LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

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-BG030419.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 | 3.195 | 13 | 18 | 26 | rBV | 252454 | 495119 | 15.56% | 2.912% |
| 2 | 3.272 | 26 | 31 | 42 | rVB | 530634 | 757905 | 23.82% | 4.457% |
| 3 | 5.692 | 436 | 443 | 451 | rBV | 437363 | 692100 | 21.75% | 4.070% |
| 4 | 7.290 | 708 | 715 | 727 | rBV | 279845 | 501285 | 15.76% | 2.948% |
| 5 | 7.672 | 773 | 780 | 789 | rBV | 745168 | 1284325 | 40.37% | 7.553% |
| 6 | 8.142 | 853 | 860 | 872 | rVB | 164578 | 290426 | 9.13% | 1.708% |
| 7 | 8.471 | 906 | 916 | 923 | rVB | 676048 | 1186576 | 37.30% | 6.978% |
| 8 | 9.322 | 1053 | 1061 | 1069 | rBV | 582491 | 1056559 | 33.21% | 6.214% |
| 9 | 10.967 | 1333 | 1341 | 1349 | rBV | 218109 | 396677 | 12.47% | 2.333% |
| 10 | 13.393 | 1746 | 1754 | 1762 | rBV | 1513403 | 2373397 | 74.60% | 13.958% |
| 11 | 14.774 | 1981 | 1989 | 1996 | rBV3 | 318627 | 534084 | 16.79% | 3.141% |
| 12 | 16.260 | 2235 | 2242 | 2248 | rBV | 1078646 | 1676367 | 52.69% | 9.859% |
| 13 | 17.517 | 2449 | 2456 | 2466 | rBV | 421399 | 651876 | 20.49% | 3.834% |
| 14 | 18.175 | 2563 | 2568 | 2573 | rVB7 | 26917 | 41819 | 1.31% | 0.246% |
| 15 | 18.369 | 2596 | 2601 | 2611 | rBV4 | 50167 | 84300 | 2.65% | 0.496% |
| 16 | 18.680 | 2650 | 2654 | 2663 | rVB2 | 30606 | 65646 | 2.06% | 0.386% |
| 17 | 18.786 | 2667 | 2672 | 2676 | rBV6 | 22358 | 37640 | 1.18% | 0.221% |
| 18 | 18.962 | 2698 | 2702 | 2706 | rVB3 | 34926 | 42057 | 1.32% | 0.247% |
| 19 | 19.632 | 2812 | 2816 | 2820 | rBV4 | 29138 | 44745 | 1.41% | 0.263% |
| 20 | 20.108 | 2892 | 2897 | 2903 | rBV | 2433638 | 3181563 | 100.00% | 18.711% |
| 21 | 21.805 | 3179 | 3186 | 3192 | rBV2 | 426922 | 713218 | 22.42% | 4.195% |
| 22 | 23.280 | 3433 | 3437 | 3446 | rVB3 | 29951 | 58284 | 1.83% | 0.343% |
| 23 | 24.108 | 3575 | 3578 | 3584 | rVB4 | 33247 | 63401 | 1.99% | 0.373% |
| 24 | 25.101 | 3741 | 3747 | 3748 | rBV4 | 29785 | 51935 | 1.63% | 0.305% |
| 25 | 25.166 | 3750 | 3758 | 3769 | rVB2 | 241376 | 722193 | 22.70% | 4.247% |

Sum of corrected areas: 17003497

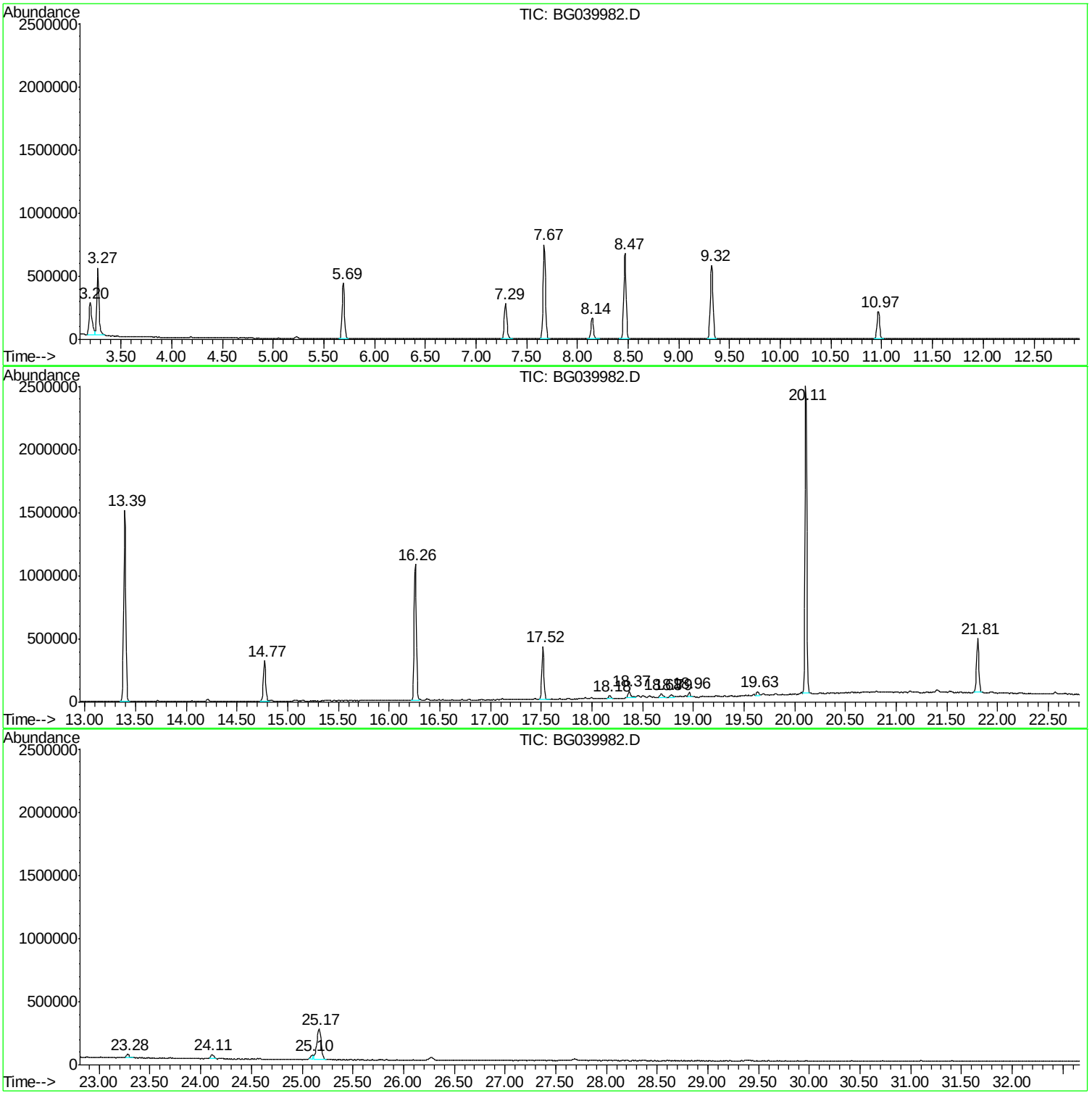
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

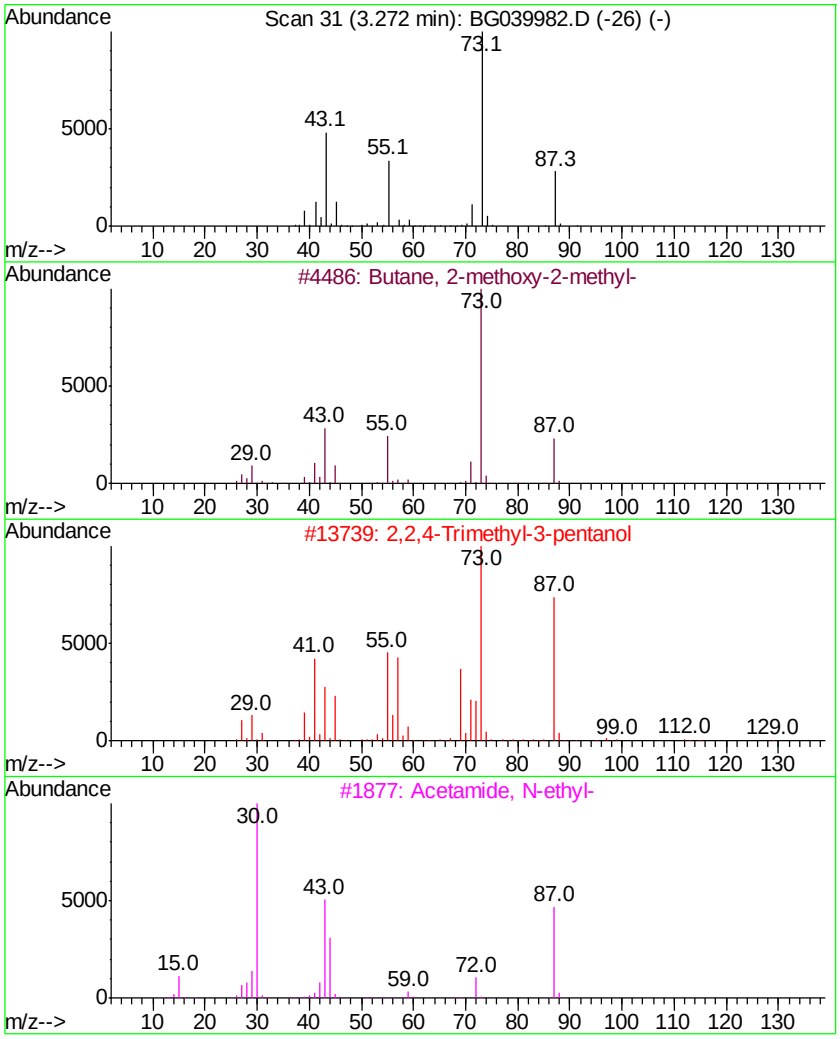
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

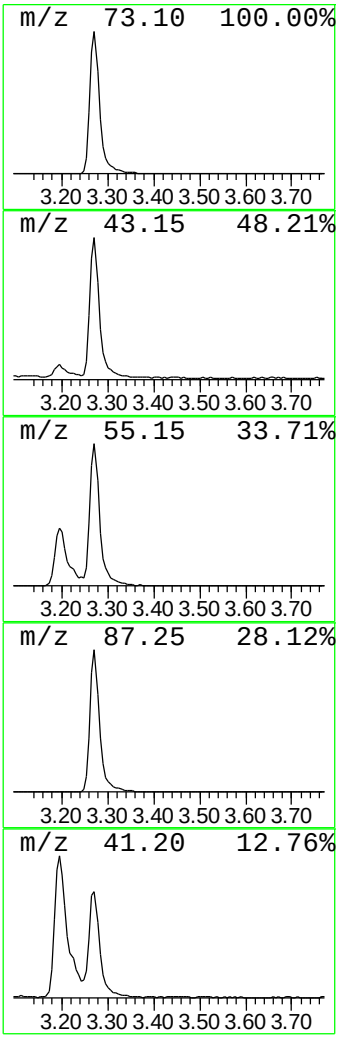
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.27 | 52.19 ng | 757905 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 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\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

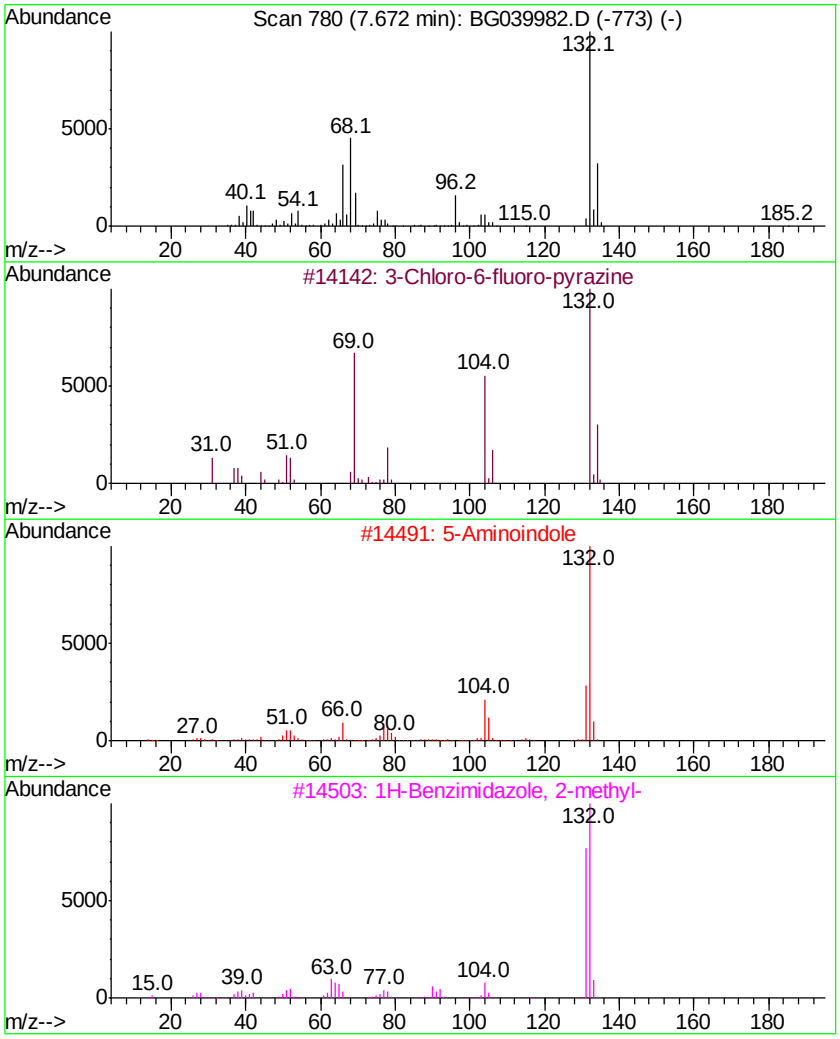
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

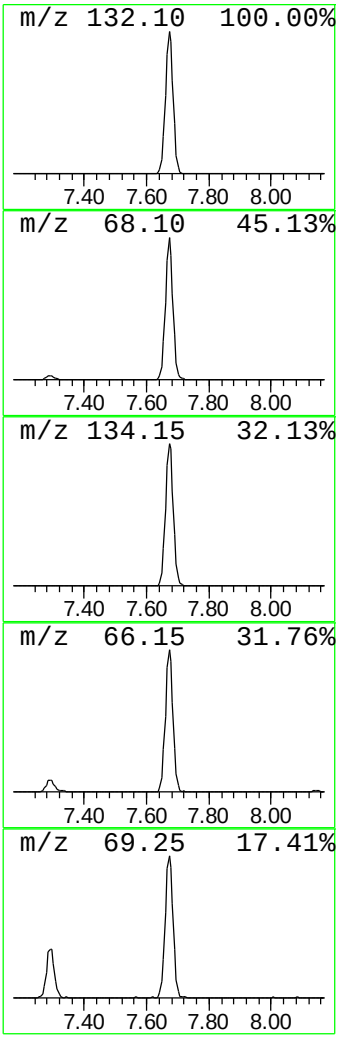
**********

Peak Number 3 unknown7.67 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.67 | 88.44 ng | 1284330 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 27 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

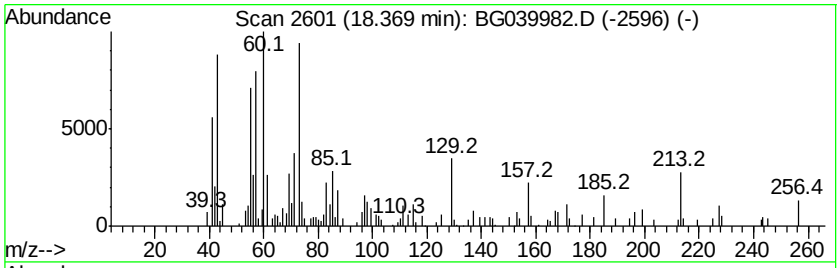
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

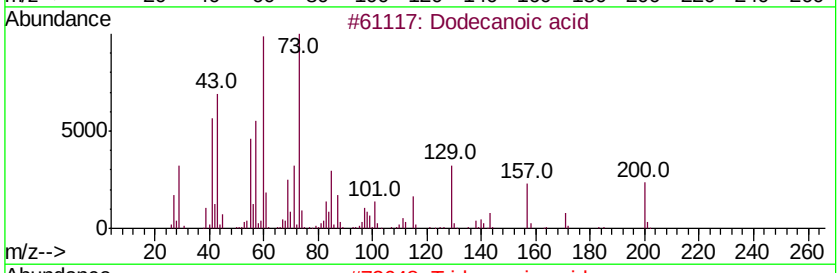
**********

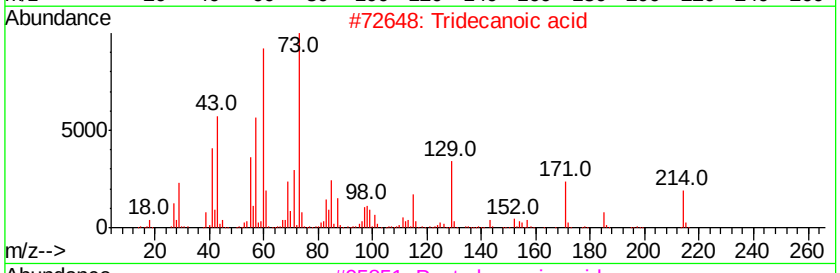
Peak Number 5 Dodecanoic acid Concentration Rank 5

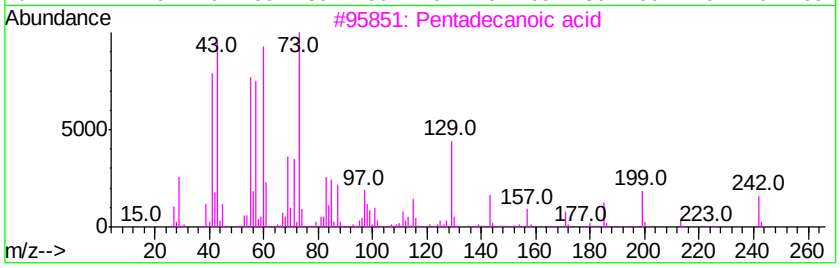
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.37 | 2.59 ng | 84300 | Phenanthrene-d10 | 17.52 |

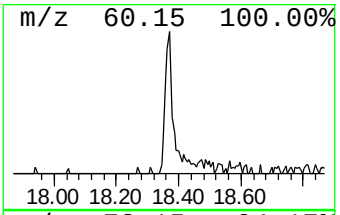
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 72 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 62 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 62 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 60 |
| 5 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 58 |

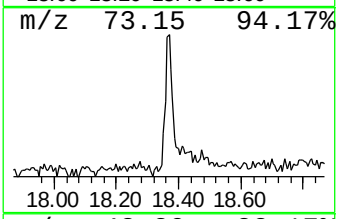


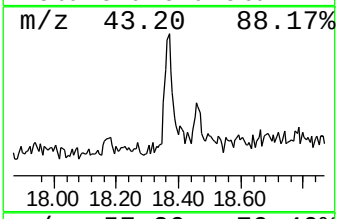



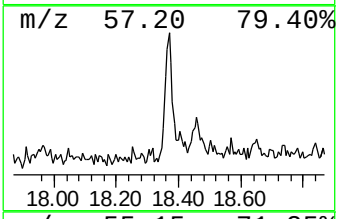



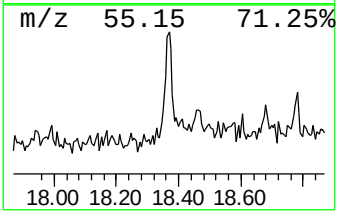



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

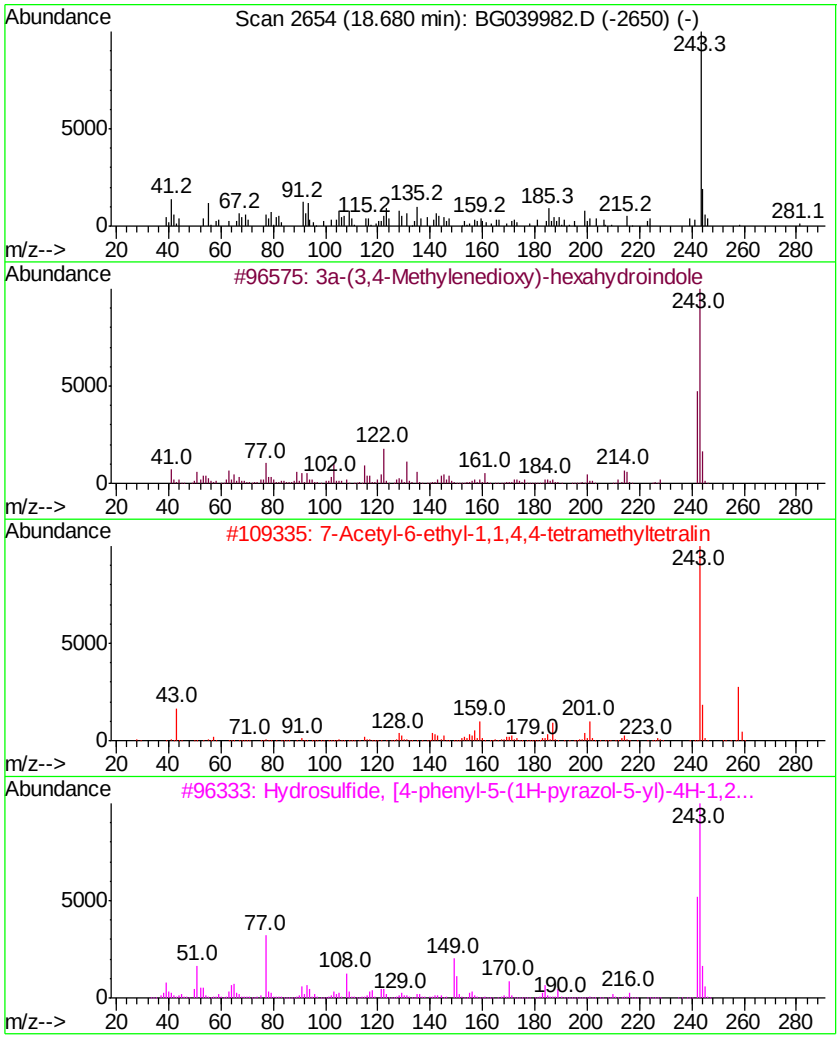
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

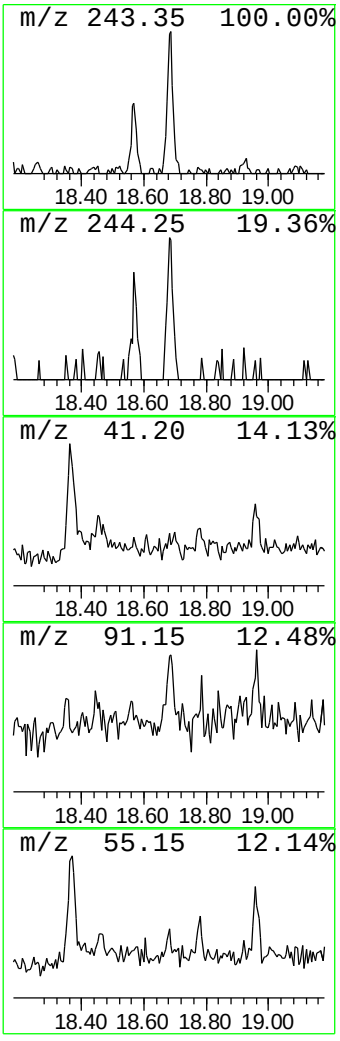
**********

Peak Number 6 3a-(3,4-Methylenedioxy)-hex... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.68 | 2.01 ng | 65646 | Phenanthrene-d10 | 17.52 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3a-(3,4-Methylenedioxy)-hexahydr... | 243 | C15H17NO2 | 109535-43-5 | 64 |
| 2 | 7-Acetyl-6-ethyl-1,1,4,4-tetrame... | 258 | C18H26O | 000088-29-9 | 59 |
| 3 | Hydrosulfide, [4-phenyl-5-(1H-py... | 243 | C11H9N5S | 1000338-10-2 | 58 |
| 4 | 3-Phenyl-4-azafluorene | 243 | C18H13N | 033777-97-8 | 58 |
| 5 | 2(1H)-Pyridinone, 3-acetyl-4-hyd... | 243 | C14H13NO3 | 013959-06-3 | 53 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG031819\
Data File : BG039982.D
Acq On : 18 Mar 2019 23:13
Operator : JU/SJ
Sample : K1932-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG030419.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... | 3.27 | 52.2 | ng | 757905 | 1 | 8.15 | 290426 | 20.0 |
| unknown7.67 | 7.67 | 88.4 | ng | 1284330 | 1 | 8.15 | 290426 | 20.0 |
| Dodecanoic acid | 18.37 | 2.6 | ng | 84300 | 4 | 17.52 | 651876 | 20.0 |
| 3a-(3,4-Methylene... | 18.68 | 2.0 | ng | 65646 | 4 | 17.52 | 651876 | 20.0 |