LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

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-BG121218.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 | 3.177 | 12 | 15 | 26 | rVB | 36360 | 55268 | 2.18% | 0.482% |
| 2 | 5.609 | 423 | 429 | 441 | rVB | 239896 | 395601 | 15.64% | 3.449% |
| 3 | 7.219 | 696 | 703 | 714 | rBV | 168610 | 328500 | 12.99% | 2.864% |
| 4 | 7.583 | 758 | 765 | 777 | rBV | 422548 | 761544 | 30.10% | 6.639% |
| 5 | 8.053 | 838 | 845 | 854 | rBV | 83036 | 140535 | 5.56% | 1.225% |
| 6 | 8.376 | 892 | 900 | 911 | rBV | 346566 | 617936 | 24.43% | 5.387% |
| 7 | 9.234 | 1038 | 1046 | 1059 | rBV | 301655 | 576942 | 22.81% | 5.030% |
| 8 | 10.873 | 1317 | 1325 | 1335 | rBV | 117714 | 215828 | 8.53% | 1.882% |
| 9 | 13.312 | 1732 | 1740 | 1752 | rBV | 1009302 | 1573614 | 62.20% | 13.718% |
| 10 | 14.692 | 1968 | 1975 | 1988 | rBV2 | 218171 | 359319 | 14.20% | 3.132% |
| 11 | 16.185 | 2222 | 2229 | 2243 | rBV3 | 852505 | 1358442 | 53.70% | 11.843% |
| 12 | 17.442 | 2435 | 2443 | 2453 | rBV | 291284 | 454637 | 17.97% | 3.963% |
| 13 | 20.039 | 2879 | 2885 | 2895 | rBV | 1864007 | 2529786 | 100.00% | 22.054% |
| 14 | 20.304 | 2926 | 2930 | 2936 | rVB | 35083 | 41307 | 1.63% | 0.360% |
| 15 | 20.691 | 2988 | 2996 | 3003 | rBV9 | 11100 | 29967 | 1.18% | 0.261% |
| 16 | 20.803 | 3010 | 3015 | 3019 | rBV2 | 58405 | 73256 | 2.90% | 0.639% |
| 17 | 21.308 | 3096 | 3101 | 3112 | rBV | 87677 | 129252 | 5.11% | 1.127% |
| 18 | 21.720 | 3164 | 3171 | 3179 | rVB | 309923 | 522185 | 20.64% | 4.552% |
| 19 | 21.855 | 3188 | 3194 | 3199 | rBV | 77455 | 112221 | 4.44% | 0.978% |
| 20 | 22.466 | 3292 | 3298 | 3304 | rVB | 73143 | 116851 | 4.62% | 1.019% |
| 21 | 23.165 | 3410 | 3417 | 3424 | rBV3 | 61431 | 119143 | 4.71% | 1.039% |
| 22 | 23.359 | 3444 | 3450 | 3455 | rVB2 | 28194 | 55846 | 2.21% | 0.487% |
| 23 | 23.970 | 3547 | 3554 | 3562 | rBV2 | 52695 | 115905 | 4.58% | 1.010% |
| 24 | 24.933 | 3709 | 3718 | 3723 | rBV2 | 41013 | 106589 | 4.21% | 0.929% |
| 25 | 25.016 | 3723 | 3732 | 3743 | rVB2 | 170221 | 495984 | 19.61% | 4.324% |
| 26 | 26.073 | 3901 | 3912 | 3924 | rVB4 | 30187 | 95129 | 3.76% | 0.829% |
| 27 | 27.436 | 4133 | 4144 | 4158 | rVB8 | 21665 | 89170 | 3.52% | 0.777% |

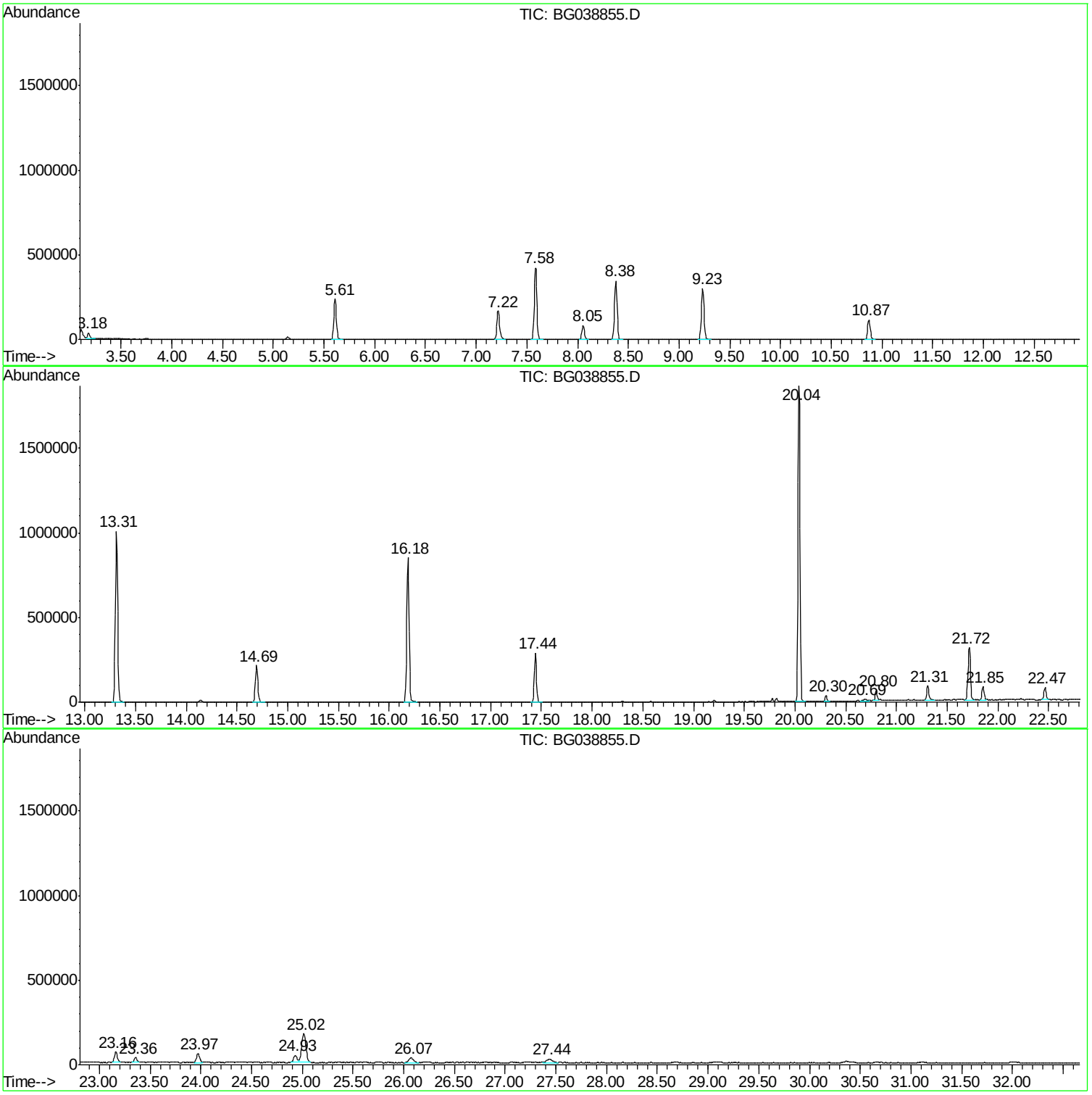
Sum of corrected areas: 11470757

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

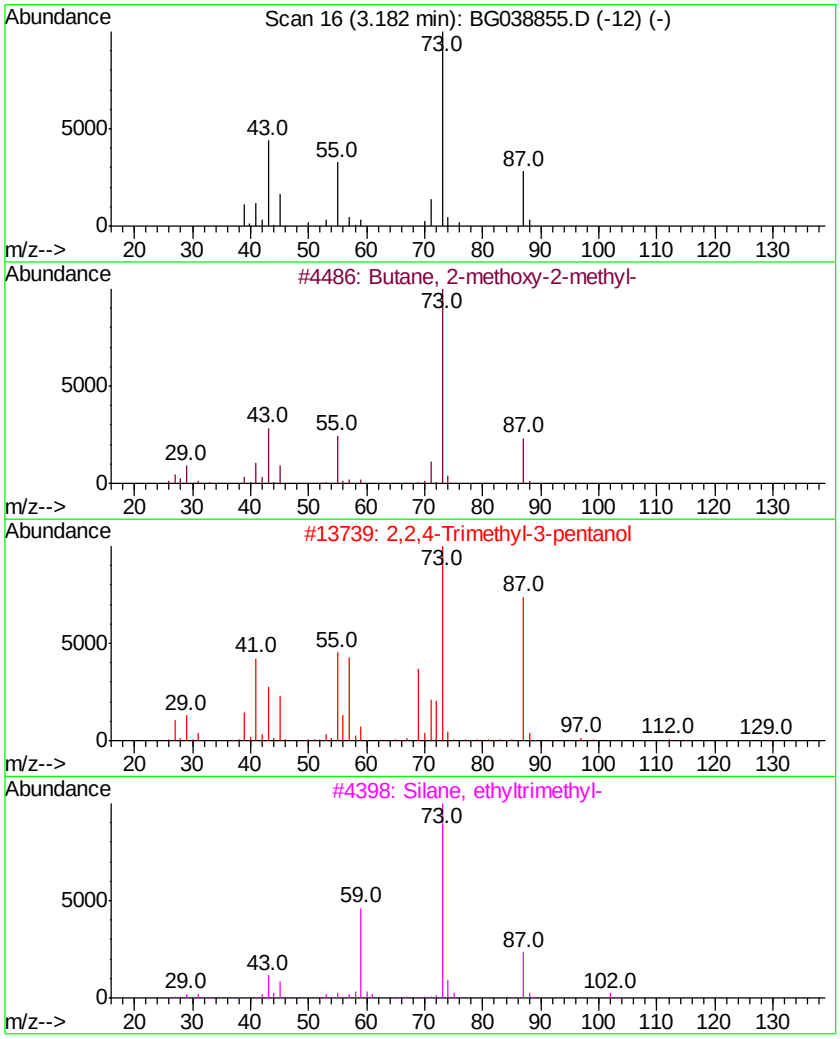
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

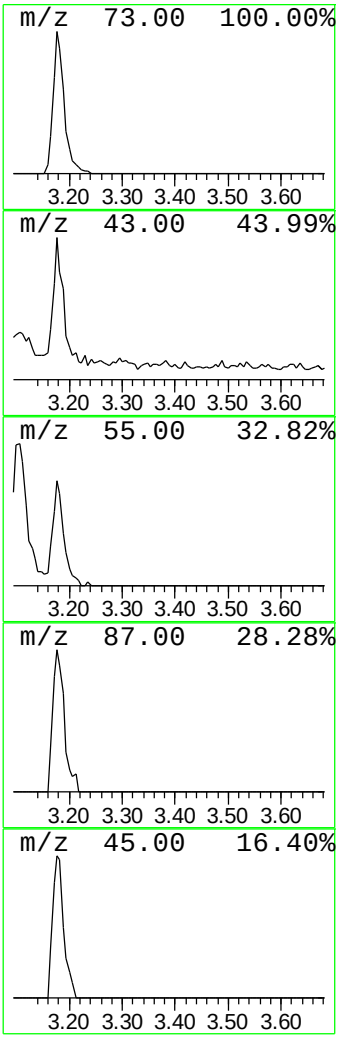
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.18 | 7.87 ng | 55268 | 1,4-Dichlorobenzene-d4 | 8.05 |

| 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 | 40 |
| 3 | Silane, ethyltrimethyl- | 102 | C5H14Si | 003439-38-1 | 38 |
| 4 | 1-Propene-1-thiol | 74 | C3H6S | 000925-89-3 | 32 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 25 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

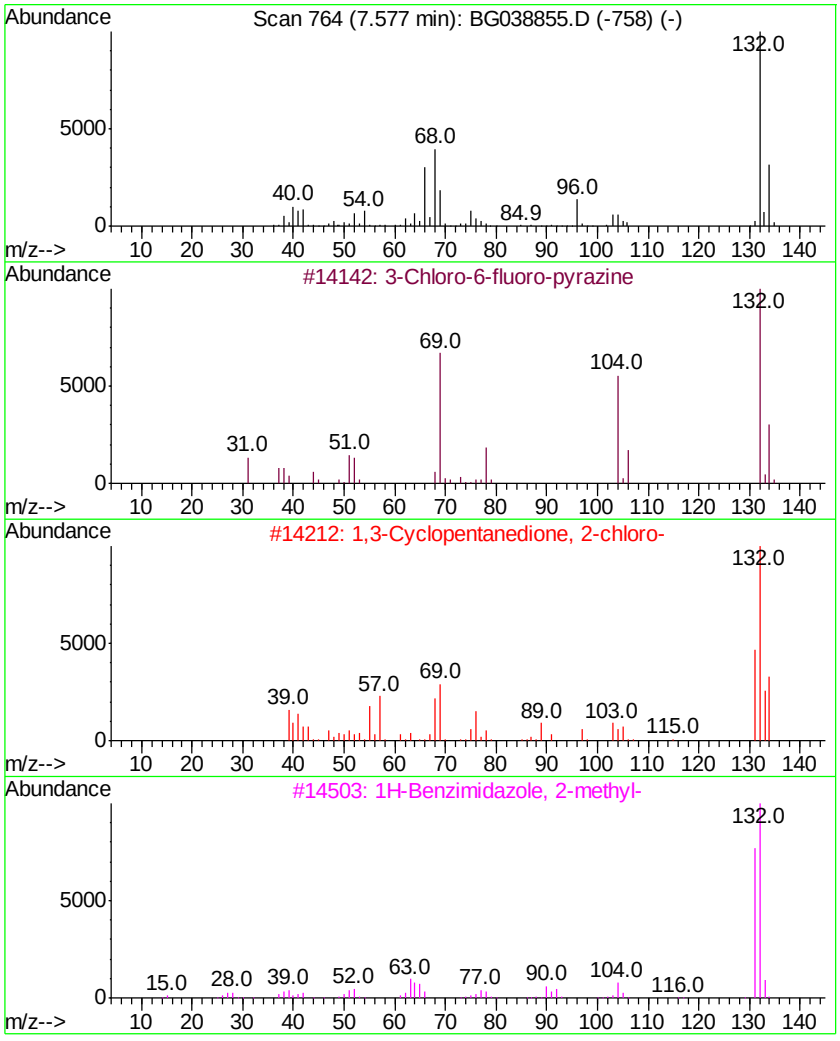
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

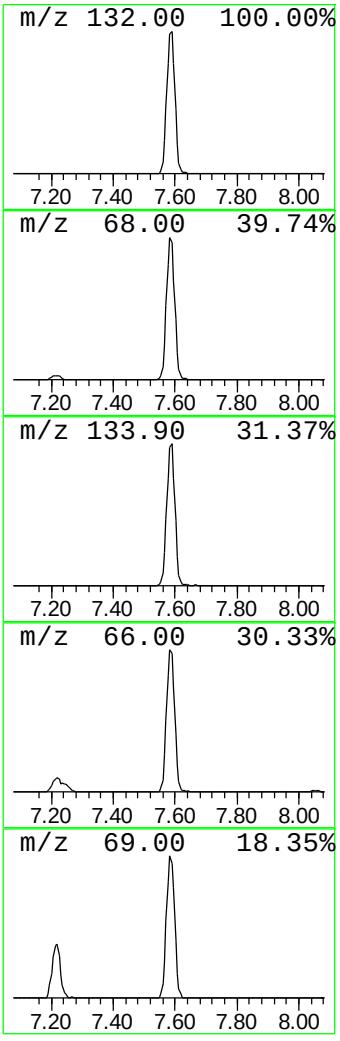
**********

Peak Number 2 unknown7.58 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.58 | 108.38 ng | 761544 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 25 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 5 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |



# Library Search Compound Report

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Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

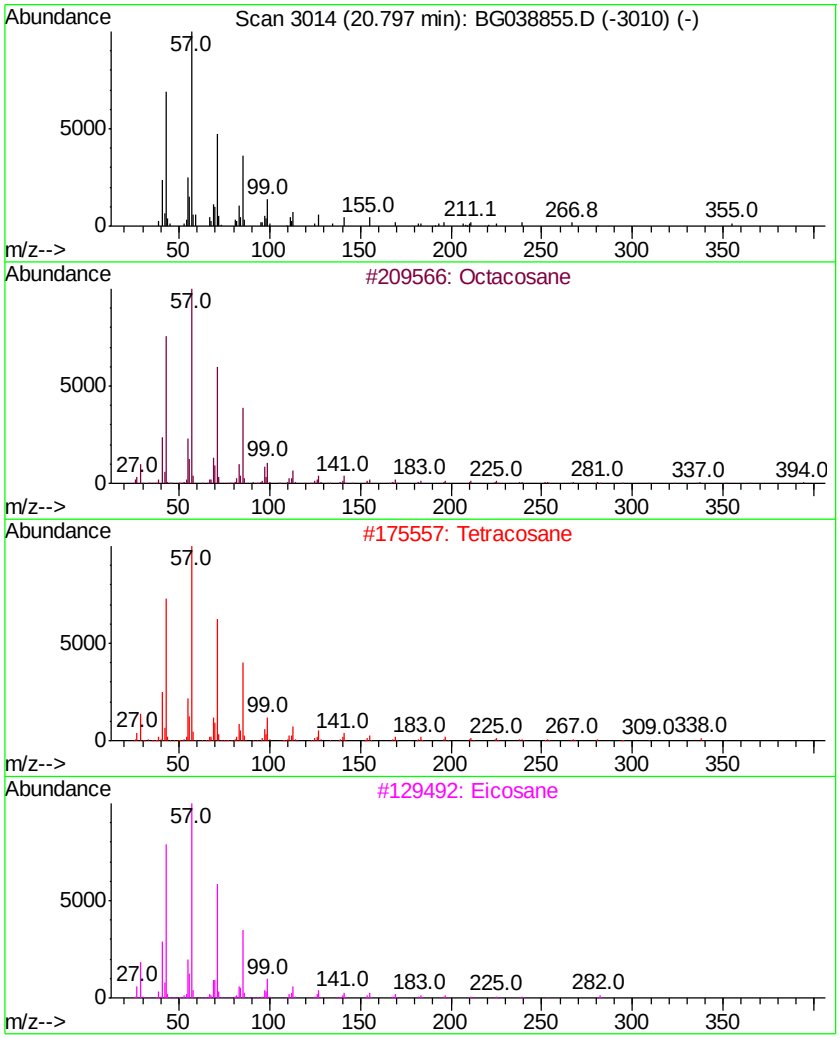
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

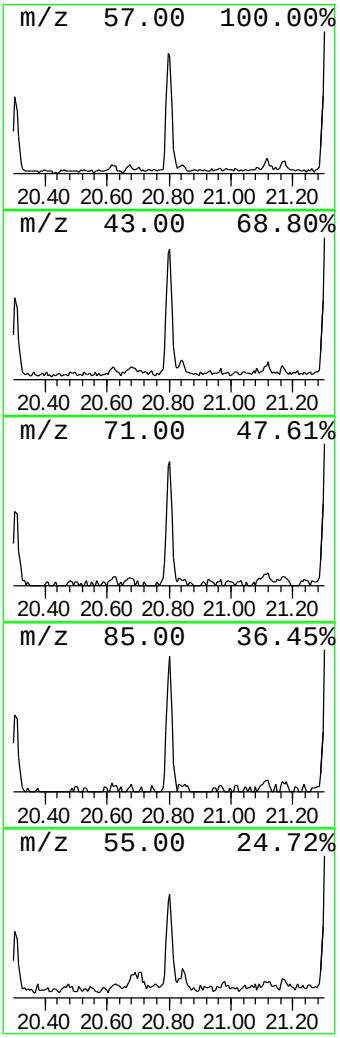
**********

Peak Number 4 Octacosane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.80 | 2.81 ng | 73256 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 83 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 83 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 83 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

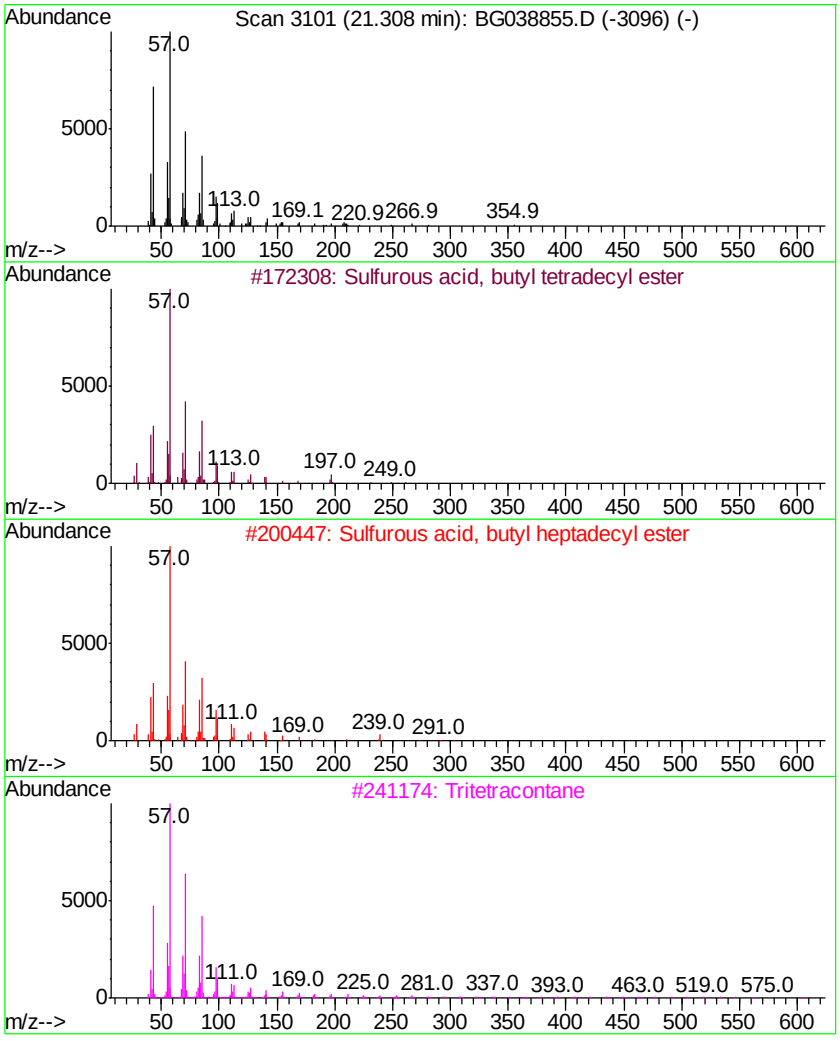
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

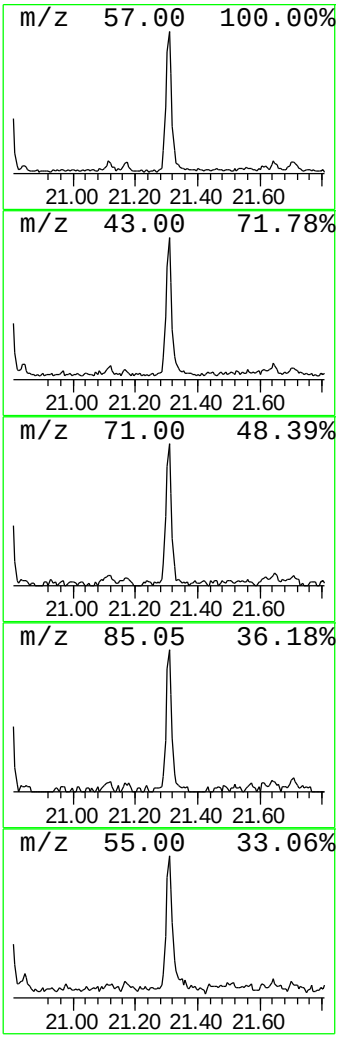
**********

Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.31 | 4.95 ng | 129252 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, butyl tetradecyl... | 334 | C18H38O3S | 1000309-18-1 | 91 |
| 2 | Sulfurous acid, butyl heptadecyl... | 376 | C21H44O3S | 1000309-18-4 | 91 |
| 3 | Tritetracontane | 605 | C43H88 | 007098-21-7 | 90 |
| 4 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

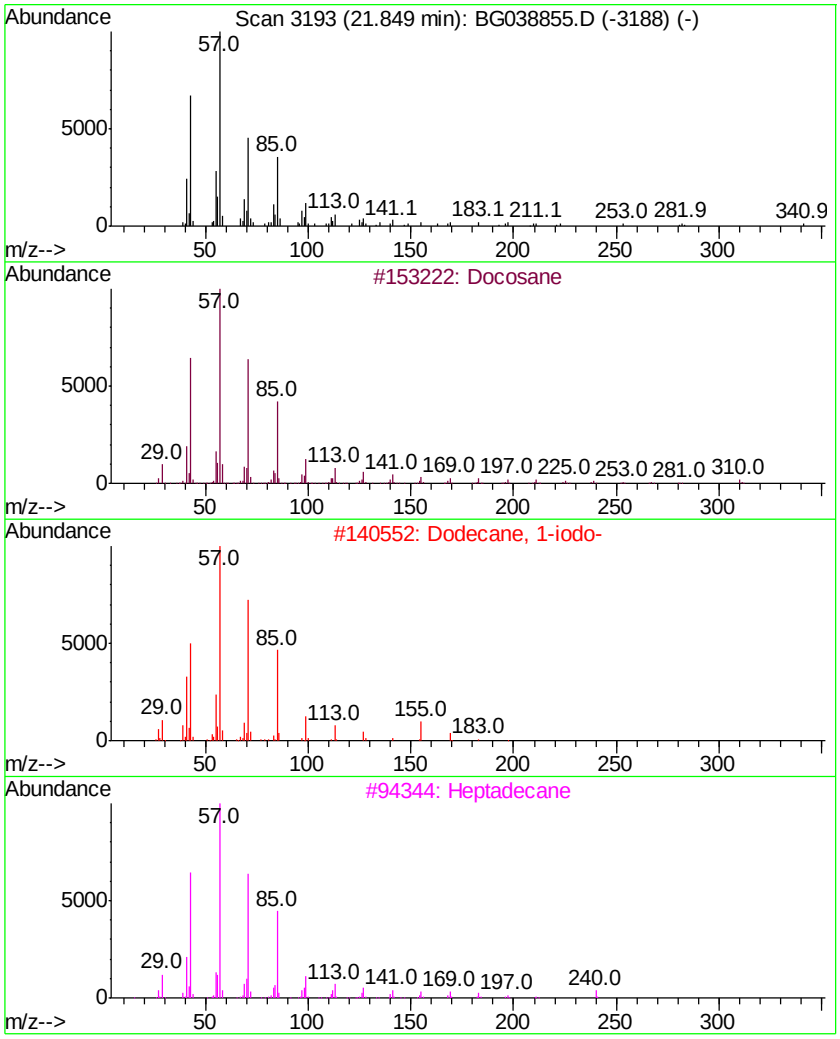
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

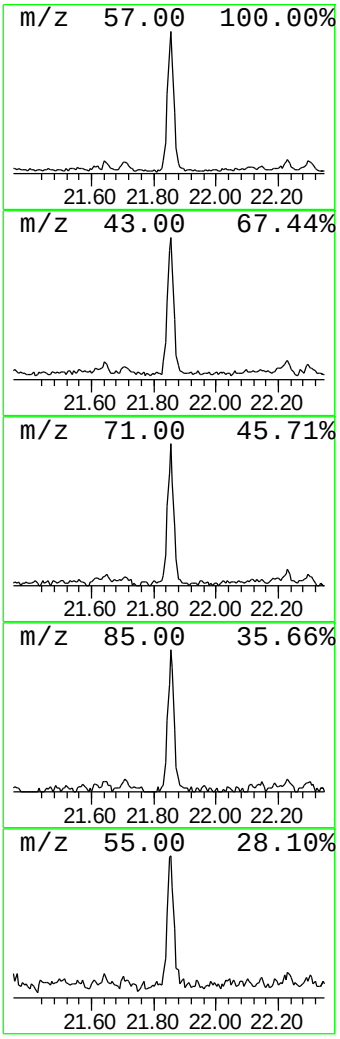
**********

Peak Number 6 Docosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.85 | 4.30 ng | 112221 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |
| 2 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 86 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 86 |
| 4 | Pentadecane | 212 | C15H32 | 000629-62-9 | 83 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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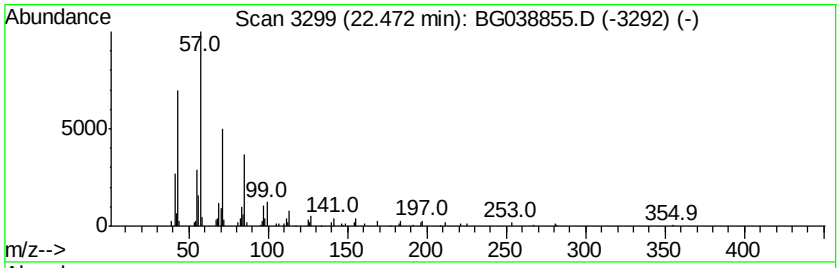
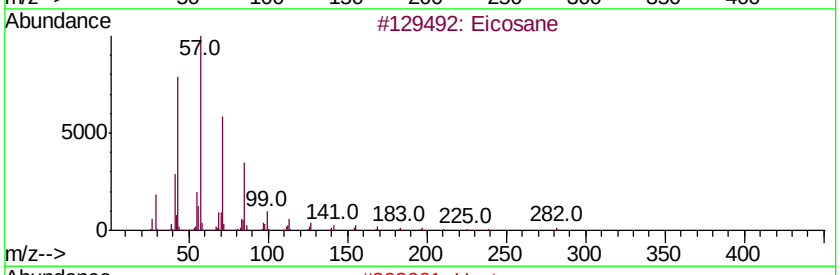
**********

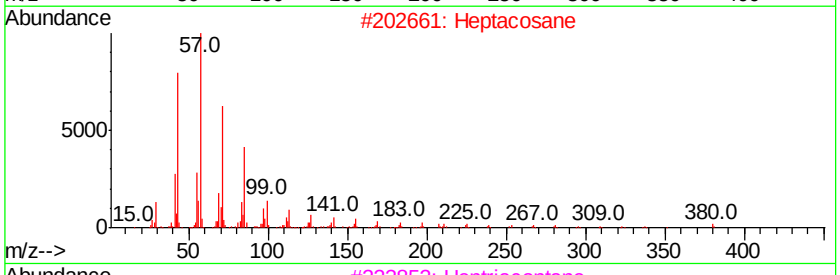
Peak Number 7 Eicosane Concentration Rank 7

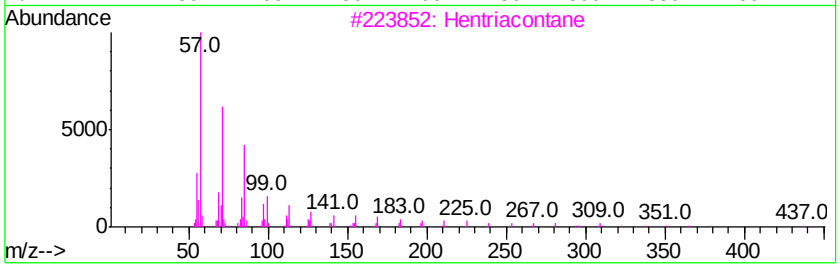
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.47 | 4.48 ng | 116851 | Chrysene-d12 | 21.72 |

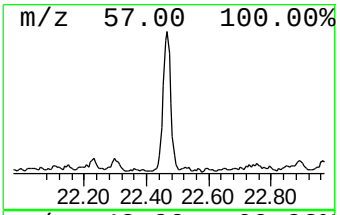
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 4 | Eicosane, 2-methyl- | 296 | C21H44 | 001560-84-5 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |

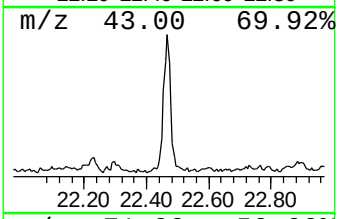


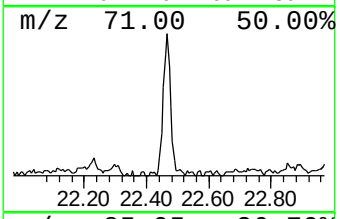



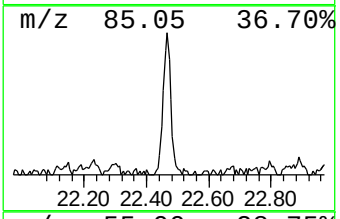



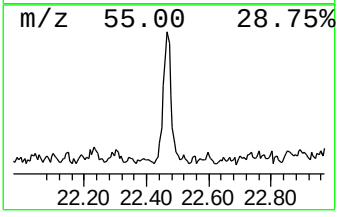



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**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

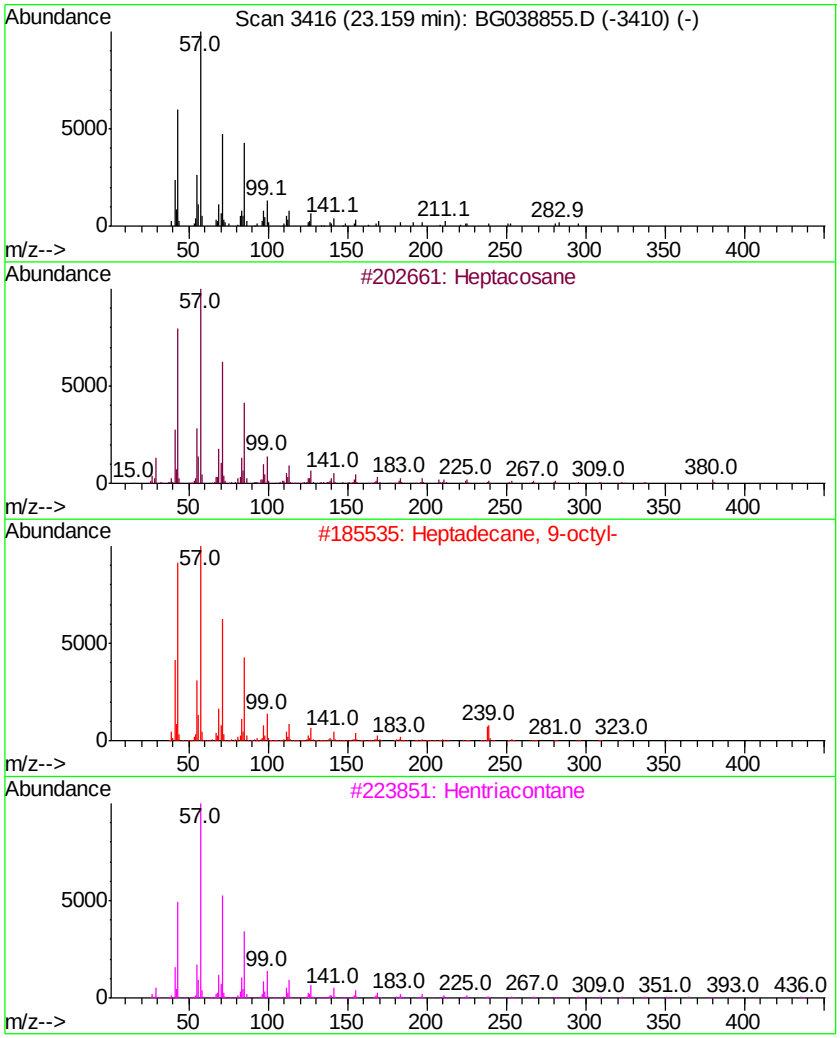
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

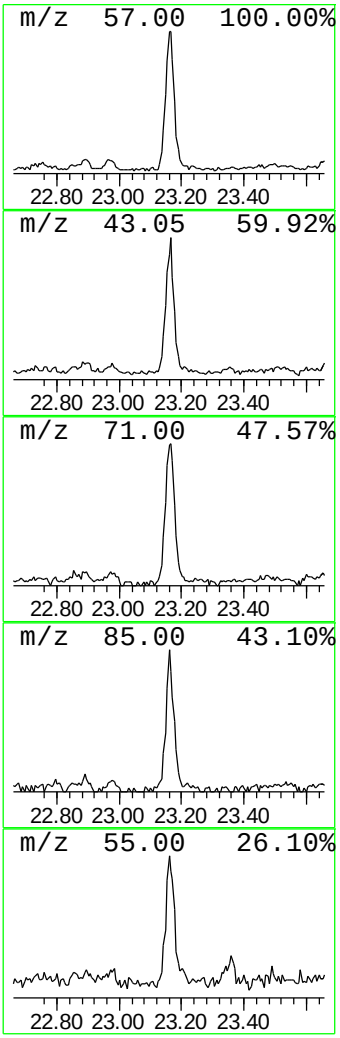
**********

Peak Number 8 Heptacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.16 | 4.56 ng | 119143 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |
| 4 | Tetracosane, 11-decyl- | 479 | C34H70 | 055429-84-0 | 87 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

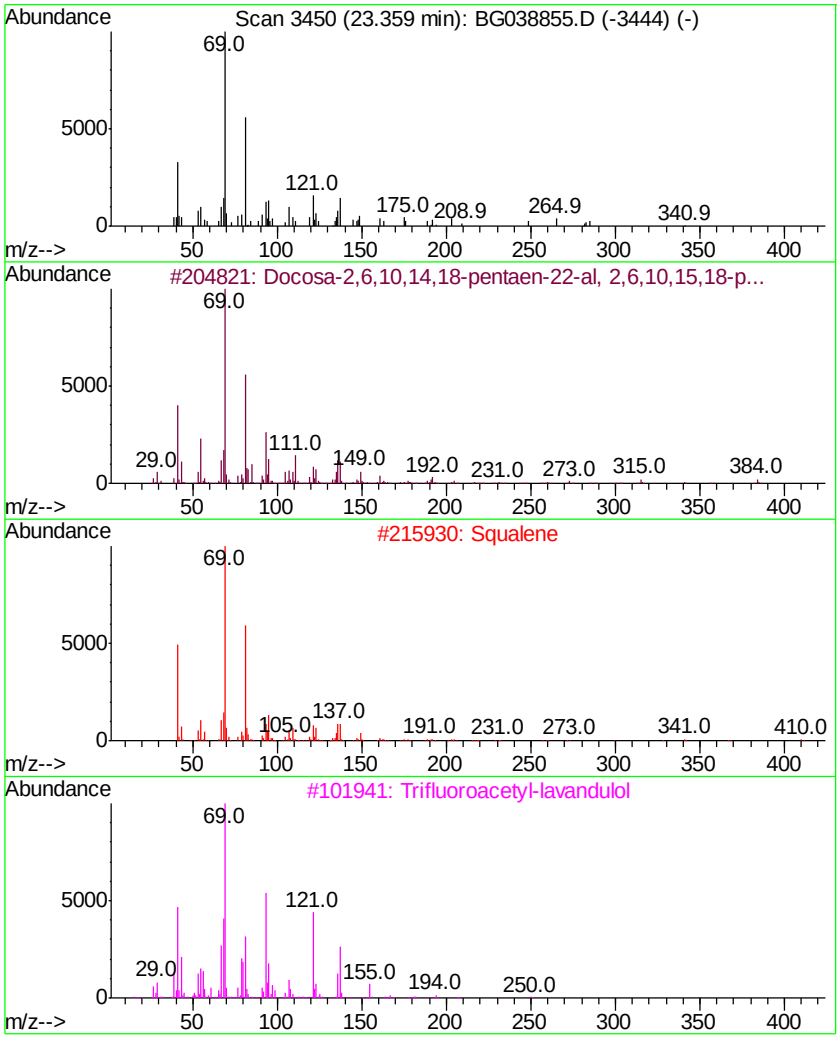
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

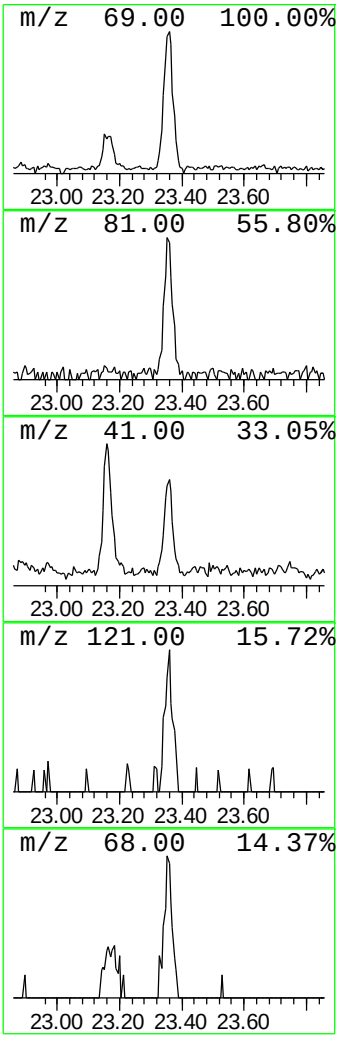
**********

Peak Number 9 Docosa-2,6,10,14,18-pentaen... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.36 | 2.14 ng | 55846 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O | 1000163-04-7 | 80 |
| 2 | Squalene | 410 | C30H50 | 000111-02-4 | 72 |
| 3 | Trifluoroacetyl-lavandulol | 250 | C12H17F3O2 | 028673-24-7 | 64 |
| 4 | Supraene | 410 | C30H50 | 007683-64-9 | 64 |
| 5 | .beta.-D-Mannofuranoside, farnesyl- | 384 | C21H36O6 | 1000155-15-5 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

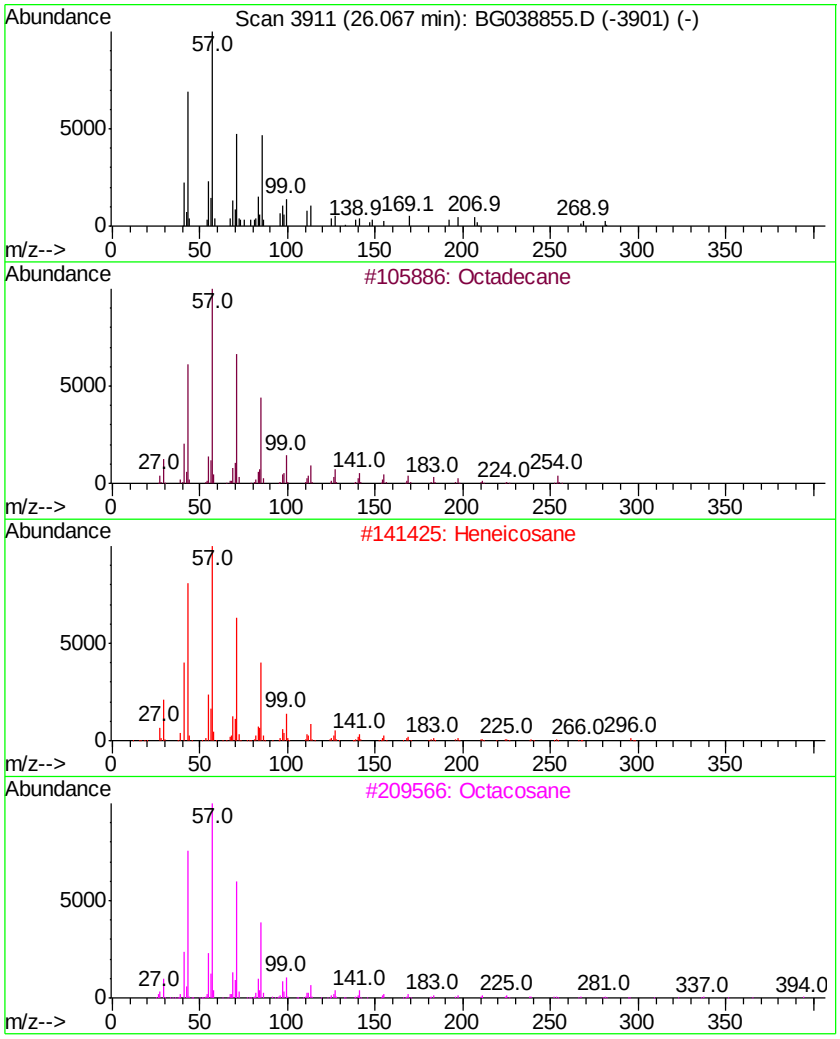
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

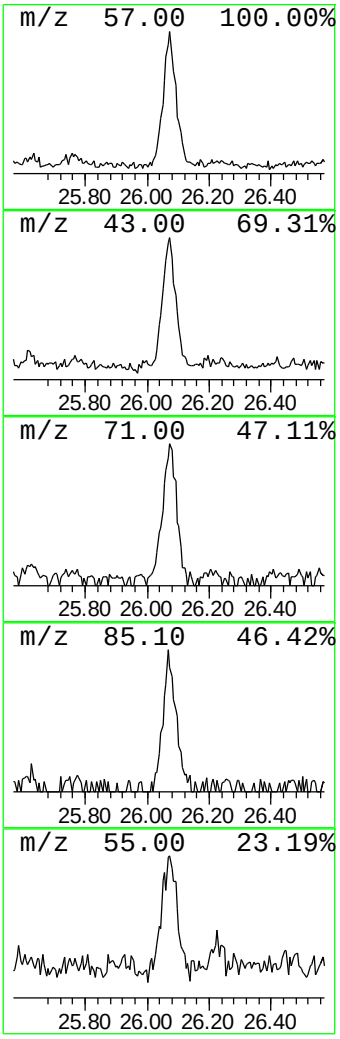
**********

Peak Number 12 Octadecane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.07 | 3.84 ng | 95129 | Perylene-d12 | 25.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 83 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 83 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 83 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 83 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG122718\
Data File : BG038855.D
Acq On : 27 Dec 2018 22:33
Operator : JU/SJ
Sample : J6549-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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... | 3.18 | 7.9 | ng | 55268 | 1 | 8.05 | 140535 | 20.0 |
| unknown7.58 | 7.58 | 108.4 | ng | 761544 | 1 | 8.05 | 140535 | 20.0 |
| Octacosane | 20.80 | 2.8 | ng | 73256 | 5 | 21.72 | 522185 | 20.0 |
| Sulfurous acid, b... | 21.31 | 5.0 | ng | 129252 | 5 | 21.72 | 522185 | 20.0 |
| Docosane | 21.85 | 4.3 | ng | 112221 | 5 | 21.72 | 522185 | 20.0 |
| Eicosane | 22.47 | 4.5 | ng | 116851 | 5 | 21.72 | 522185 | 20.0 |
| Heptacosane | 23.16 | 4.6 | ng | 119143 | 5 | 21.72 | 522185 | 20.0 |
| Docosa-2,6,10,14,... | 23.36 | 2.1 | ng | 55846 | 5 | 21.72 | 522185 | 20.0 |
| Octadecane | 26.07 | 3.8 | ng | 95129 | 6 | 25.02 | 495984 | 20.0 |