LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-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-BG120919.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 | 3.196 | 13 | 18 | 27 | rVB | 211119 | 298651 | 4.37% | 0.776% |
| 2 | 5.111 | 338 | 344 | 353 | rBV | 327913 | 489621 | 7.16% | 1.272% |
| 3 | 5.581 | 416 | 424 | 434 | rBV | 1493787 | 2385899 | 34.90% | 6.199% |
| 4 | 7.162 | 685 | 693 | 704 | rBV | 1681489 | 2924571 | 42.78% | 7.598% |
| 5 | 7.538 | 749 | 757 | 767 | rBV | 1533927 | 2698397 | 39.47% | 7.011% |
| 6 | 8.002 | 828 | 836 | 843 | rBV | 365234 | 631378 | 9.24% | 1.640% |
| 7 | 8.325 | 882 | 891 | 899 | rBV | 1140594 | 1958606 | 28.65% | 5.089% |
| 8 | 9.153 | 1022 | 1032 | 1040 | rBV | 930448 | 1681273 | 24.59% | 4.368% |
| 9 | 10.804 | 1303 | 1313 | 1322 | rBV | 528566 | 984894 | 14.41% | 2.559% |
| 10 | 13.255 | 1722 | 1730 | 1743 | rBV | 2657683 | 4188746 | 61.27% | 10.883% |
| 11 | 14.077 | 1863 | 1870 | 1882 | rVB | 228269 | 349676 | 5.11% | 0.908% |
| 12 | 14.623 | 1956 | 1963 | 1974 | rBV | 1047925 | 1655272 | 24.21% | 4.301% |
| 13 | 16.110 | 2209 | 2216 | 2236 | rBV | 1871812 | 3055360 | 44.69% | 7.938% |
| 14 | 17.367 | 2423 | 2430 | 2441 | rBV | 1456740 | 2191452 | 32.05% | 5.694% |
| 15 | 19.982 | 2869 | 2875 | 2885 | rBV | 5305947 | 6836729 | 100.00% | 17.762% |
| 16 | 21.292 | 3093 | 3098 | 3111 | rBV2 | 412332 | 781861 | 11.44% | 2.031% |
| 17 | 21.627 | 3148 | 3155 | 3163 | rBV | 1345762 | 2290780 | 33.51% | 5.952% |
| 18 | 21.856 | 3189 | 3194 | 3203 | rVB | 135388 | 208916 | 3.06% | 0.543% |
| 19 | 22.455 | 3292 | 3296 | 3302 | rBV2 | 153528 | 258069 | 3.77% | 0.670% |
| 20 | 23.149 | 3409 | 3414 | 3423 | rVB | 152926 | 284372 | 4.16% | 0.739% |
| 21 | 23.948 | 3544 | 3550 | 3562 | rBV2 | 121788 | 267500 | 3.91% | 0.695% |
| 22 | 24.782 | 3683 | 3692 | 3704 | rBV2 | 667608 | 2068067 | 30.25% | 5.373% |

Sum of corrected areas: 38490090

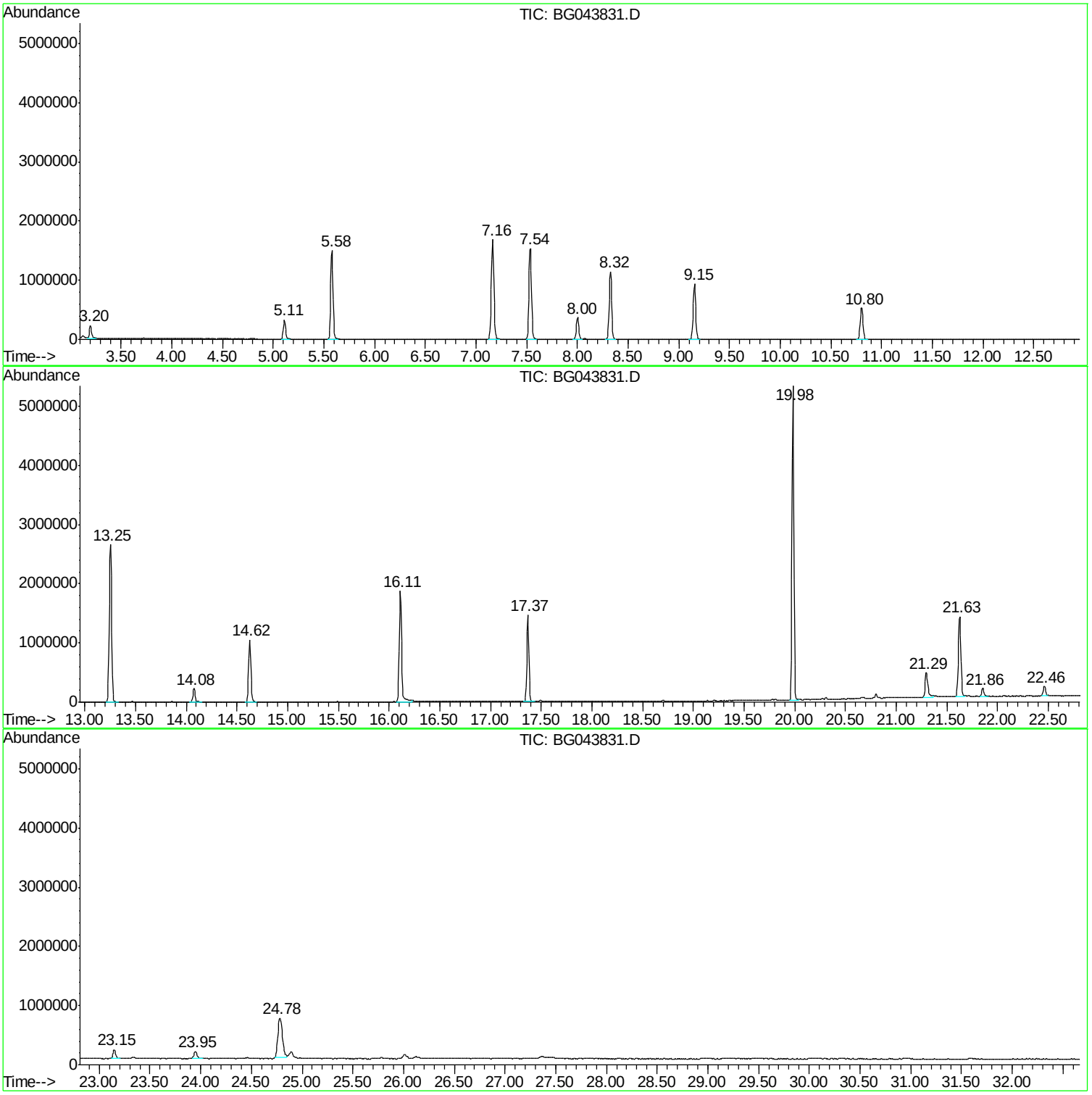
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

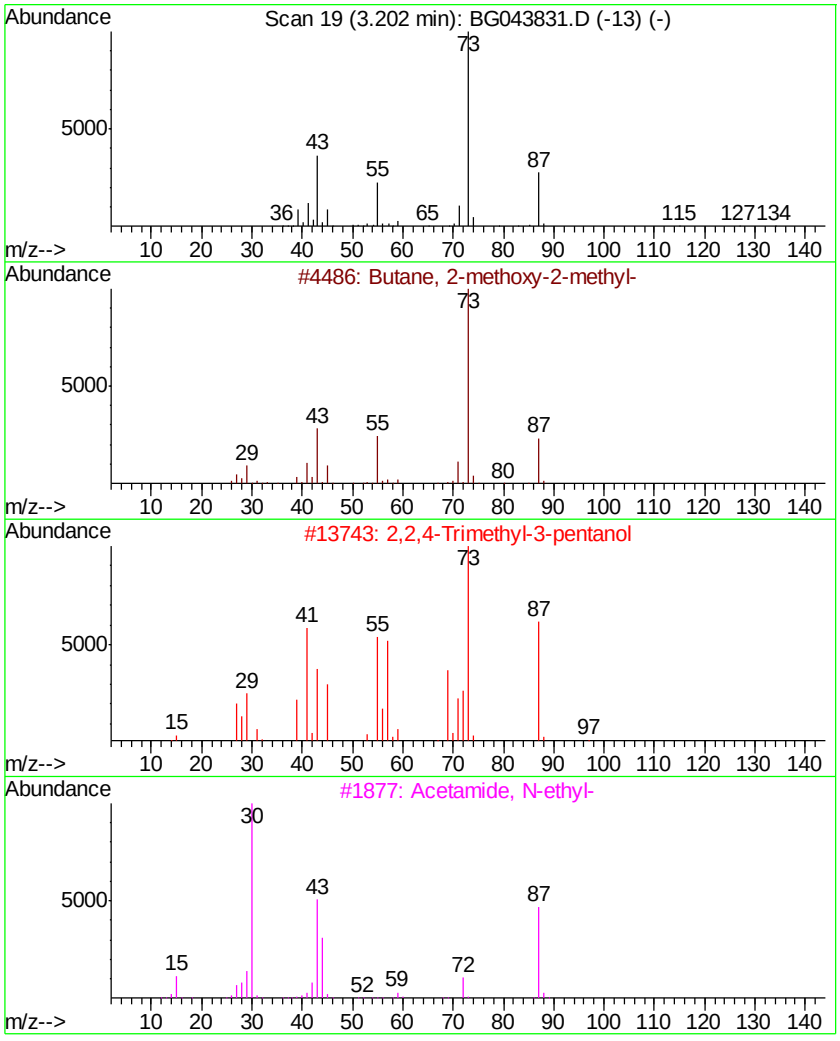
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

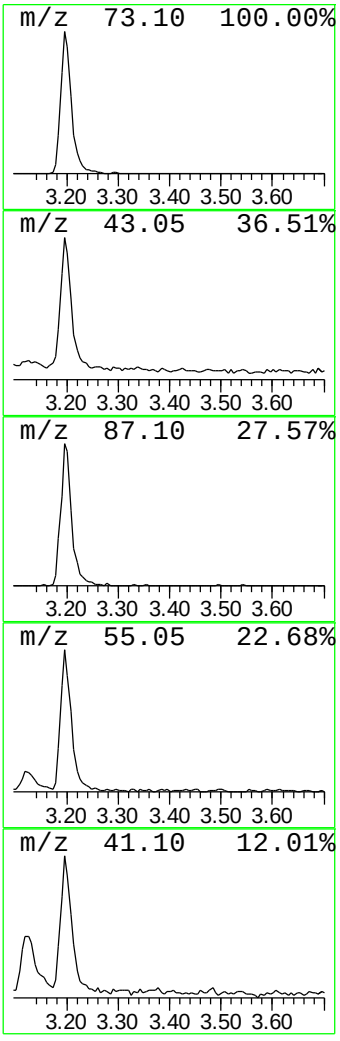
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.20 | 9.46 ng | 298651 | 1,4-Dichlorobenzene-d4 | 8.00 |

| 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 | 56 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

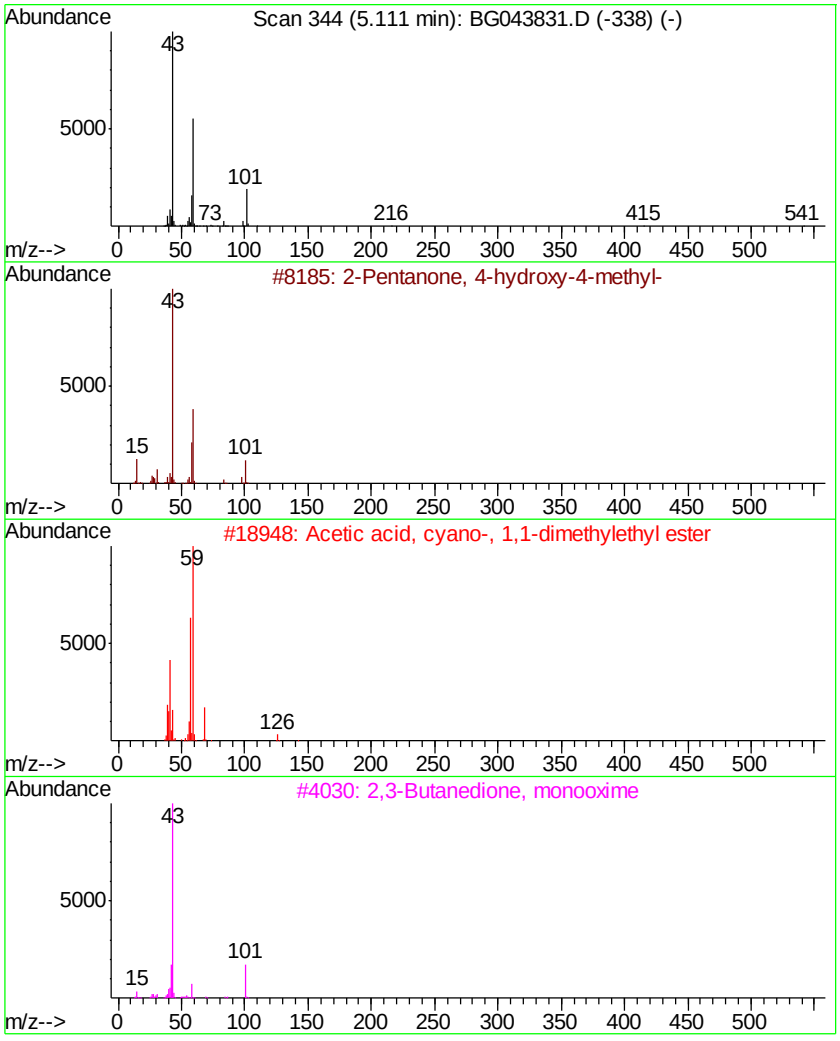
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

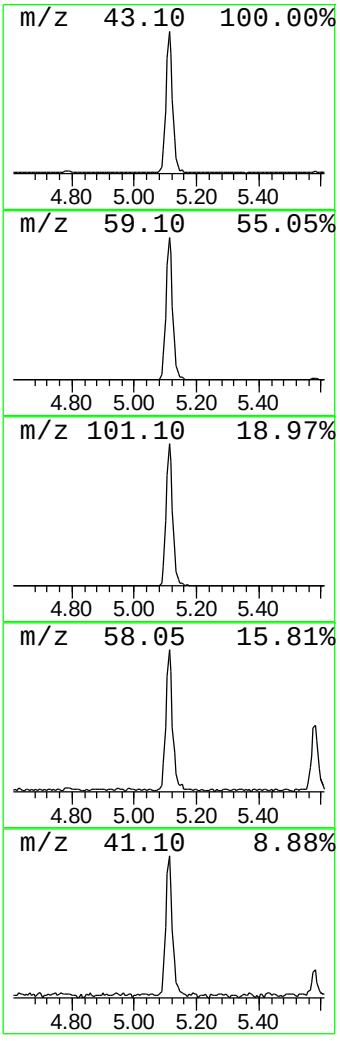
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 15.51 ng | 489621 | 1,4-Dichlorobenzene-d4 | 8.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 12 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

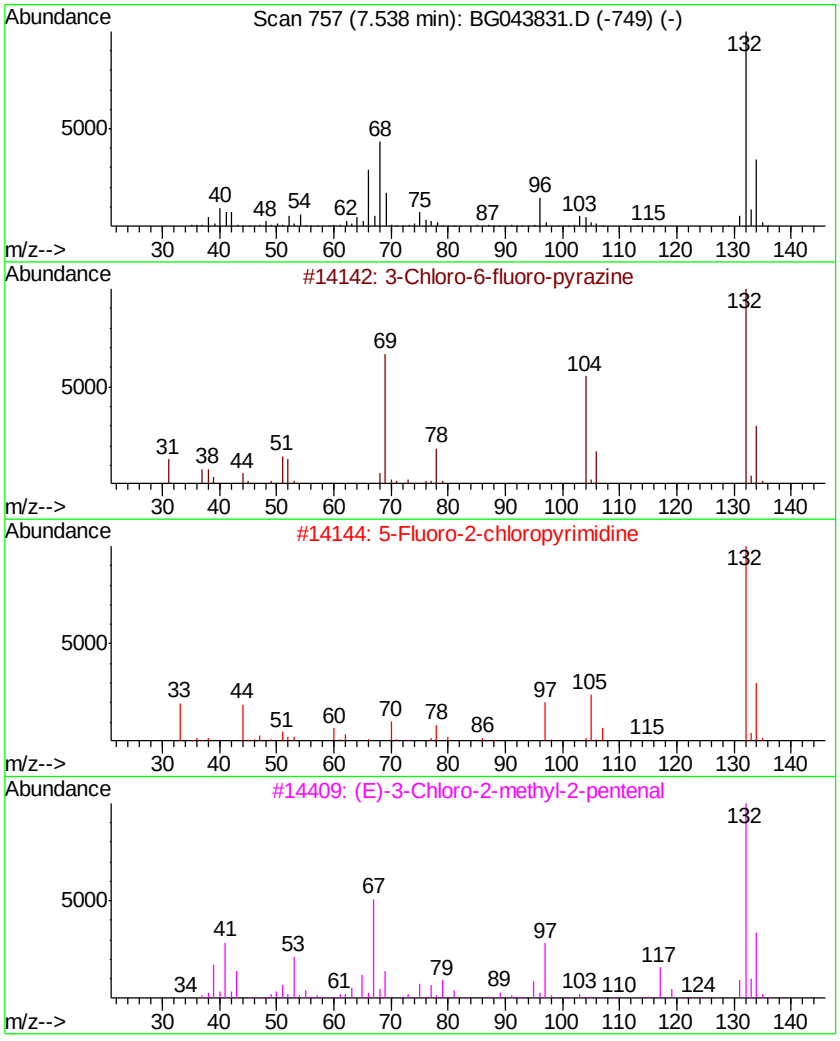
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

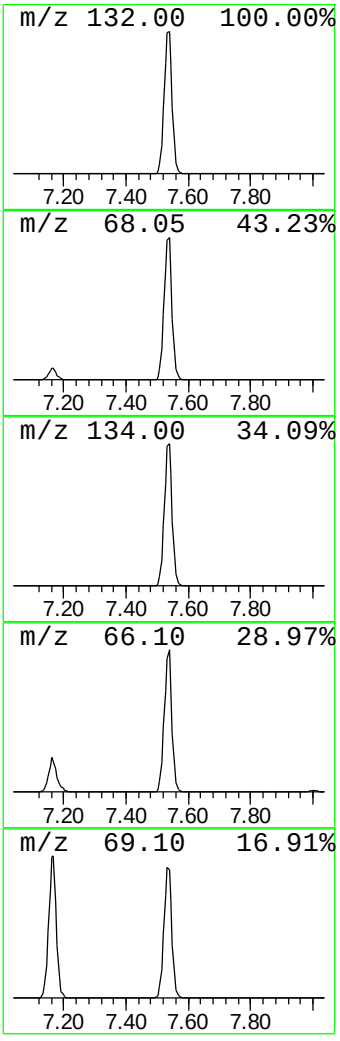
**********

Peak Number 3 unknown7.54 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.54 | 85.48 ng | 2698400 | 1,4-Dichlorobenzene-d4 | 8.00 |

| 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 | 16 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

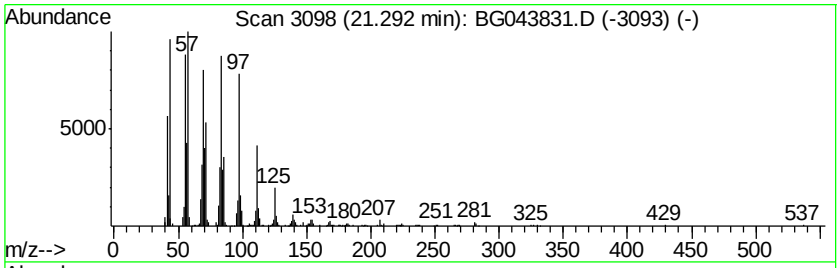
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

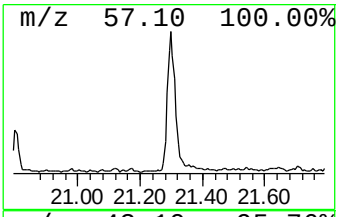
**********

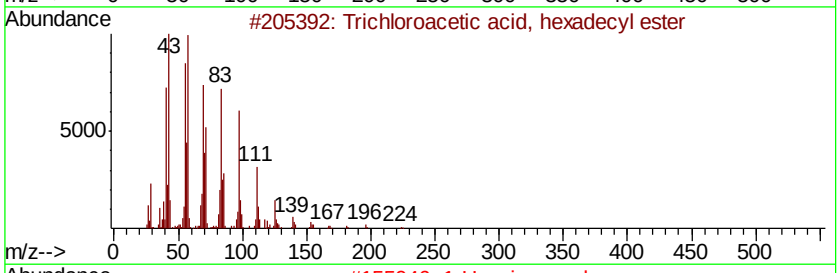
Peak Number 5 1-Heneicosanol Concentration Rank 5

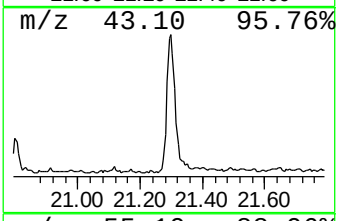
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.29 | 6.83 ng | 781861 | Chrysene-d12 | 21.63 |

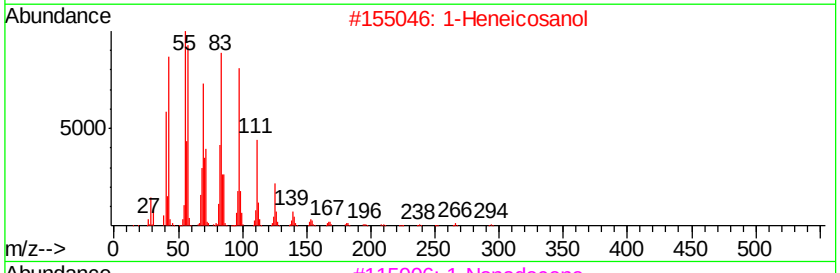
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 3 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 4 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 91 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91 |

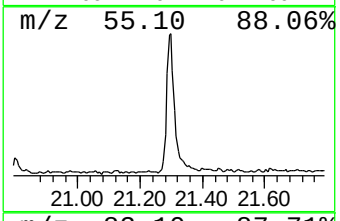


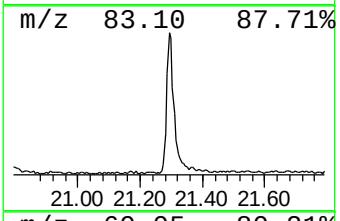



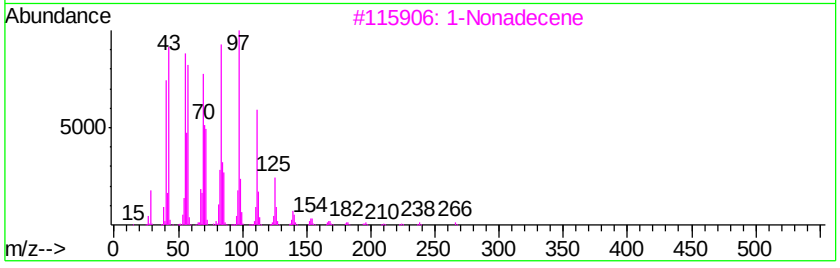



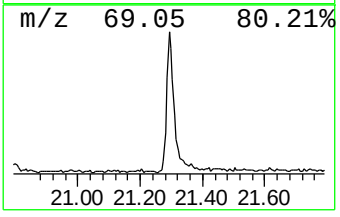



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

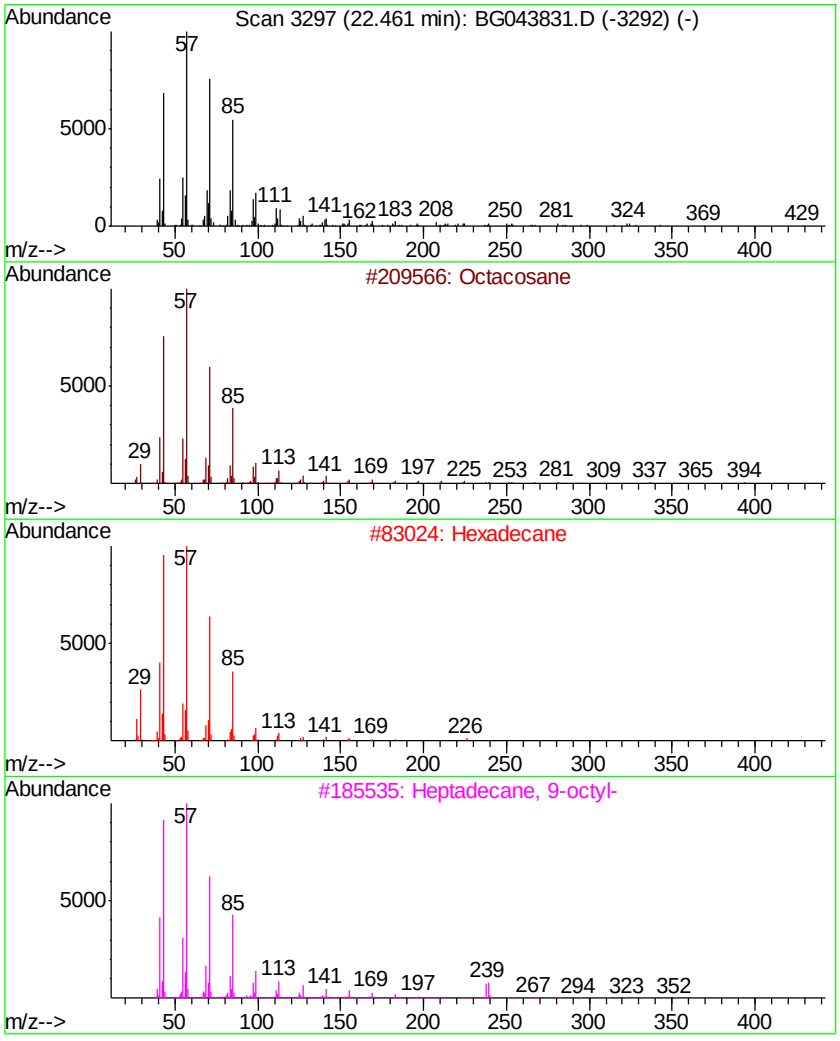
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

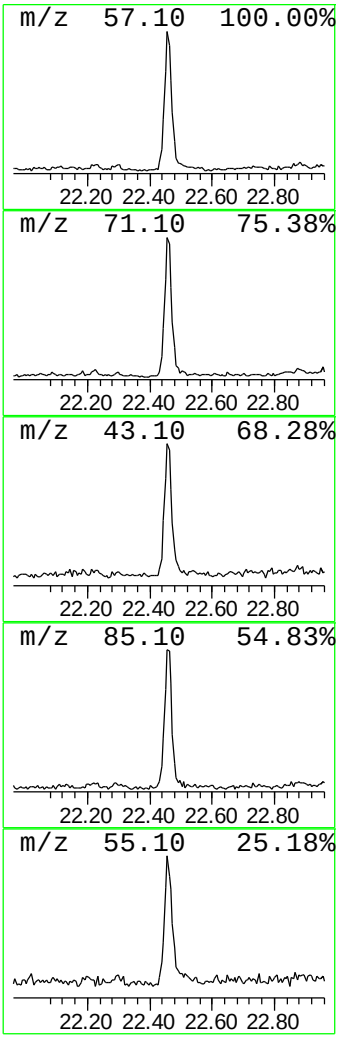
**********

Peak Number 6 Octacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.46 | 2.25 ng | 258069 | Chrysene-d12 | 21.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

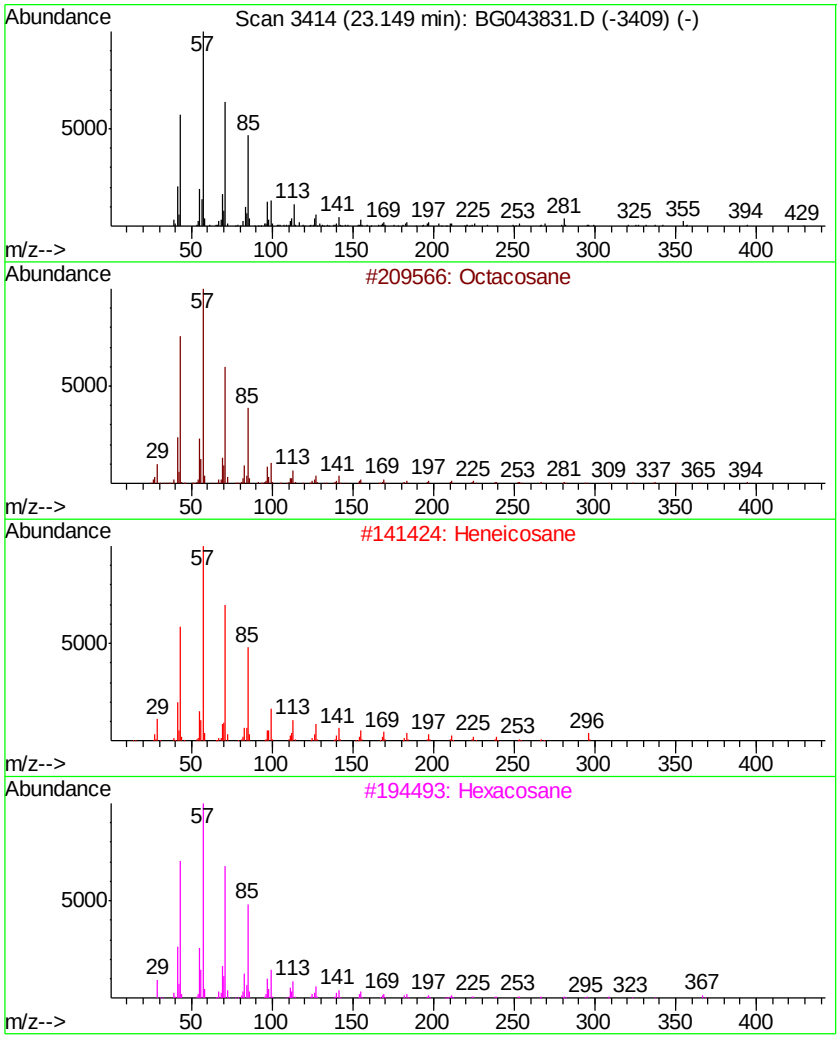
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

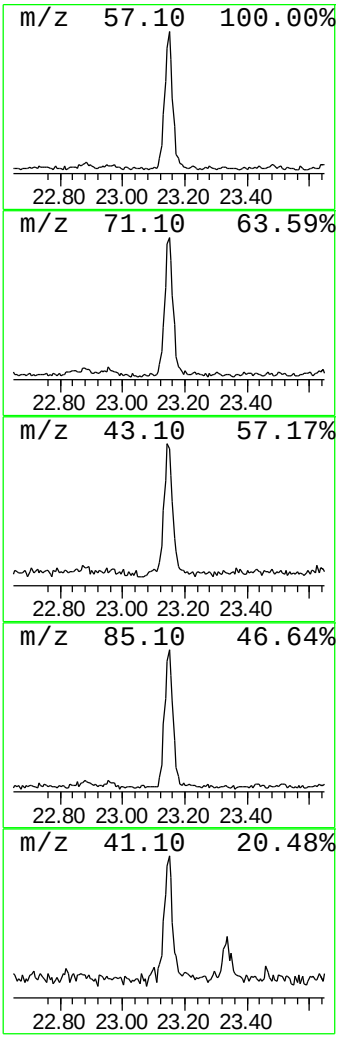
**********

Peak Number 7 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.15 | 2.48 ng | 284372 | Chrysene-d12 | 21.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 93 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |
| 5 | 5,5,7,7-Tetraethylundecane | 268 | C19H40 | 1000360-42-0 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

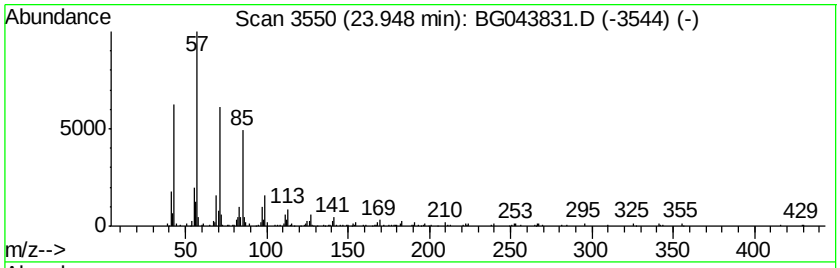
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

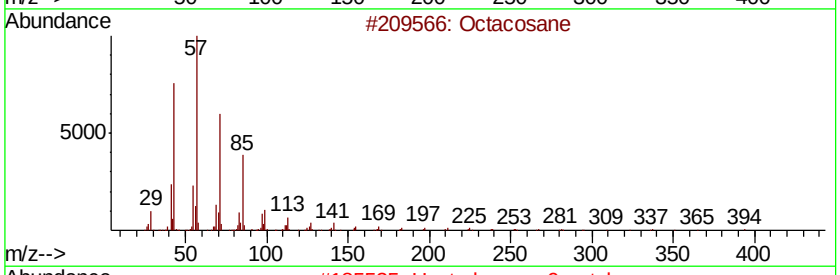
**********

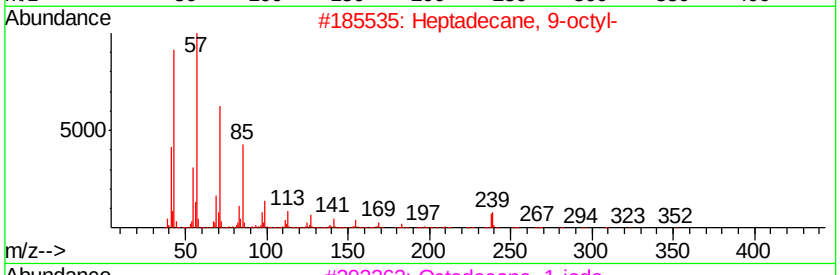
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 6

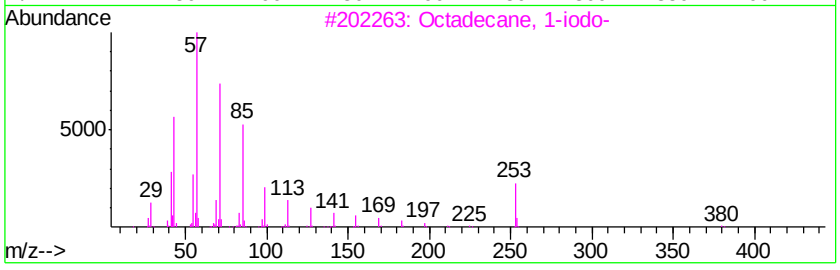
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.95 | 2.59 ng | 267500 | Perylene-d12 | 24.79 |

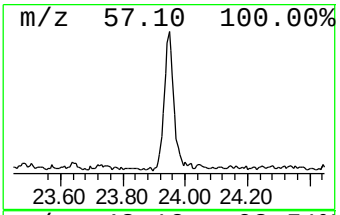
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 3 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 83 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 81 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |

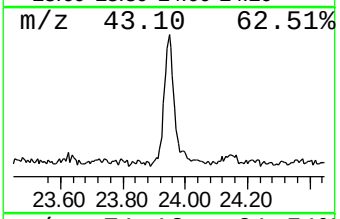


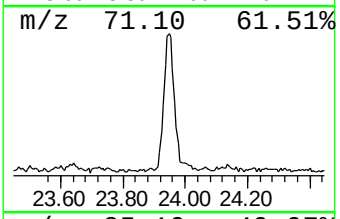



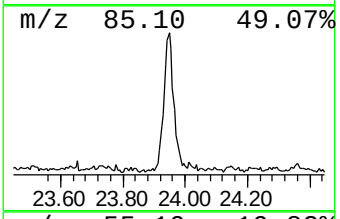



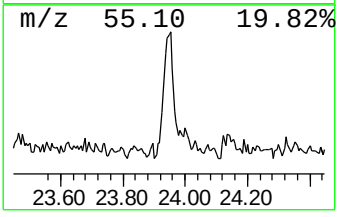



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121719\
Data File : BG043831.D
Acq On : 17 Dec 2019 22:35
Operator : JU
Sample : K6318-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** X089-WC-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.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... | 3.20 | 9.5 | ng | 298651 | 1 | 8.00 | 631378 | 20.0 |
| 2-Pentanone, 4-hy... | 5.11 | 15.5 | ng | 489621 | 1 | 8.00 | 631378 | 20.0 |
| unknown7.54 | 7.54 | 85.5 | ng | 2698400 | 1 | 8.00 | 631378 | 20.0 |
| 1-Heneicosanol | 21.29 | 6.8 | ng | 781861 | 5 | 21.63 | 2290780 | 20.0 |
| Octacosane | 22.46 | 2.3 | ng | 258069 | 5 | 21.63 | 2290780 | 20.0 |
| Heneicosane | 23.15 | 2.5 | ng | 284372 | 5 | 21.63 | 2290780 | 20.0 |
| Heptadecane, 9-oc... | 23.95 | 2.6 | ng | 267500 | 6 | 24.79 | 2068070 | 20.0 |