LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

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-BG060718.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 | 5.168 | 314 | 320 | 328 | rBV2 | 37279 | 59437 | 1.42% | 0.339% |
| 2 | 5.632 | 392 | 399 | 412 | rVB | 312866 | 513374 | 12.26% | 2.930% |
| 3 | 7.212 | 659 | 668 | 678 | rBV | 213605 | 390354 | 9.32% | 2.228% |
| 4 | 7.588 | 725 | 732 | 741 | rBV | 540758 | 931335 | 22.23% | 5.316% |
| 5 | 8.052 | 804 | 811 | 820 | rBV | 178284 | 310333 | 7.41% | 1.771% |
| 6 | 8.381 | 858 | 867 | 874 | rBV | 748784 | 1341211 | 32.02% | 7.656% |
| 7 | 9.215 | 998 | 1009 | 1021 | rBV | 630855 | 1104405 | 26.37% | 6.304% |
| 8 | 10.860 | 1282 | 1289 | 1298 | rBV | 209386 | 386987 | 9.24% | 2.209% |
| 9 | 13.298 | 1694 | 1704 | 1716 | rBV | 1689491 | 2695534 | 64.35% | 15.387% |
| 10 | 14.120 | 1839 | 1844 | 1853 | rVB | 64585 | 91097 | 2.17% | 0.520% |
| 11 | 14.673 | 1929 | 1938 | 1948 | rBV2 | 355226 | 582571 | 13.91% | 3.325% |
| 12 | 15.959 | 2152 | 2157 | 2163 | rVB2 | 118684 | 147275 | 3.52% | 0.841% |
| 13 | 16.159 | 2184 | 2191 | 2200 | rBV | 935988 | 1418312 | 33.86% | 8.096% |
| 14 | 17.416 | 2398 | 2405 | 2414 | rBV2 | 512673 | 773159 | 18.46% | 4.413% |
| 15 | 18.297 | 2550 | 2555 | 2564 | rBV2 | 92647 | 138141 | 3.30% | 0.789% |
| 16 | 19.566 | 2764 | 2771 | 2778 | rBV2 | 59859 | 89932 | 2.15% | 0.513% |
| 17 | 20.024 | 2843 | 2849 | 2858 | rBV | 3294084 | 4188790 | 100.00% | 23.911% |
| 18 | 21.328 | 3067 | 3071 | 3083 | rBV9 | 24113 | 60863 | 1.45% | 0.347% |
| 19 | 21.681 | 3125 | 3131 | 3144 | rVB | 530007 | 900922 | 21.51% | 5.143% |
| 20 | 22.486 | 3261 | 3268 | 3271 | rBV3 | 33672 | 53506 | 1.28% | 0.305% |
| 21 | 23.173 | 3379 | 3385 | 3392 | rVB3 | 52000 | 99177 | 2.37% | 0.566% |
| 22 | 23.984 | 3514 | 3523 | 3532 | rBV3 | 59057 | 127427 | 3.04% | 0.727% |
| 23 | 24.900 | 3668 | 3679 | 3696 | rBV2 | 295713 | 951966 | 22.73% | 5.434% |
| 24 | 26.057 | 3867 | 3876 | 3886 | rBV4 | 39375 | 120173 | 2.87% | 0.686% |
| 25 | 27.414 | 4102 | 4107 | 4115 | rVB4 | 16172 | 42044 | 1.00% | 0.240% |

Sum of corrected areas: 17518325

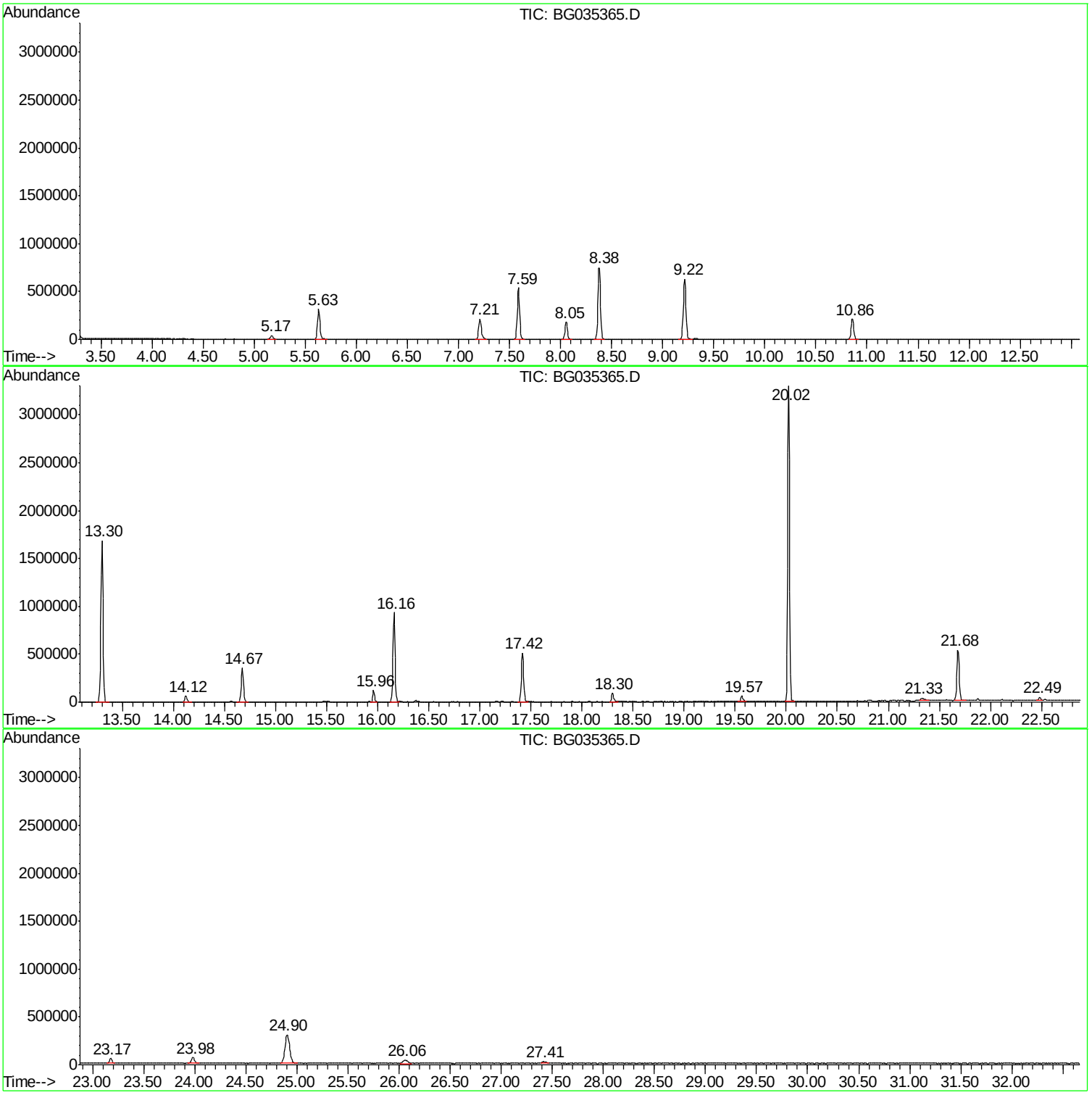
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

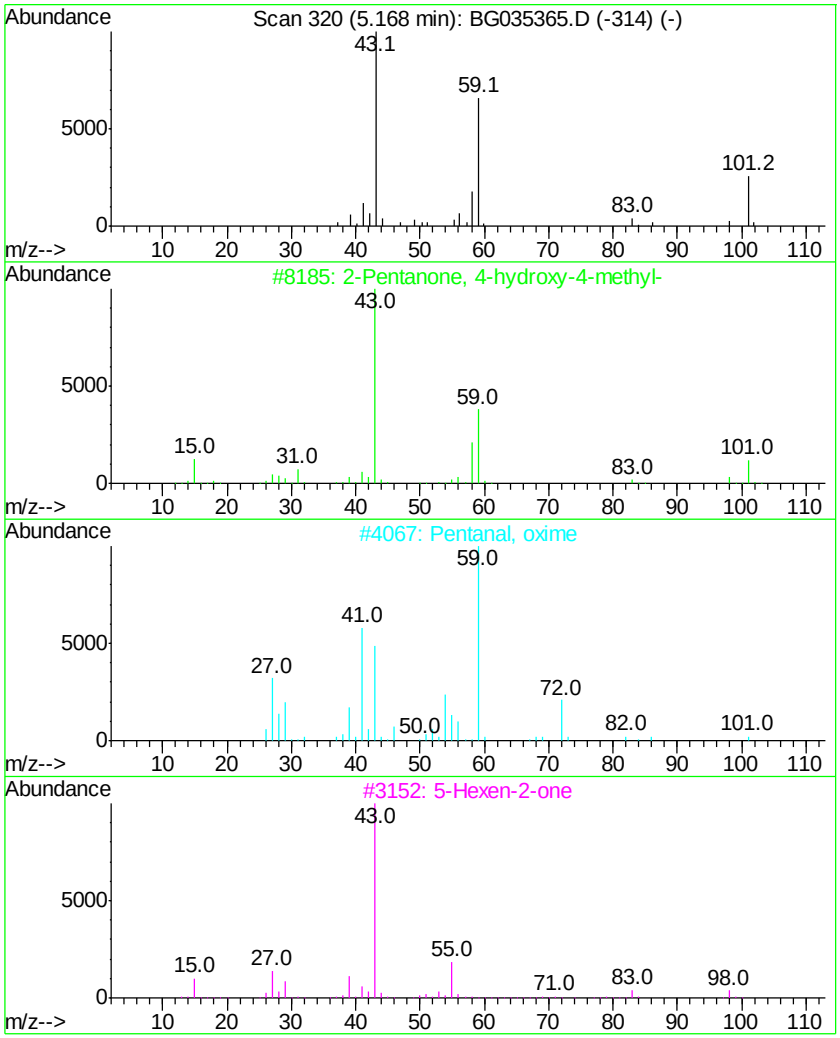
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

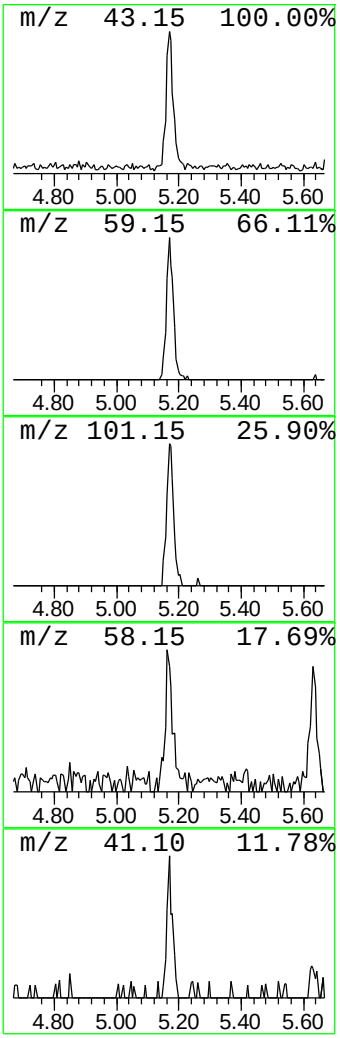
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 3.83 ng | 59437 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Pentanal, oxime | 101 | C5H11NO | 000628-79-5 | 17 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

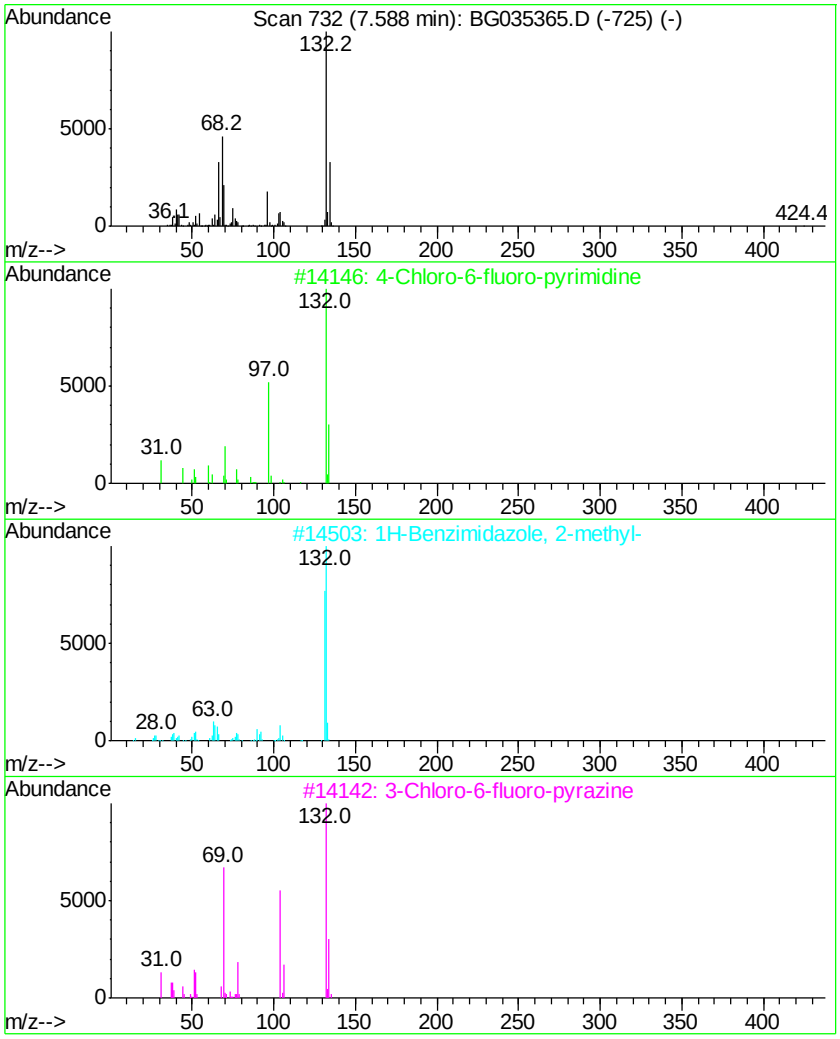
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

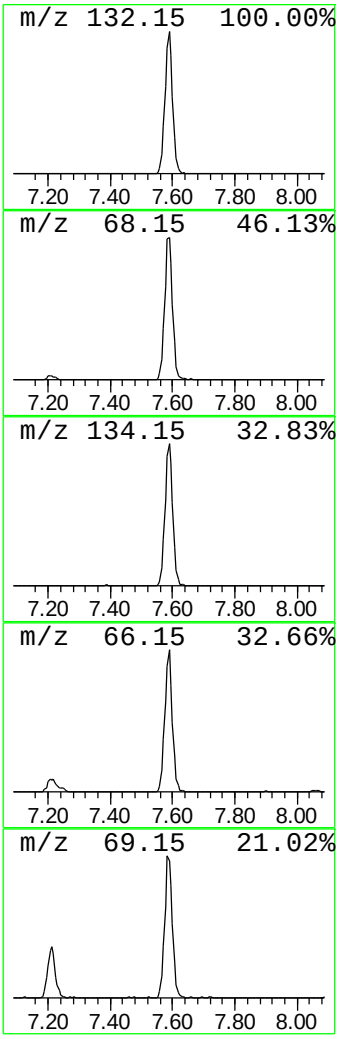
**********

Peak Number 2 unknown7.59 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.59 | 60.02 ng | 931335 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 4 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 13 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

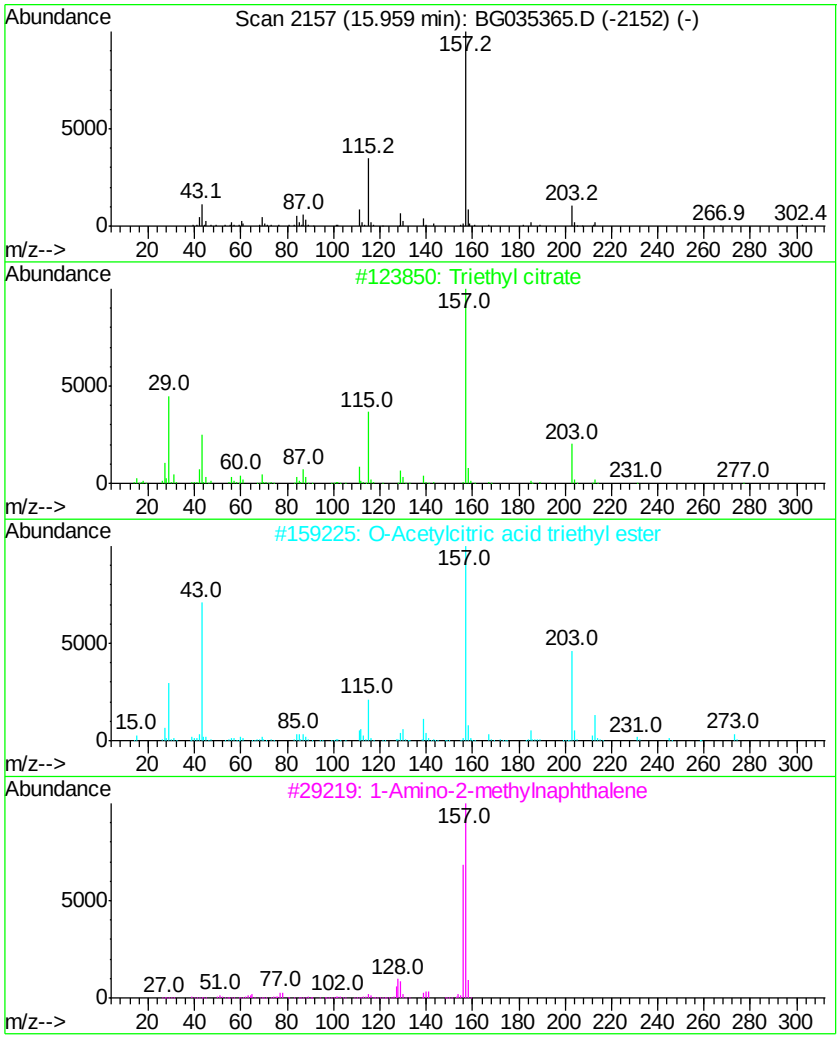
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

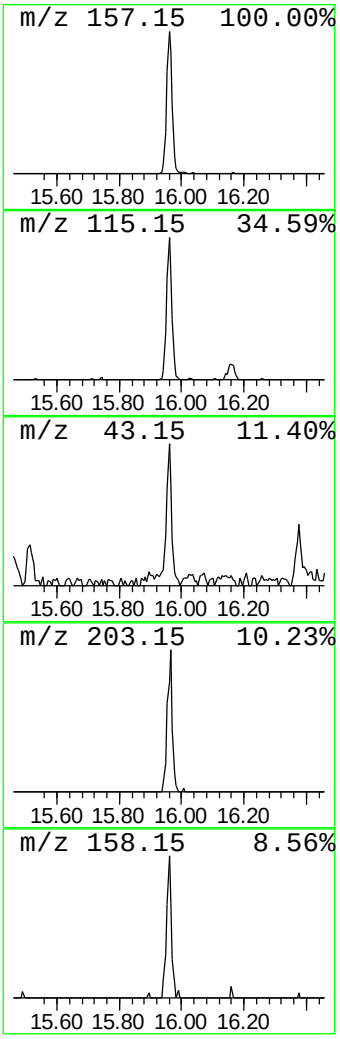
**********

Peak Number 4 Triethyl citrate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.96 | 5.06 ng | 147275 | Acenaphthene-d10 | 14.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triethyl citrate | 276 | C12H20O7 | 000077-93-0 | 86 |
| 2 | O-Acetylcitric acid triethyl ester | 318 | C14H22O8 | 000077-89-4 | 50 |
| 3 | 1-Amino-2-methylnaphthalene | 157 | C11H11N | 002246-44-8 | 50 |
| 4 | 2-Chlorobenzoic acid, tridecyl e... | 338 | C20H31ClO2 | 1000292-42-8 | 40 |
| 5 | 3-Chloro2-fluorobenzoic acid, 3-... | 398 | C23H36ClFO2 | 1000338-65-4 | 36 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

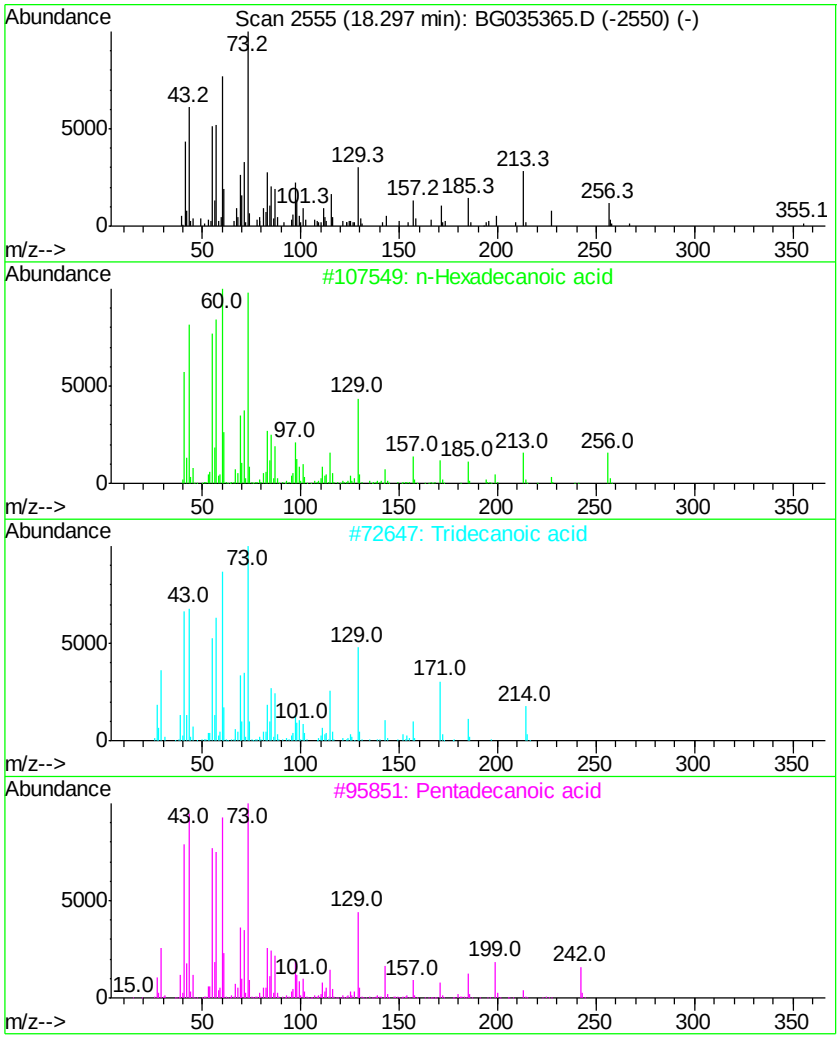
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

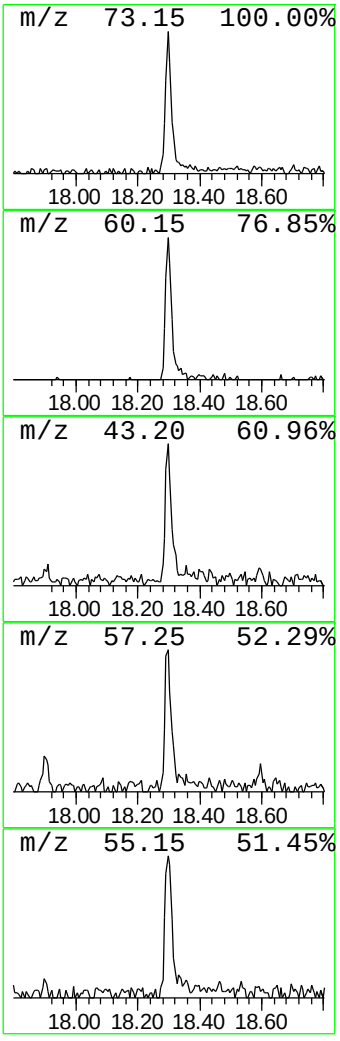
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.30 | 3.57 ng | 138141 | Phenanthrene-d10 | 17.42 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 89 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 76 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 53 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 47 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

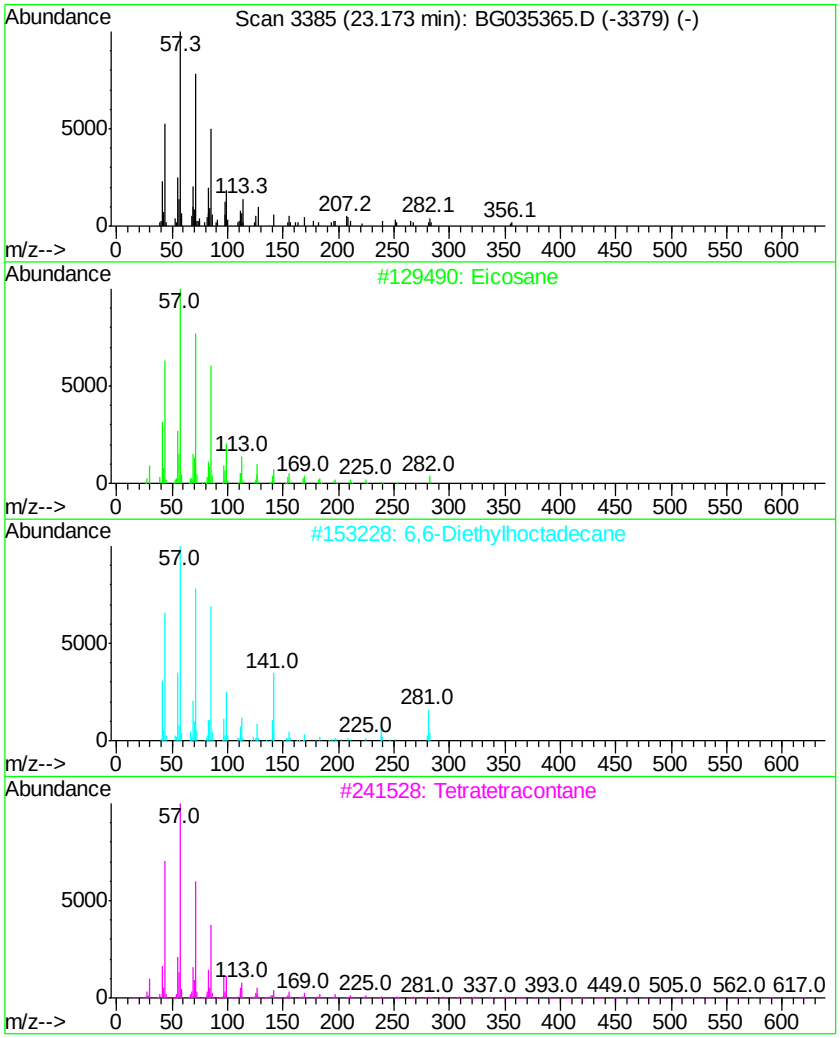
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

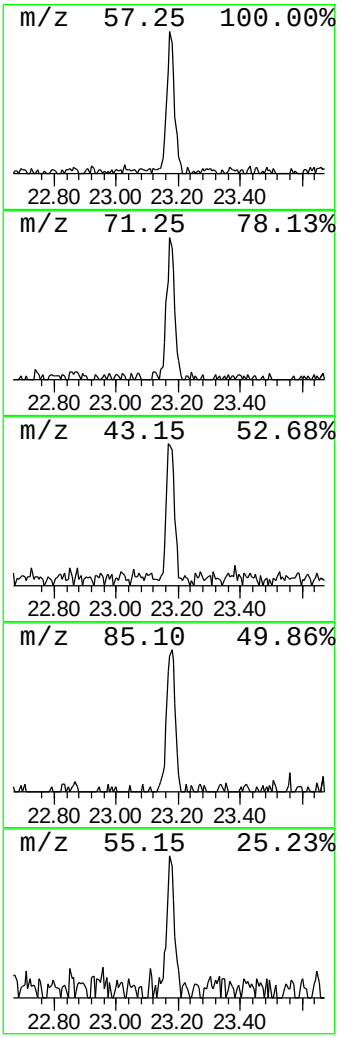
**********

Peak Number 6 Eicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.17 | 2.20 ng | 99177 | Chrysene-d12 | 21.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 98 |
| 2 | 6,6-Diethylhoctadecane | 310 | C22H46 | 1000360-41-8 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 4 | Docosane, 11-decyl- | 451 | C32H66 | 055401-55-3 | 87 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |



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Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

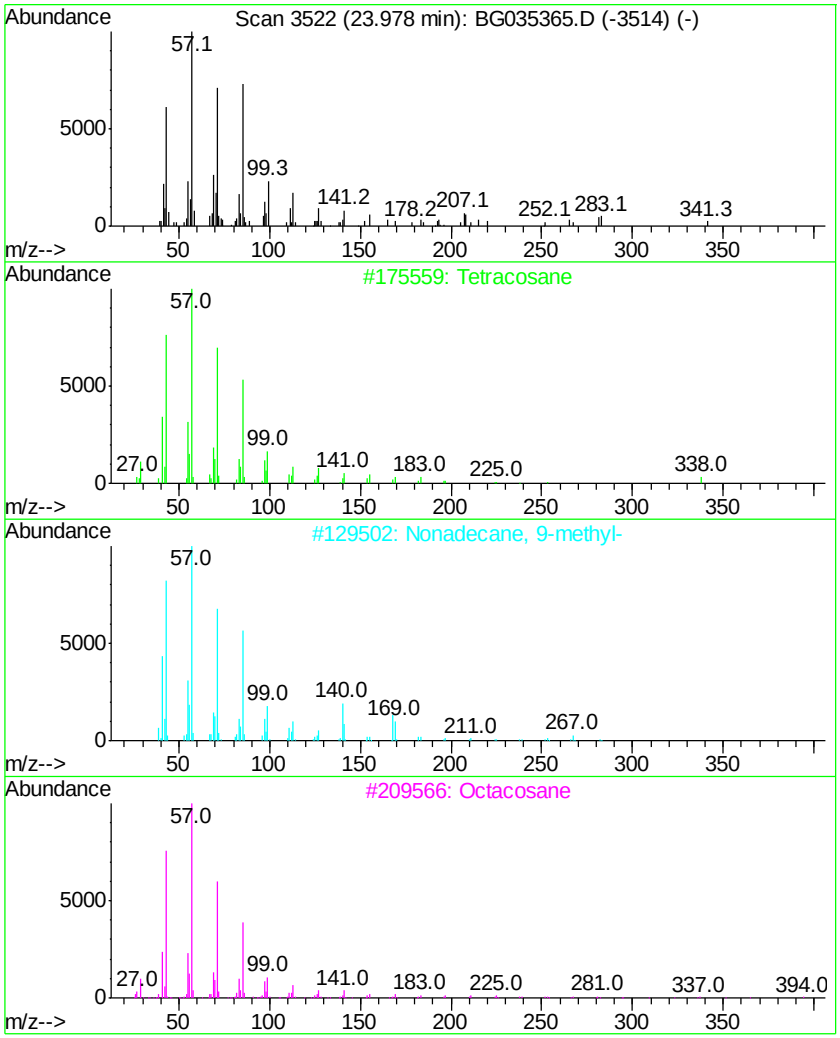
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

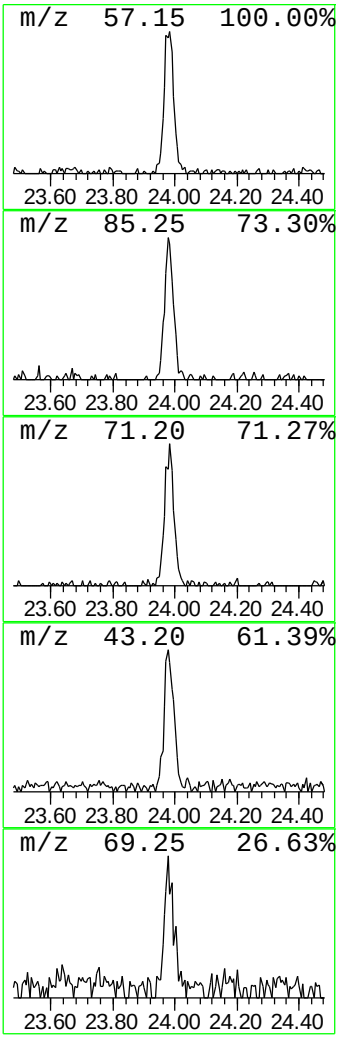
**********

Peak Number 7 Tetracosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.98 | 2.68 ng | 127427 | Perylene-d12 | 24.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 2 | Nonadecane, 9-methyl- | 282 | C20H42 | 013287-24-6 | 86 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 86 |
| 4 | Triacontane | 422 | C30H62 | 000638-68-6 | 80 |
| 5 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 80 |



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Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

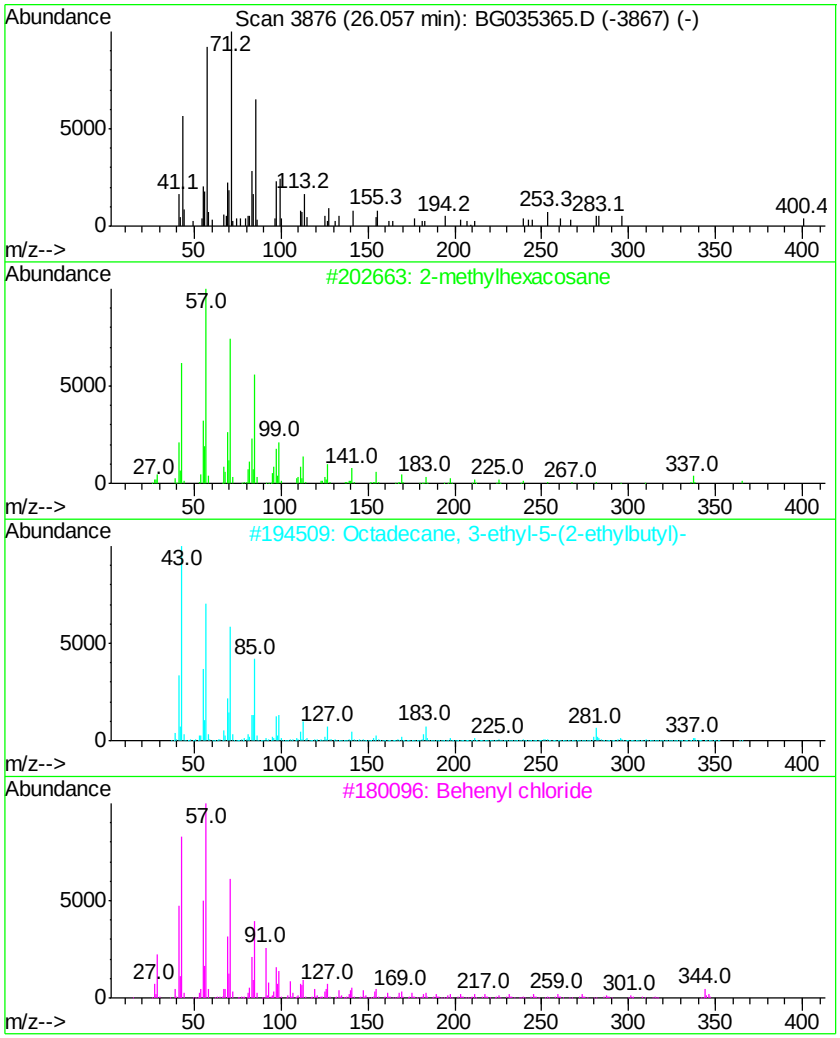
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

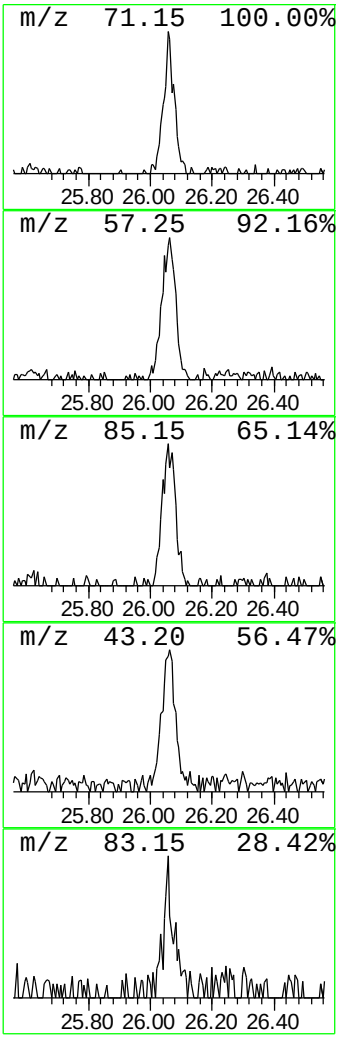
**********

Peak Number 8 2-methylhexacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.06 | 2.52 ng | 120173 | Perylene-d12 | 24.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-methylhexacosane | 380 | C27H56 | 1000376-72-7 | 83 |
| 2 | Octadecane, 3-ethyl-5-(2-ethylbu... | 366 | C26H54 | 055282-12-7 | 80 |
| 3 | Behenyl chloride | 344 | C22H45Cl | 042217-03-8 | 80 |
| 4 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 80 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 76 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062218\
Data File : BG035365.D
Acq On : 23 Jun 2018 12:53
Operator : JU/SJ
Sample : J3623-04
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 061918-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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... | 5.17 | 3.8 | ng | 59437 | 1 | 8.05 | 310333 | 20.0 |
| unknown7.59 | 7.59 | 60.0 | ng | 931335 | 1 | 8.05 | 310333 | 20.0 |
| Triethyl citrate | 15.96 | 5.1 | ng | 147275 | 3 | 14.67 | 582571 | 20.0 |
| n-Hexadecanoic acid | 18.30 | 3.6 | ng | 138141 | 4 | 17.42 | 773159 | 20.0 |
| Eicosane | 23.17 | 2.2 | ng | 99177 | 5 | 21.68 | 900922 | 20.0 |
| Tetracosane | 23.98 | 2.7 | ng | 127427 | 6 | 24.90 | 951966 | 20.0 |
| 2-methylhexacosane | 26.06 | 2.5 | ng | 120173 | 6 | 24.90 | 951966 | 20.0 |