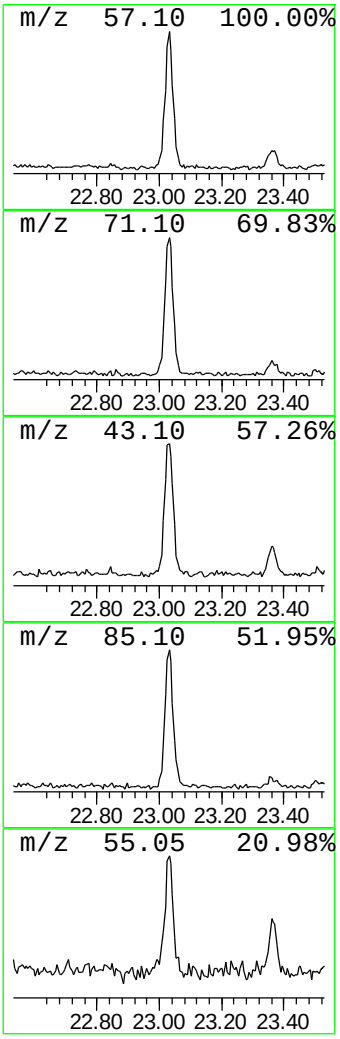
**********

Peak Number 5 Hexacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.03 | 2.67 ng | 164089 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

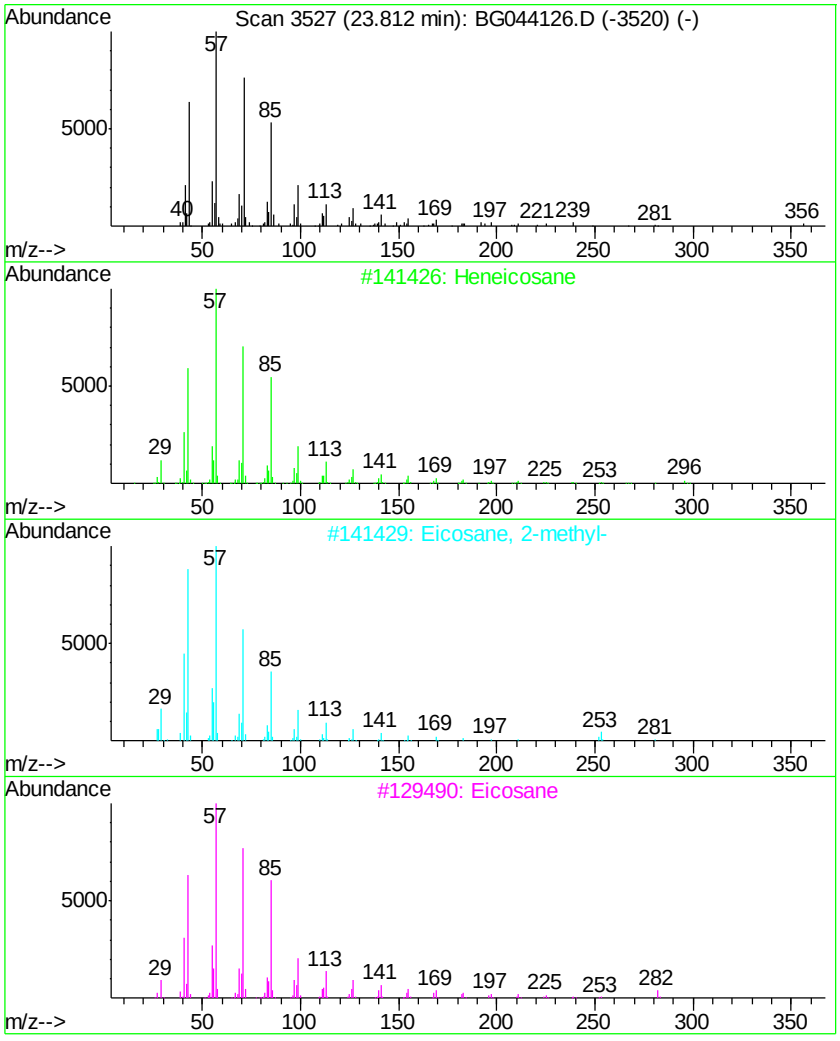
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

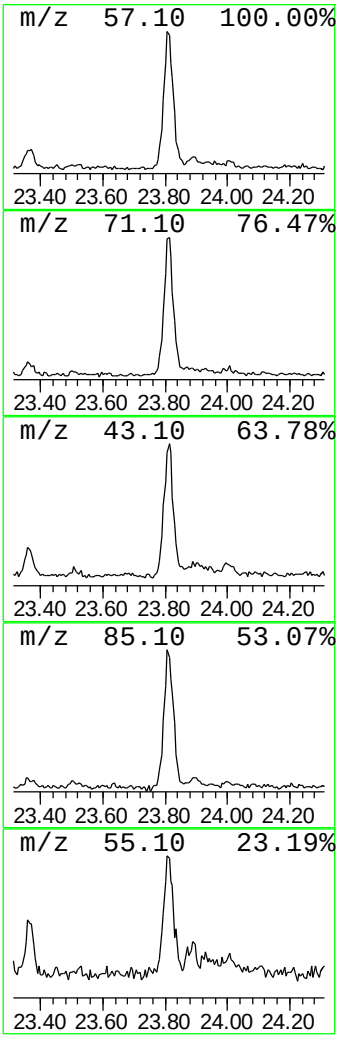
**********

Peak Number 6 Heneicosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.81 | 2.73 ng | 178550 | Perylene-d12 | 24.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Eicosane, 2-methyl- | 296 | C21H44 | 001560-84-5 | 91 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

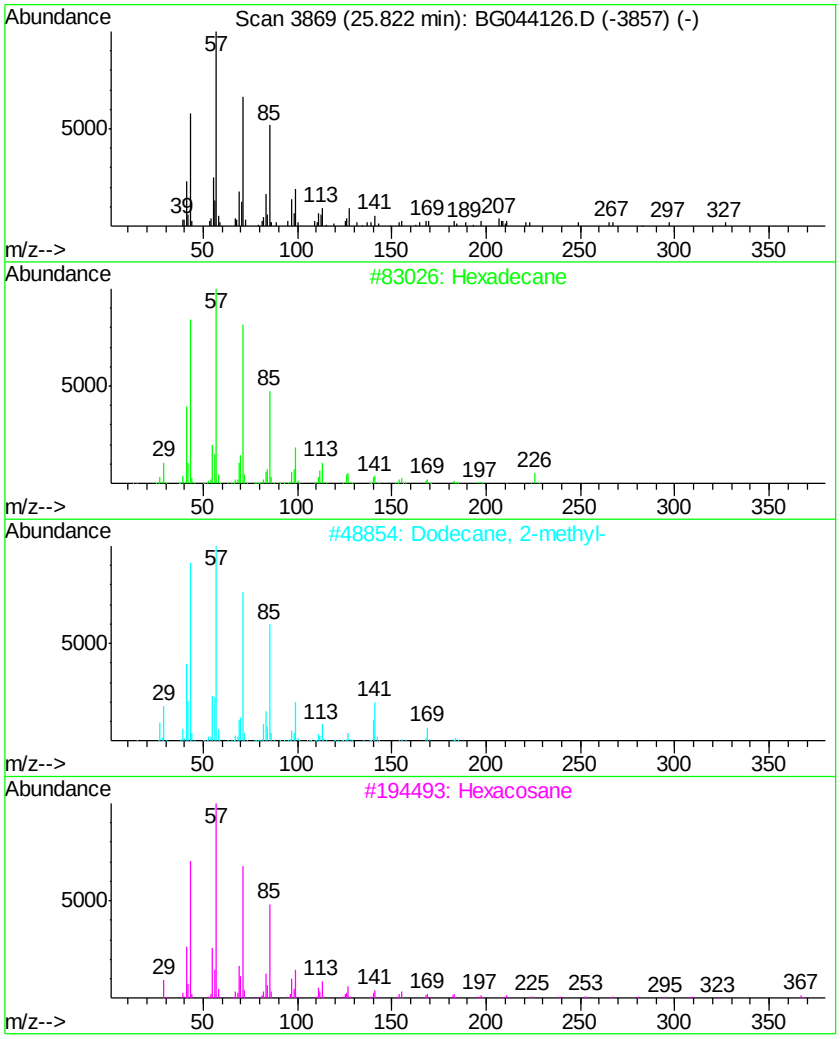
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

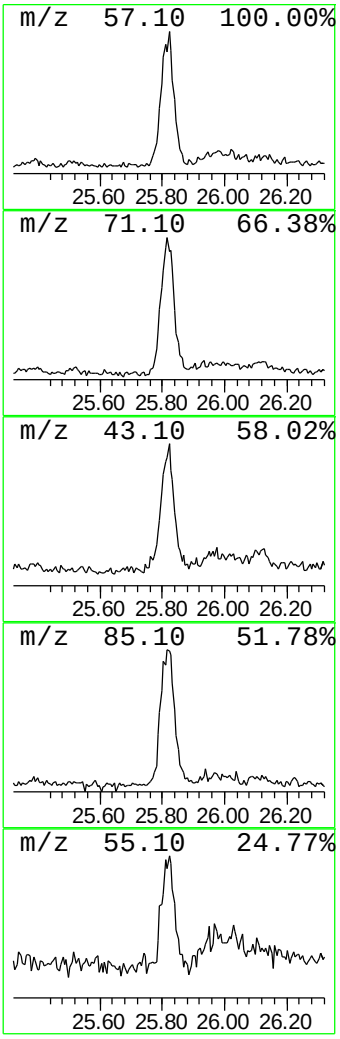
**********

Peak Number 7 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 25.82 | 2.49 ng | 163030 | Perylene-d12 | 24.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 90 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG012020\
Data File : BG044126.D
Acq On : 21 Jan 2020 10:11
Operator : JU
Sample : L1154-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** B4-15-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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 |
| 2-Pentanone, 4-hy... | 5.03 | 23.4 | ng | 533304 | 1 | 7.93 | 455711 | 20.0 |
| unknown7.47 | 7.47 | 122.3 | ng | 2786040 | 1 | 7.93 | 455711 | 20.0 |
| 1-Heneicosanol | 21.23 | 8.5 | ng | 523990 | 5 | 21.56 | 1229550 | 20.0 |
| Hexacosane | 23.03 | 2.7 | ng | 164089 | 5 | 21.56 | 1229550 | 20.0 |
| Heneicosane | 23.81 | 2.7 | ng | 178550 | 6 | 24.66 | 1307400 | 20.0 |
| Hexadecane | 25.82 | 2.5 | ng | 163030 | 6 | 24.66 | 1307400 | 20.0 |