LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

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-BG012919.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 | 3.226 | 17 | 23 | 32 | rBV | 76637 | 143183 | 4.03% | 0.646% |
| 2 | 3.297 | 32 | 35 | 42 | rVB | 47012 | 64382 | 1.81% | 0.291% |
| 3 | 5.259 | 363 | 369 | 378 | rBV | 75144 | 124132 | 3.49% | 0.560% |
| 4 | 5.717 | 440 | 447 | 459 | rBV | 1041832 | 1680820 | 47.30% | 7.588% |
| 5 | 7.315 | 711 | 719 | 731 | rBV | 1102689 | 1948061 | 54.83% | 8.795% |
| 6 | 7.703 | 777 | 785 | 792 | rBV | 1044636 | 1759210 | 49.51% | 7.942% |
| 7 | 8.179 | 859 | 866 | 879 | rVB | 183758 | 315997 | 8.89% | 1.427% |
| 8 | 8.502 | 914 | 921 | 929 | rVB | 716101 | 1248237 | 35.13% | 5.635% |
| 9 | 9.353 | 1058 | 1066 | 1081 | rBV | 604216 | 1079041 | 30.37% | 4.871% |
| 10 | 10.998 | 1339 | 1346 | 1355 | rVB | 248668 | 456328 | 12.84% | 2.060% |
| 11 | 13.430 | 1752 | 1760 | 1767 | rVB | 1507229 | 2419137 | 68.08% | 10.921% |
| 12 | 14.247 | 1893 | 1899 | 1904 | rBV | 109237 | 158006 | 4.45% | 0.713% |
| 13 | 14.799 | 1986 | 1993 | 2002 | rVB2 | 410378 | 681735 | 19.19% | 3.078% |
| 14 | 16.285 | 2239 | 2246 | 2255 | rBV | 1390559 | 2079772 | 58.53% | 9.389% |
| 15 | 16.473 | 2273 | 2278 | 2285 | rVB2 | 23323 | 47985 | 1.35% | 0.217% |
| 16 | 17.542 | 2452 | 2460 | 2466 | rBV2 | 552155 | 863761 | 24.31% | 3.899% |
| 17 | 18.001 | 2533 | 2538 | 2546 | rBV | 25368 | 39609 | 1.11% | 0.179% |
| 18 | 18.400 | 2601 | 2606 | 2613 | rBV2 | 97998 | 157169 | 4.42% | 0.710% |
| 19 | 18.694 | 2651 | 2656 | 2659 | rBV | 30596 | 41592 | 1.17% | 0.188% |
| 20 | 19.316 | 2758 | 2762 | 2766 | rBV2 | 28705 | 41150 | 1.16% | 0.186% |
| 21 | 19.663 | 2817 | 2821 | 2827 | rBV6 | 41018 | 64833 | 1.82% | 0.293% |
| 22 | 20.139 | 2896 | 2902 | 2908 | rVB | 2666550 | 3553228 | 100.00% | 16.041% |
| 23 | 20.914 | 3031 | 3034 | 3037 | rBV | 34780 | 45132 | 1.27% | 0.204% |
| 24 | 21.437 | 3118 | 3123 | 3134 | rBV | 155110 | 233733 | 6.58% | 1.055% |
| 25 | 21.696 | 3163 | 3167 | 3173 | rVB | 101968 | 148192 | 4.17% | 0.669% |
| 26 | 21.837 | 3184 | 3191 | 3198 | rBV2 | 574633 | 976761 | 27.49% | 4.410% |
| 27 | 22.007 | 3216 | 3220 | 3231 | rVB | 55620 | 94259 | 2.65% | 0.426% |
| 28 | 22.641 | 3324 | 3328 | 3338 | rVB | 62923 | 115036 | 3.24% | 0.519% |
| 29 | 23.376 | 3448 | 3453 | 3458 | rVB2 | 66636 | 131641 | 3.70% | 0.594% |
| 30 | 24.227 | 3593 | 3598 | 3605 | rVB3 | 66880 | 137916 | 3.88% | 0.623% |
| 31 | 25.226 | 3758 | 3768 | 3780 | rVB3 | 374074 | 1104621 | 31.09% | 4.987% |
| 32 | 26.442 | 3970 | 3975 | 3985 | rVB5 | 48756 | 129390 | 3.64% | 0.584% |
| 33 | 27.899 | 4216 | 4223 | 4232 | rVB9 | 21303 | 66777 | 1.88% | 0.301% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

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-BG012919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

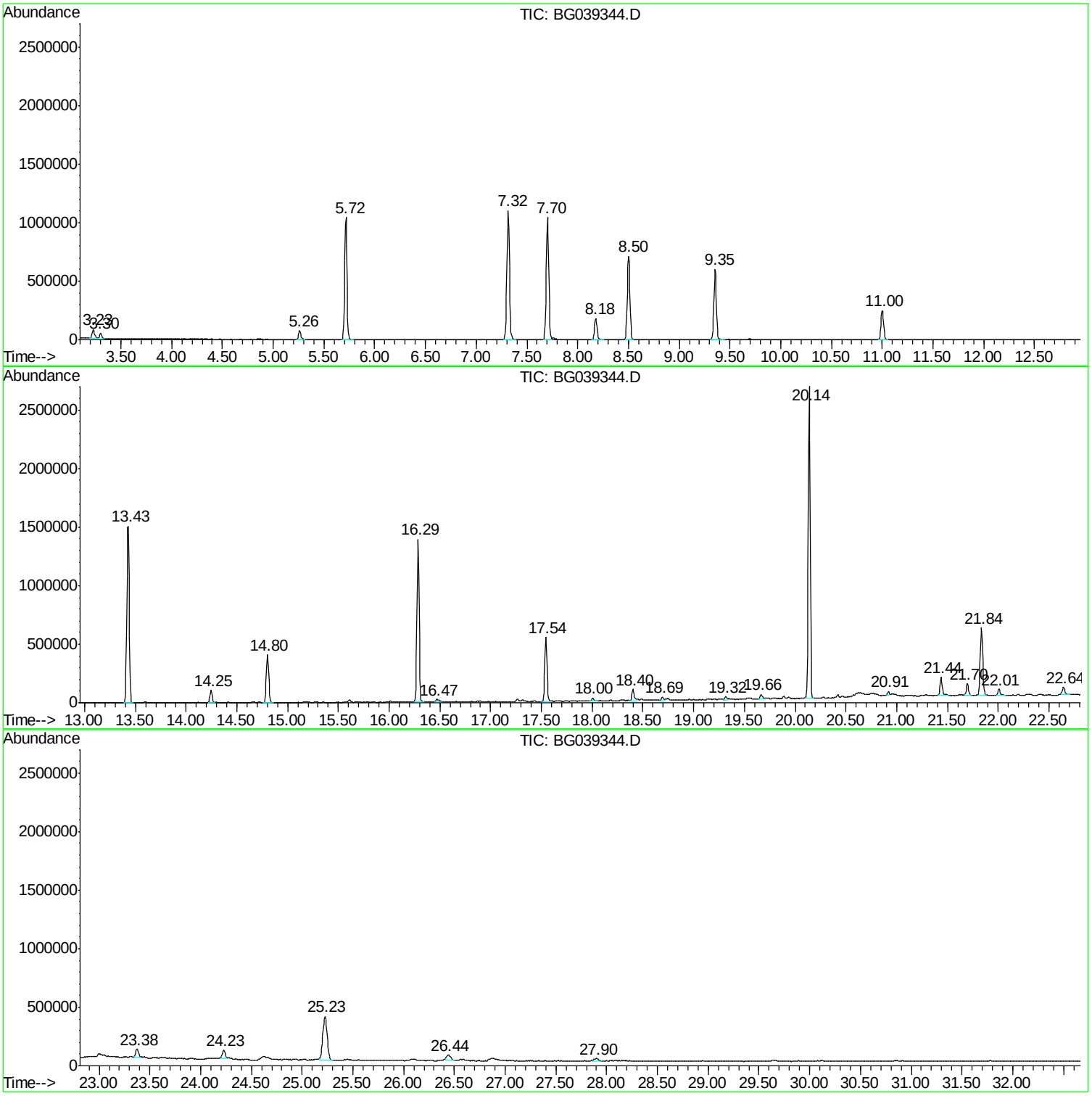
Sum of corrected areas: 22150826

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

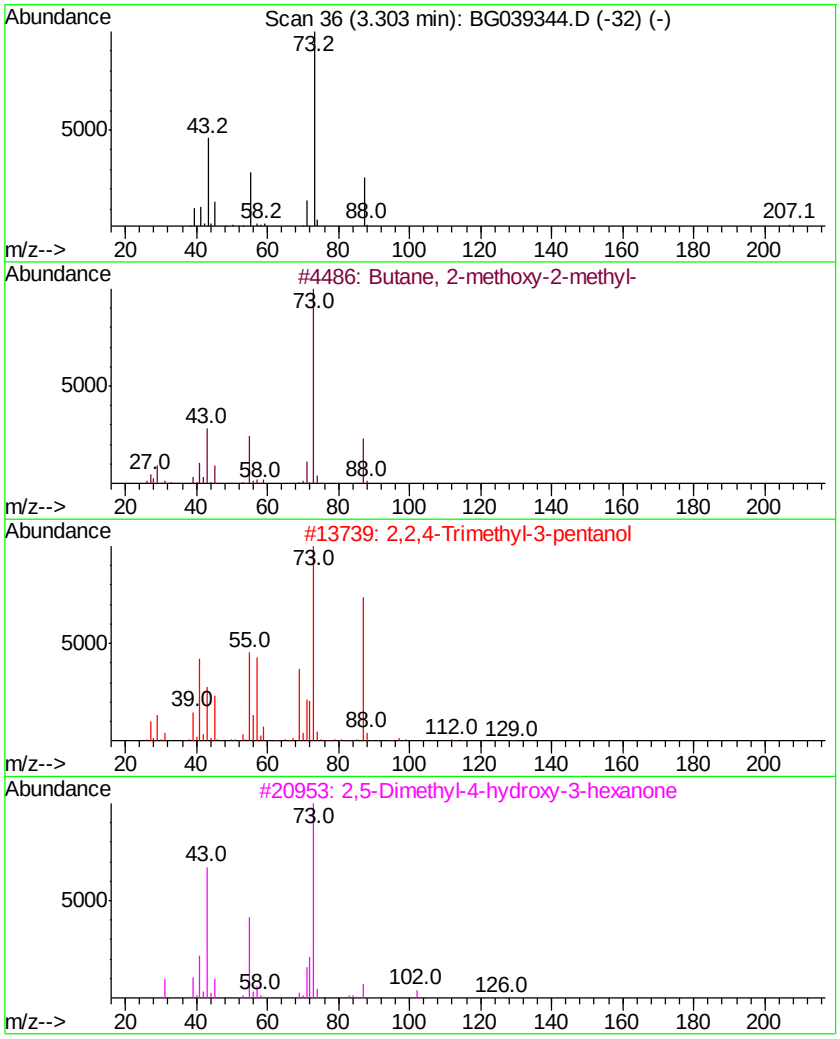
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

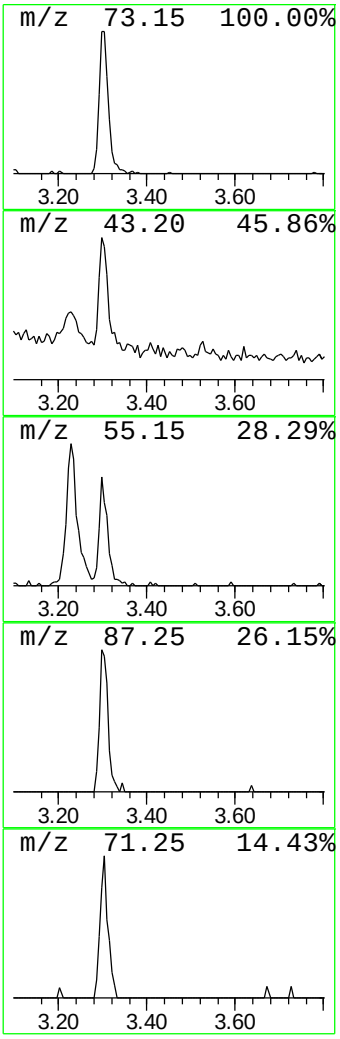
**********

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.30 | 4.07 ng | 64382 | 1,4-Dichlorobenzene-d4 | 8.18 |

| 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 | 45 |
| 3 | 2,5-Dimethyl-4-hydroxy-3-hexanone | 144 | C8H16O2 | 000815-77-0 | 33 |
| 4 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 17 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 16 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

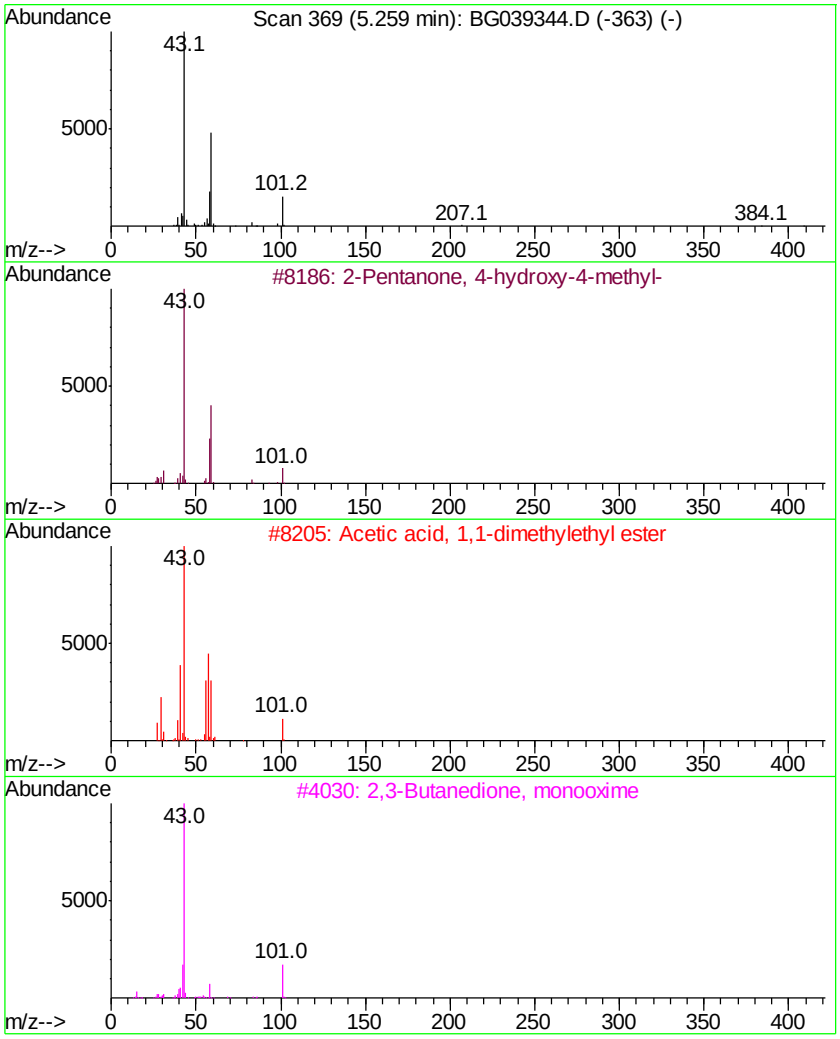
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

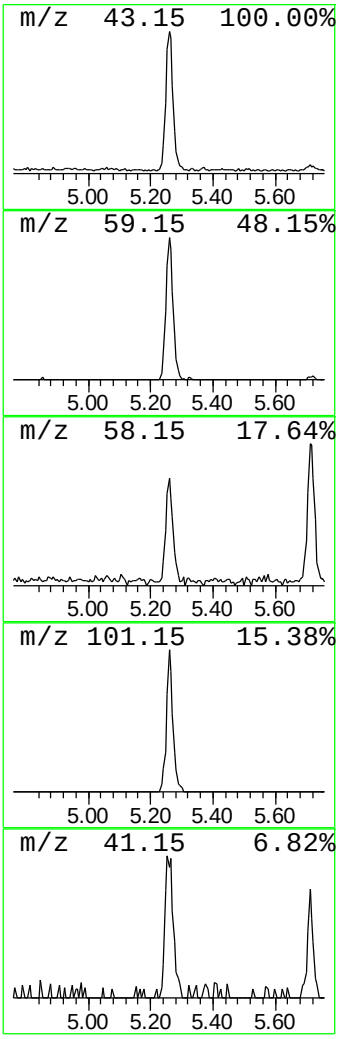
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.26 | 7.86 ng | 124132 | 1,4-Dichlorobenzene-d4 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 10 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

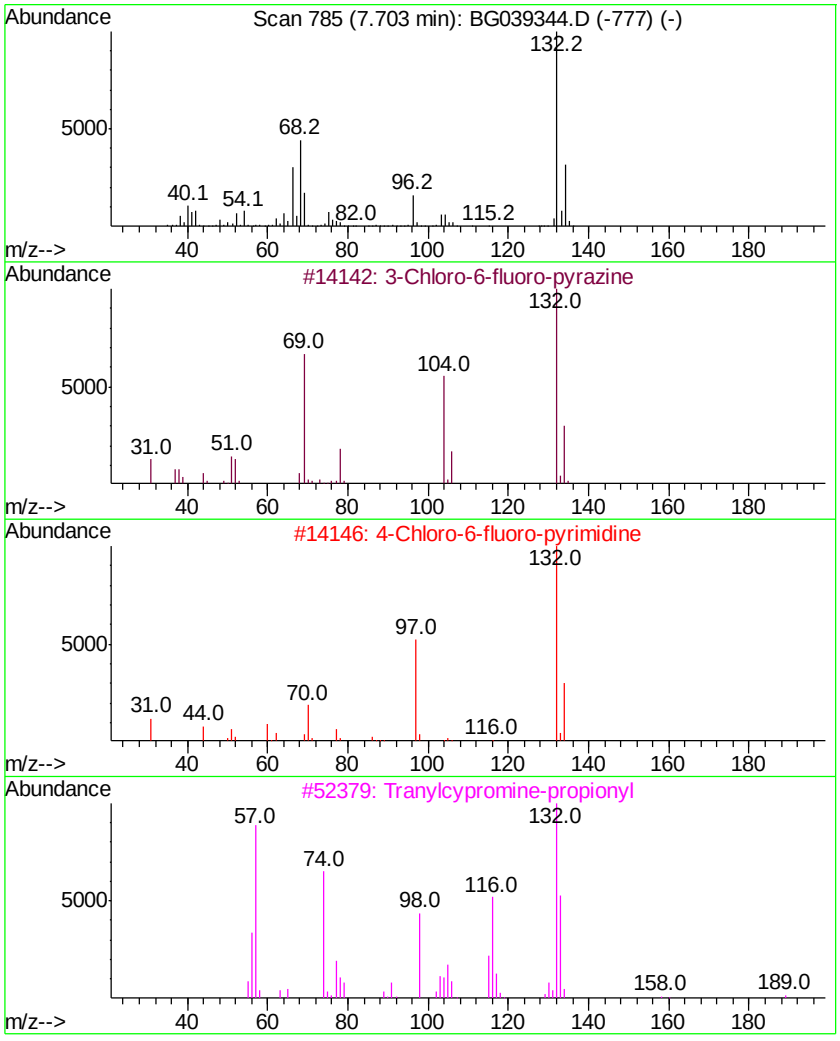
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

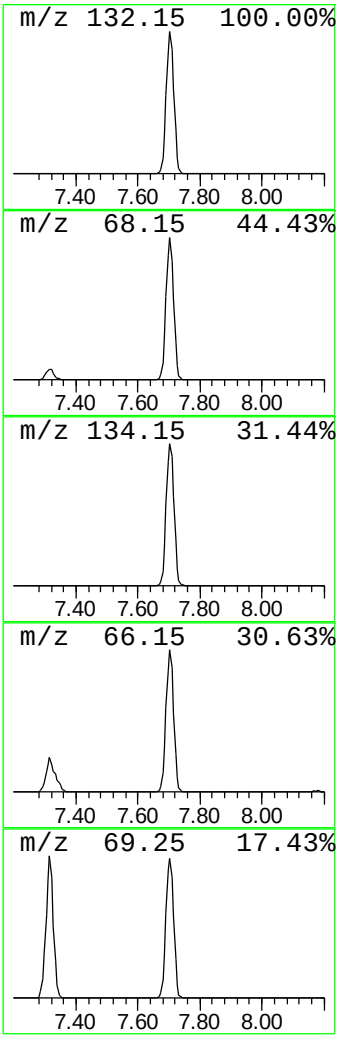
**********

Peak Number 4 unknown7.70 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.70 | 111.34 ng | 1759210 | 1,4-Dichlorobenzene-d4 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 5 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

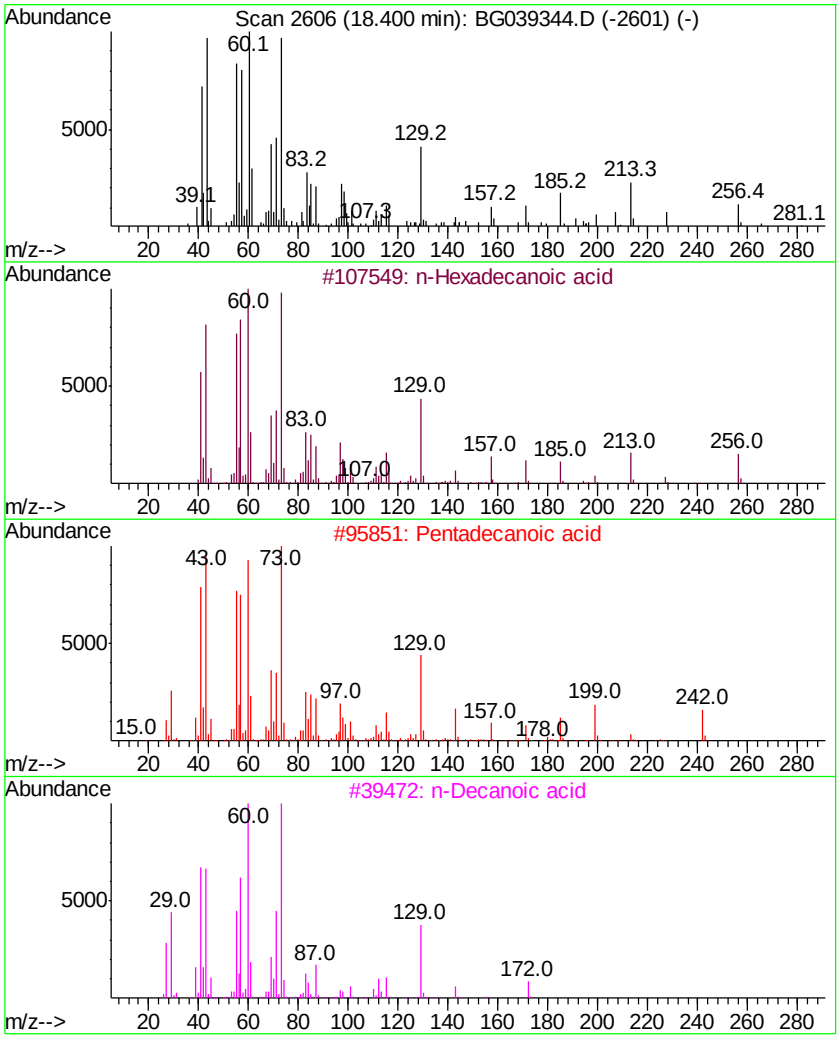
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

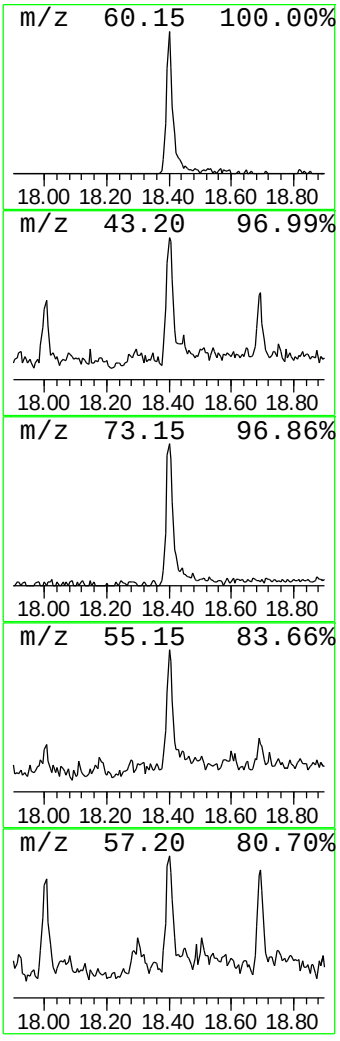
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.40 | 3.64 ng | 157169 | Phenanthrene-d10 | 17.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 68 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

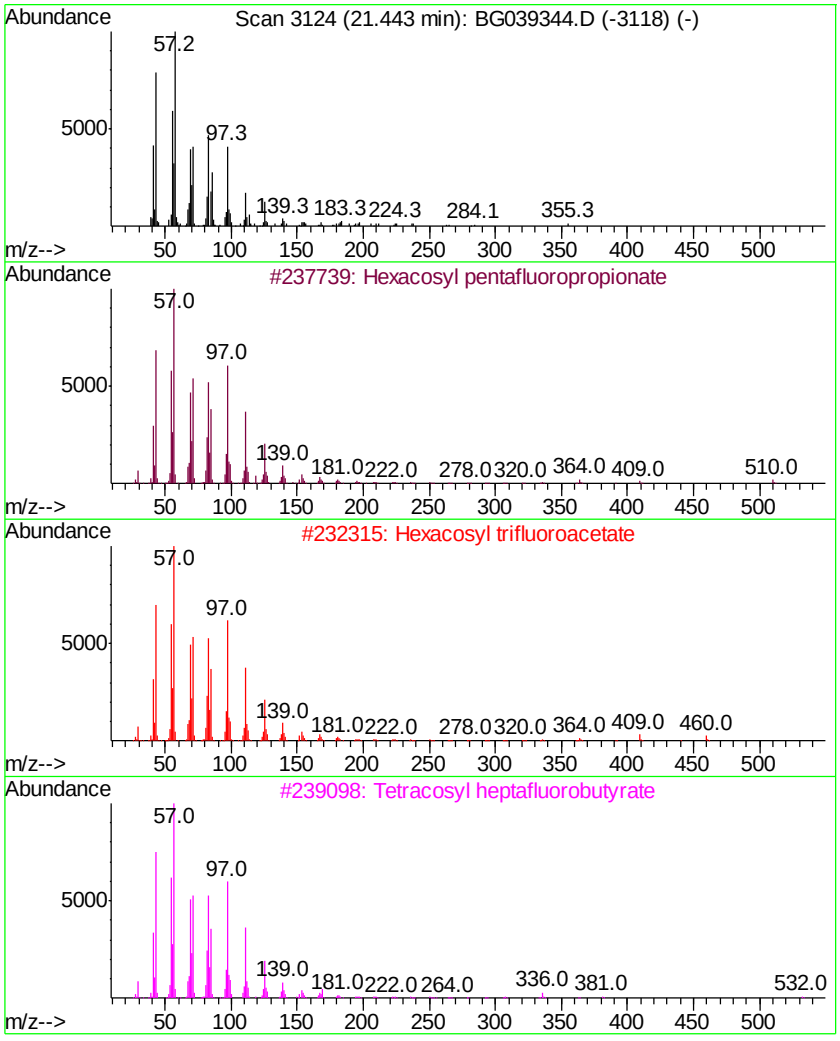
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

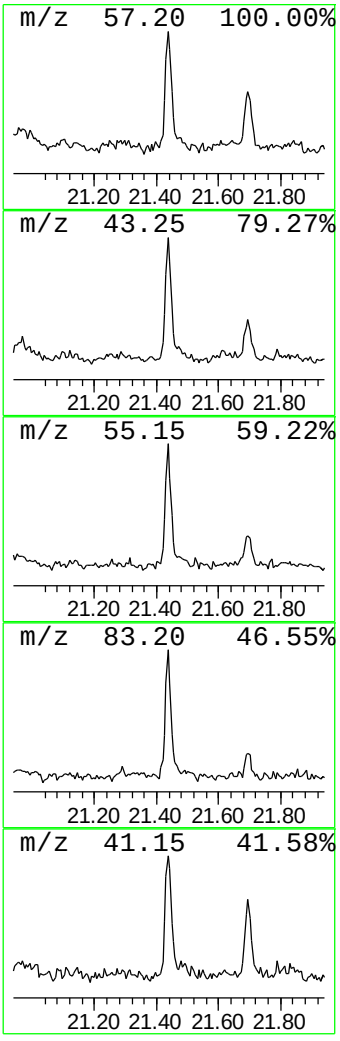
**********

Peak Number 7 Hexacosyl pentafluoropropio... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.44 | 4.79 ng | 233733 | Chrysene-d12 | 21.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosyl pentafluoropropionate | 528 | C29H53F5O2 | 1000351-81-2 | 91 |
| 2 | Hexacosyl trifluoroacetate | 478 | C28H53F3O2 | 1000351-75-0 | 91 |
| 3 | Tetracosyl heptafluorobutyrate | 550 | C28H49F7O2 | 1000351-83-7 | 91 |
| 4 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 91 |
| 5 | Octacosyl heptafluorobutyrate | 606 | C32H57F7O2 | 1000351-83-6 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

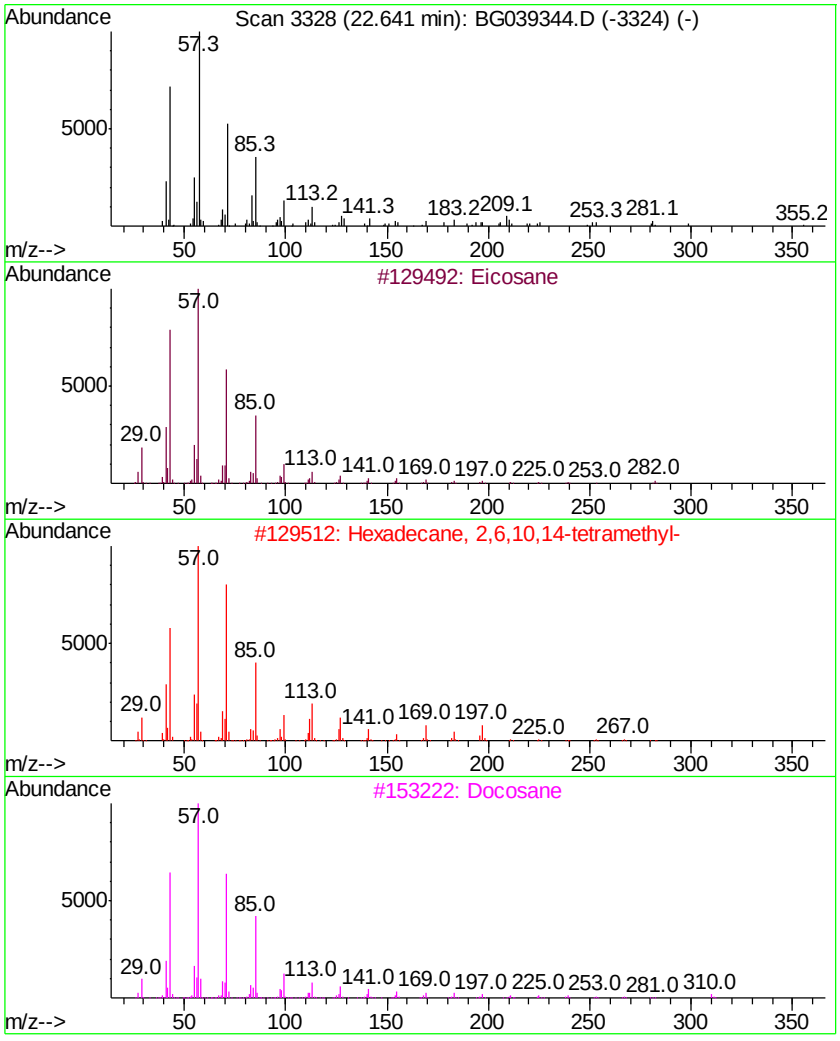
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

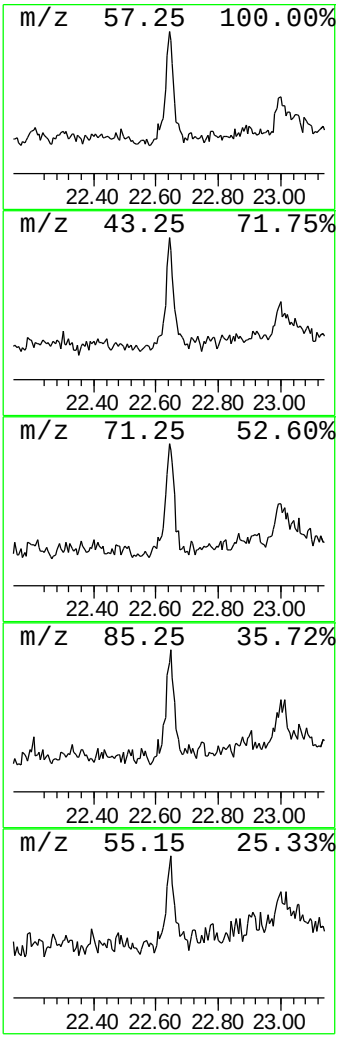
**********

Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.64 | 2.36 ng | 115036 | Chrysene-d12 | 21.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 2 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 83 |
| 3 | Docosane | 310 | C22H46 | 000629-97-0 | 80 |
| 4 | Nonadecane, 3-methyl- | 282 | C20H42 | 006418-45-7 | 80 |
| 5 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

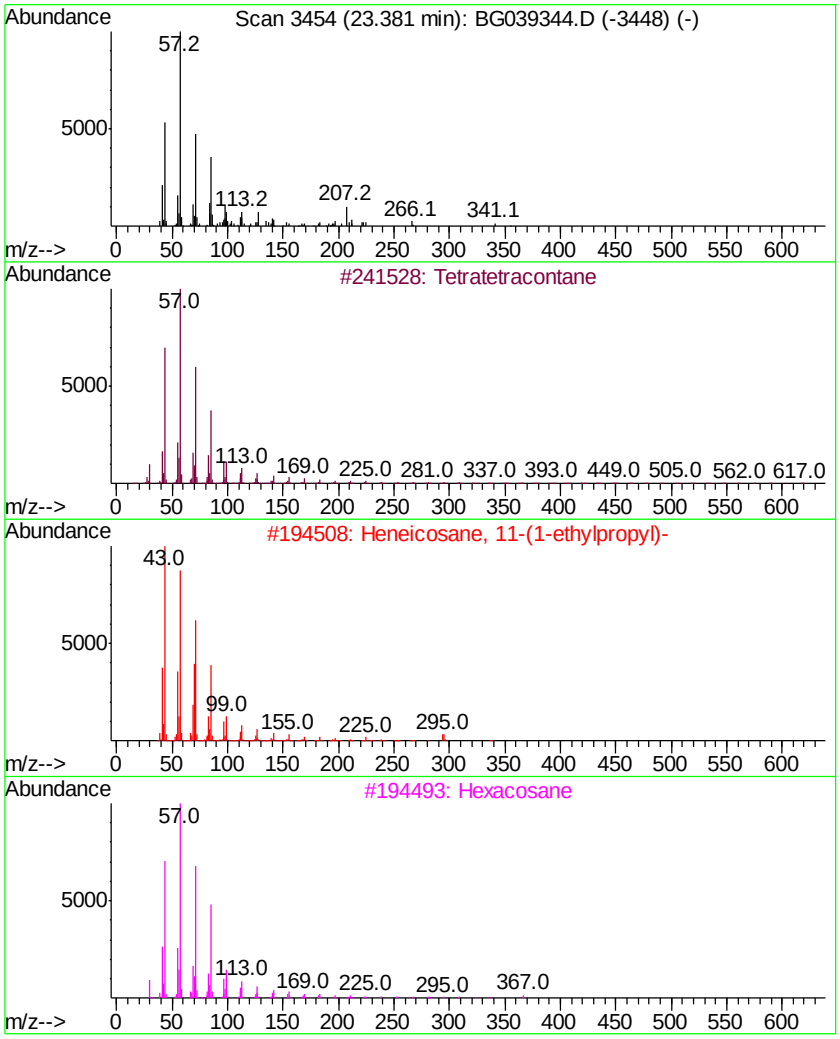
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

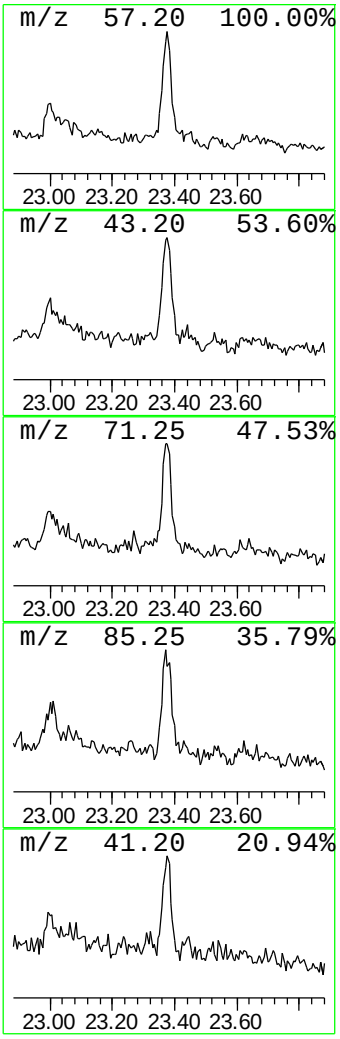
**********

Peak Number 9 Tetratetracontane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.38 | 2.70 ng | 131641 | Chrysene-d12 | 21.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 74 |
| 2 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 72 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |
| 4 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 72 |
| 5 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 72 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

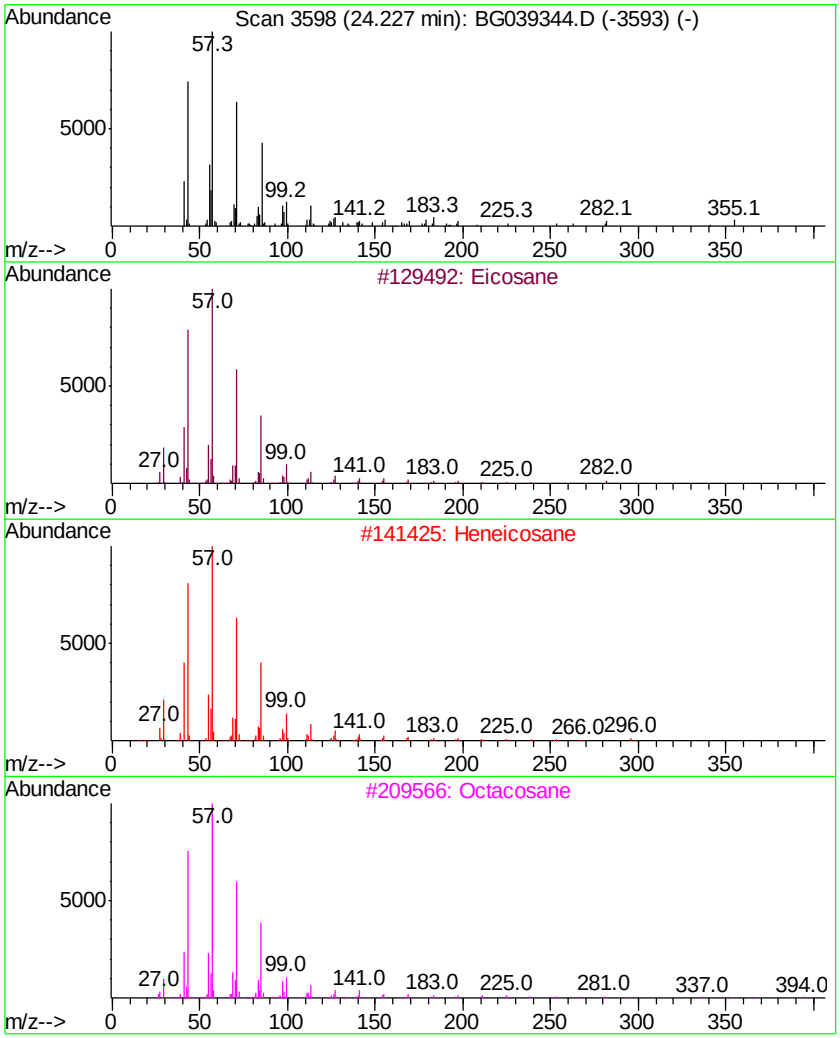
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

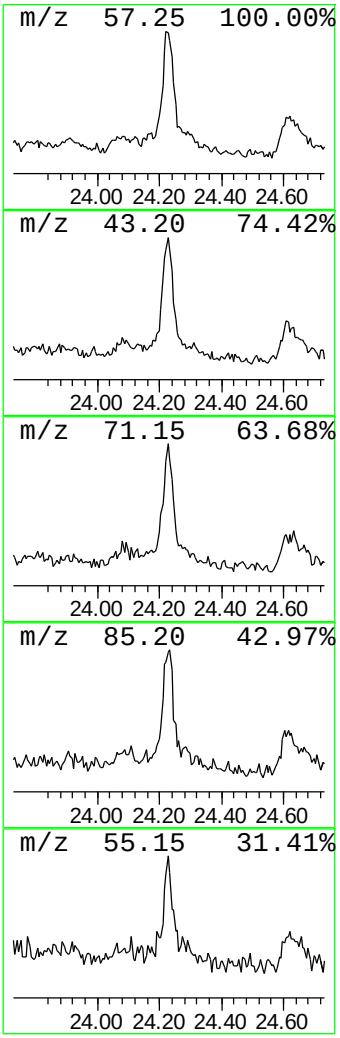
**********

Peak Number 10 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.23 | 2.50 ng | 137916 | Perylene-d12 | 25.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |
| 5 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

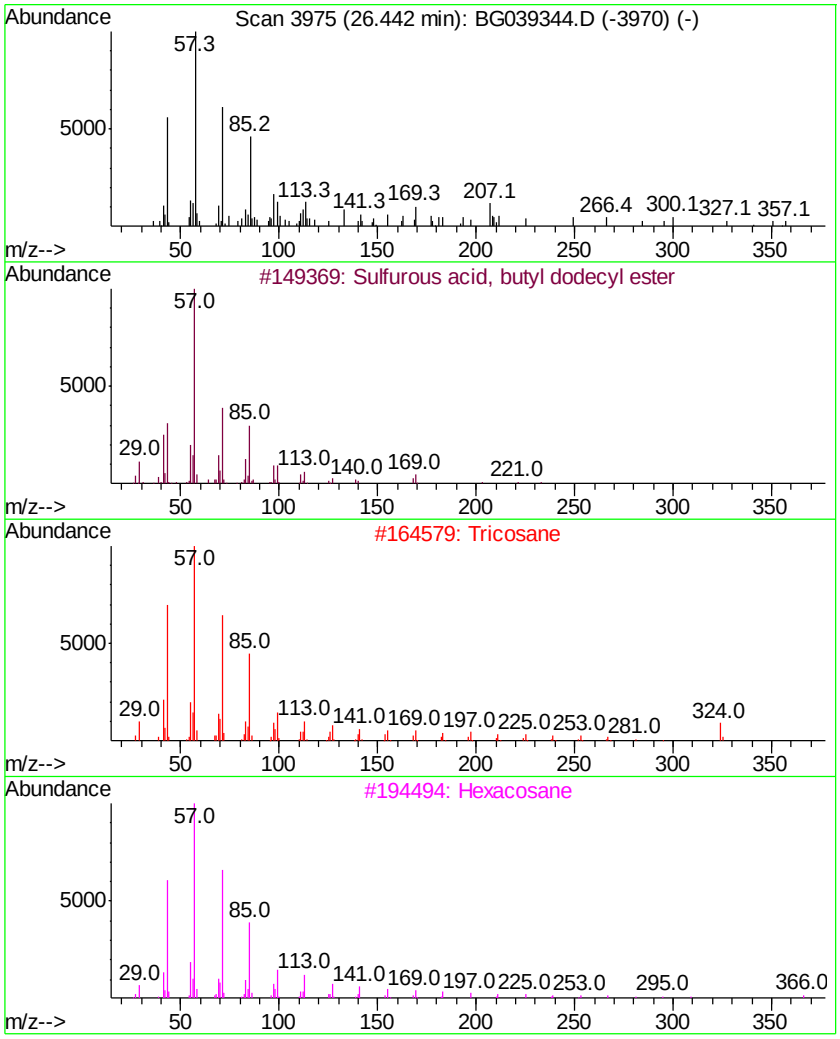
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

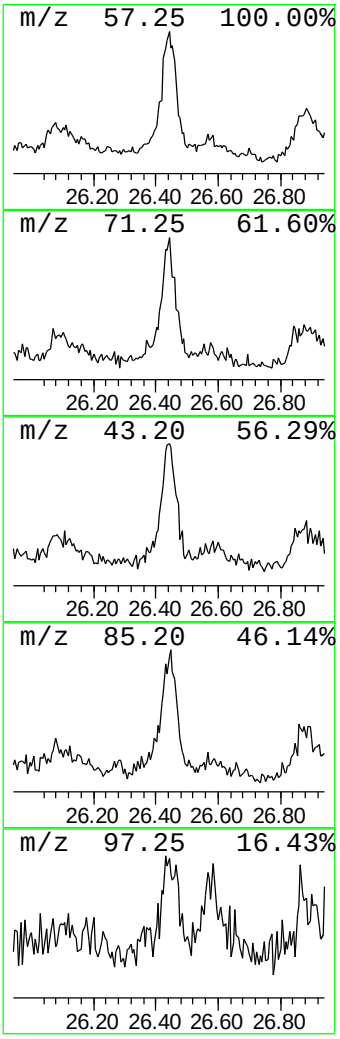
**********

Peak Number 11 Sulfurous acid, butyl dodec... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.44 | 2.34 ng | 129390 | Perylene-d12 | 25.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, butyl dodecyl ester | 306 | C16H34O3S | 1000309-17-9 | 64 |
| 2 | Tricosane | 324 | C23H48 | 000638-67-5 | 58 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 58 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 53 |
| 5 | Sulfurous acid, 2-ethylhexyl iso... | 278 | C14H30O3S | 1000309-19-0 | 52 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG020119\
Data File : BG039344.D
Acq On : 1 Feb 2019 15:56
Operator : JU/SJ
Sample : K1292-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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... | 3.30 | 4.1 | ng | 64382 | 1 | 8.18 | 315997 | 20.0 |
| 2-Pentanone, 4-hy... | 5.26 | 7.9 | ng | 124132 | 1 | 8.18 | 315997 | 20.0 |
| unknown7.70 | 7.70 | 111.3 | ng | 1759210 | 1 | 8.18 | 315997 | 20.0 |
| n-Hexadecanoic acid | 18.40 | 3.6 | ng | 157169 | 4 | 17.54 | 863761 | 20.0 |
| Hexacosyl pentafl... | 21.44 | 4.8 | ng | 233733 | 5 | 21.84 | 976761 | 20.0 |
| Hexadecane, 2,6,1... | 22.64 | 2.4 | ng | 115036 | 5 | 21.84 | 976761 | 20.0 |
| Tetratetracontane | 23.38 | 2.7 | ng | 131641 | 5 | 21.84 | 976761 | 20.0 |
| Eicosane | 24.23 | 2.5 | ng | 137916 | 6 | 25.23 | 1104620 | 20.0 |
| Sulfurous acid, b... | 26.44 | 2.3 | ng | 129390 | 6 | 25.23 | 1104620 | 20.0 |