LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038675.D
Acq On : 17 Dec 2018 23:39
Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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 | 5.144 | 345 | 350 | 358 | rVB | 25307 | 40524 | 2.28% | 0.425% |
| 2 | 5.609 | 422 | 429 | 443 | rVB | 457997 | 756552 | 42.65% | 7.926% |
| 3 | 7.213 | 695 | 702 | 716 | rVB | 465495 | 880415 | 49.63% | 9.223% |
| 4 | 7.589 | 757 | 766 | 776 | rBV | 430672 | 783312 | 44.16% | 8.206% |
| 5 | 8.059 | 840 | 846 | 853 | rBV | 74612 | 124883 | 7.04% | 1.308% |
| 6 | 8.382 | 894 | 901 | 912 | rVB | 337856 | 599827 | 33.82% | 6.284% |
| 7 | 9.234 | 1038 | 1046 | 1055 | rBV | 288662 | 559017 | 31.52% | 5.856% |
| 8 | 10.873 | 1318 | 1325 | 1335 | rBV | 90980 | 170991 | 9.64% | 1.791% |
| 9 | 13.317 | 1732 | 1741 | 1751 | rBV | 723501 | 1139610 | 64.25% | 11.938% |
| 10 | 14.140 | 1875 | 1881 | 1894 | rVB | 42004 | 65653 | 3.70% | 0.688% |
| 11 | 14.692 | 1969 | 1975 | 1984 | rBV3 | 149821 | 248543 | 14.01% | 2.604% |
| 12 | 16.184 | 2223 | 2229 | 2245 | rBV2 | 653693 | 1035162 | 58.36% | 10.844% |
| 13 | 17.442 | 2436 | 2443 | 2456 | rBV2 | 224935 | 342708 | 19.32% | 3.590% |
| 14 | 18.300 | 2584 | 2589 | 2598 | rBV2 | 27861 | 49923 | 2.81% | 0.523% |
| 15 | 20.045 | 2880 | 2886 | 2892 | rBV | 1384479 | 1773810 | 100.00% | 18.582% |
| 16 | 21.320 | 3098 | 3103 | 3112 | rBV2 | 26092 | 45386 | 2.56% | 0.475% |
| 17 | 21.725 | 3165 | 3172 | 3184 | rVB | 210697 | 373370 | 21.05% | 3.911% |
| 18 | 22.477 | 3295 | 3300 | 3306 | rBV | 19152 | 29146 | 1.64% | 0.305% |
| 19 | 23.012 | 3385 | 3391 | 3400 | rVB3 | 13984 | 28323 | 1.60% | 0.297% |
| 20 | 23.176 | 3412 | 3419 | 3433 | rBV2 | 28873 | 66995 | 3.78% | 0.702% |
| 21 | 23.993 | 3550 | 3558 | 3565 | rVB4 | 16776 | 39327 | 2.22% | 0.412% |
| 22 | 25.021 | 3723 | 3733 | 3743 | rVB3 | 122495 | 361685 | 20.39% | 3.789% |
| 23 | 26.090 | 3907 | 3915 | 3921 | rBV3 | 11610 | 30528 | 1.72% | 0.320% |

Sum of corrected areas: 9545690

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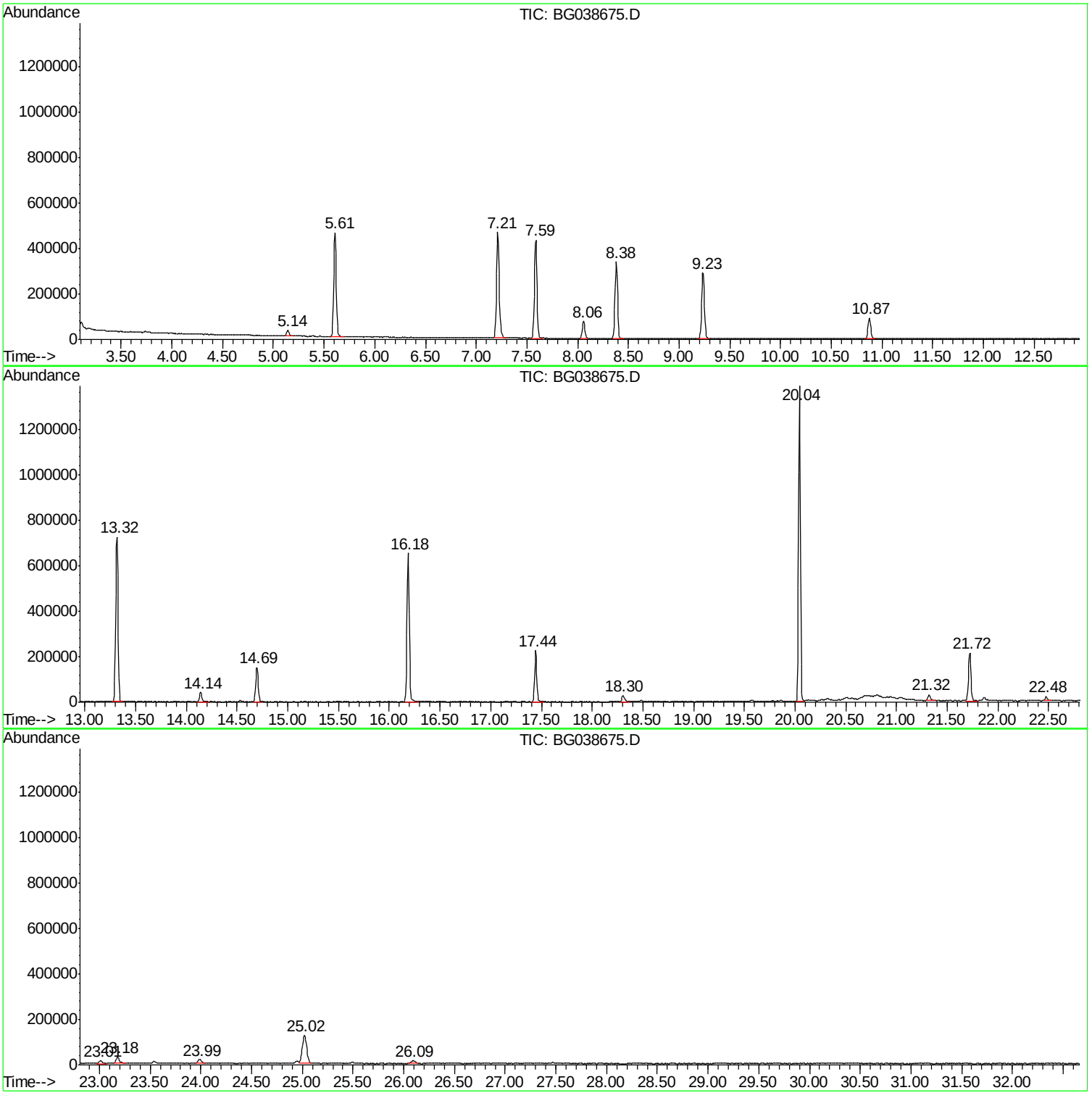
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
P001-SS002-1824-01

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038675.D
Acq On : 17 Dec 2018 23:39
Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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

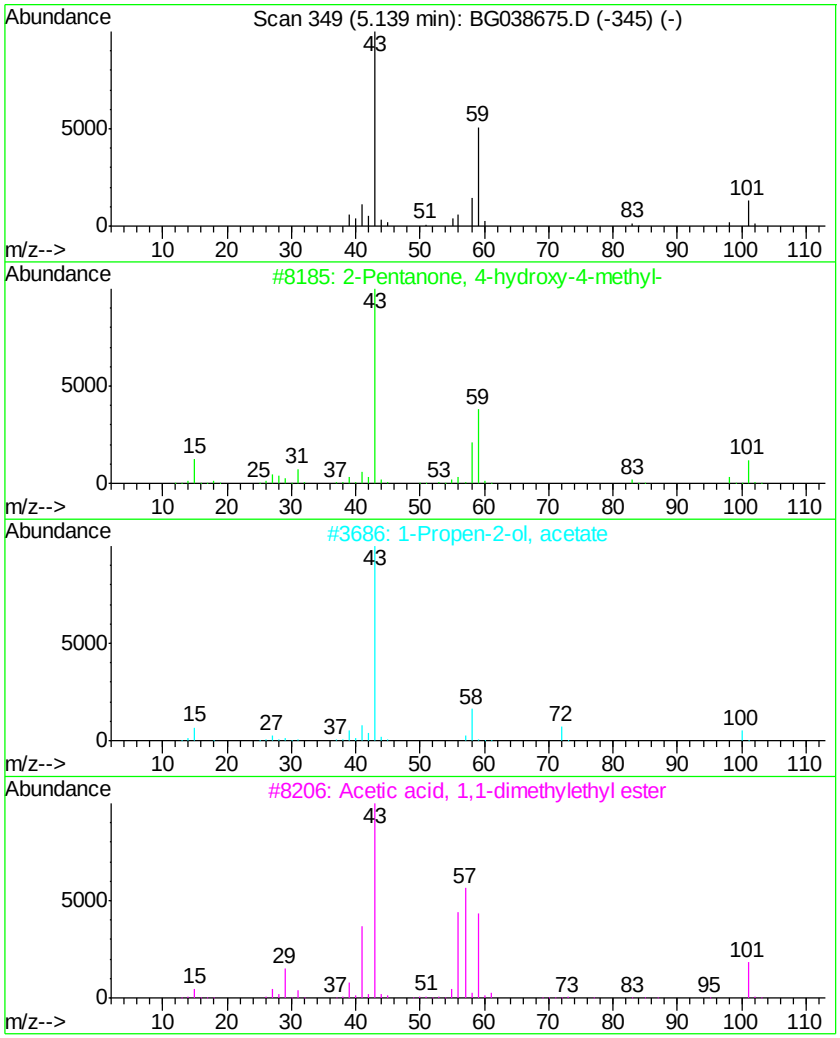
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

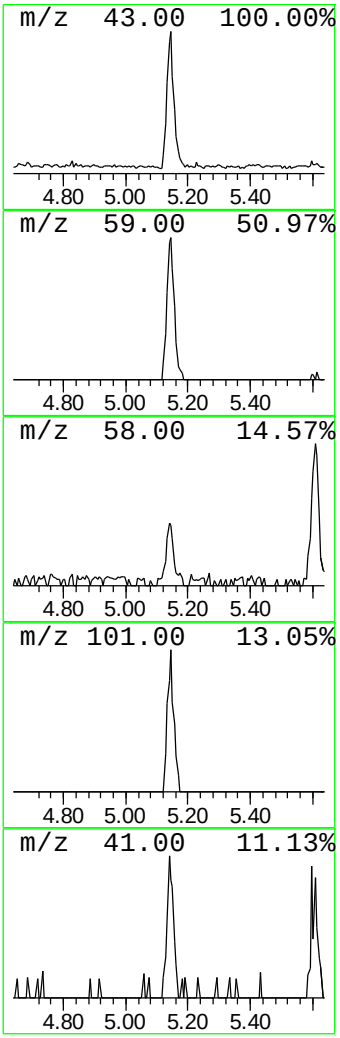
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.14 | 6.49 ng | 40524 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 4 | 1-Butene, 4-ethoxy- | 100 | C6H12O | 044611-46-3 | 9 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 7 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038675.D
Acq On : 17 Dec 2018 23:39
Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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

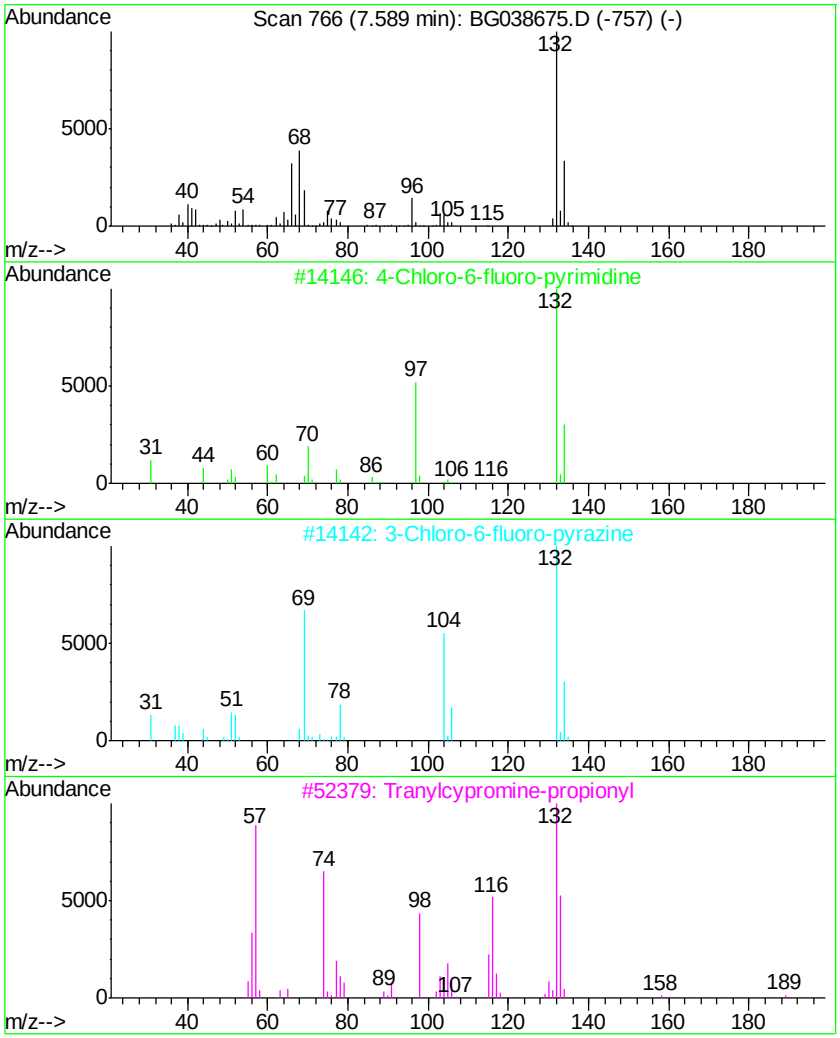
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

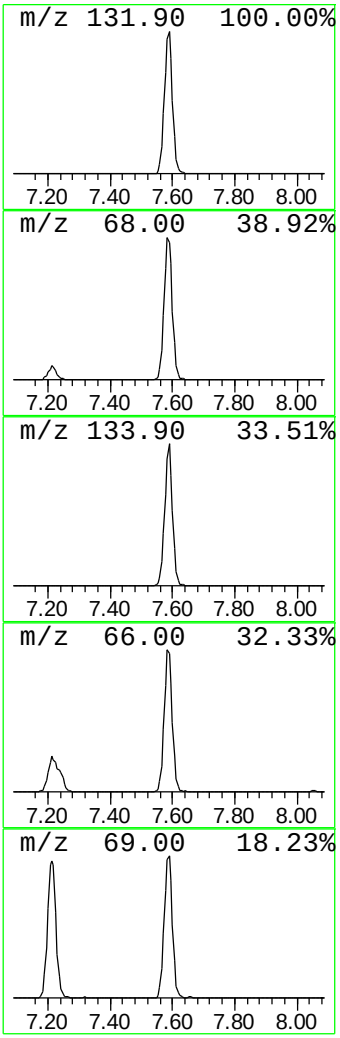
**********

Peak Number 2 unknown7.59 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.59 | 125.45 ng | 783312 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 22 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 5 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 22 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038675.D
Acq On : 17 Dec 2018 23:39
Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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

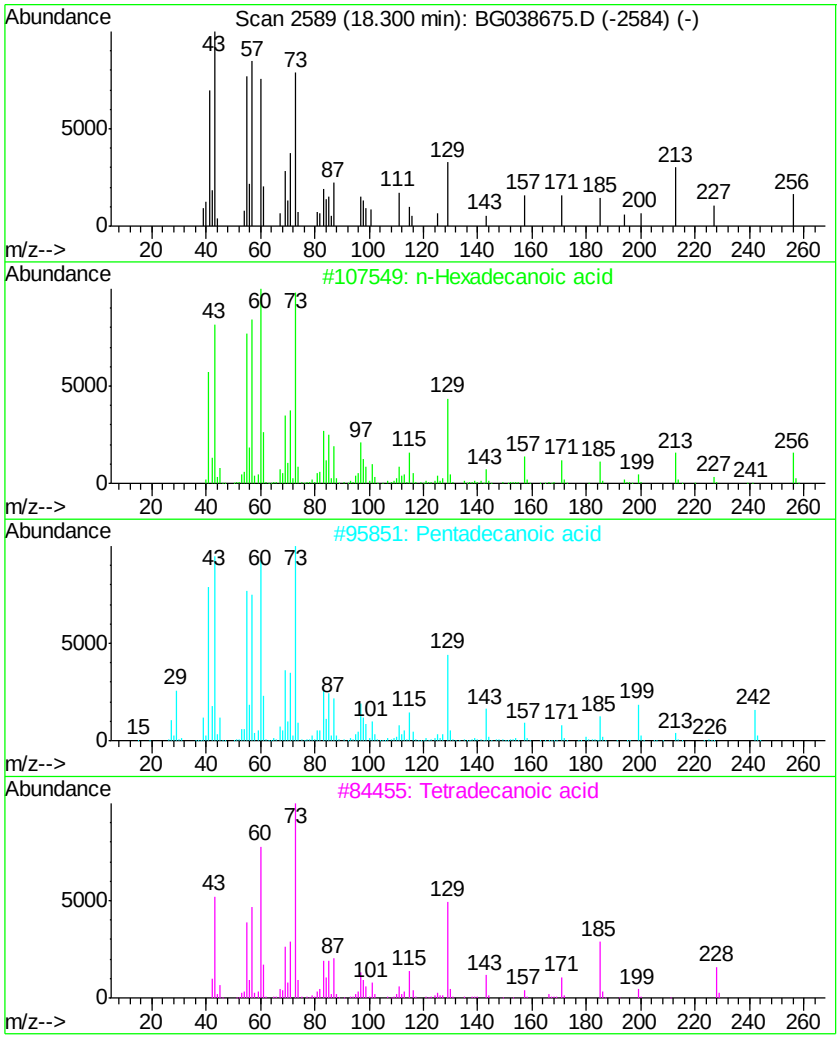
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

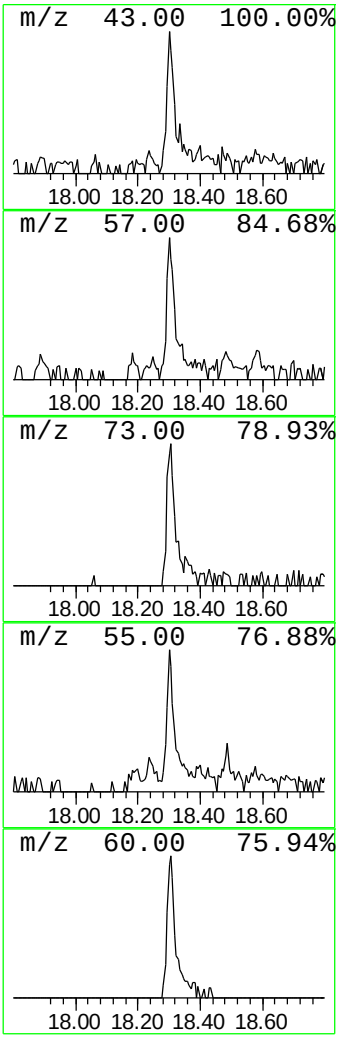
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.30 | 2.91 ng | 49923 | Phenanthrene-d10 | 17.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 64 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 53 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038675.D
Acq On : 17 Dec 2018 23:39
Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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

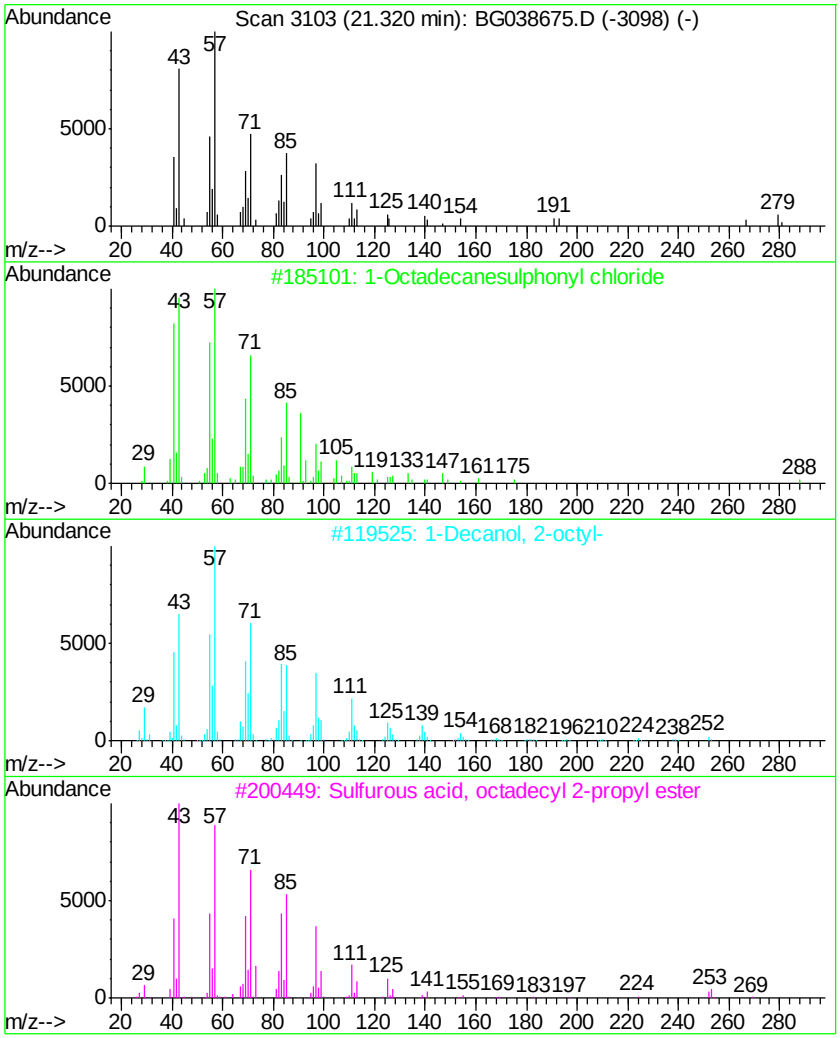
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

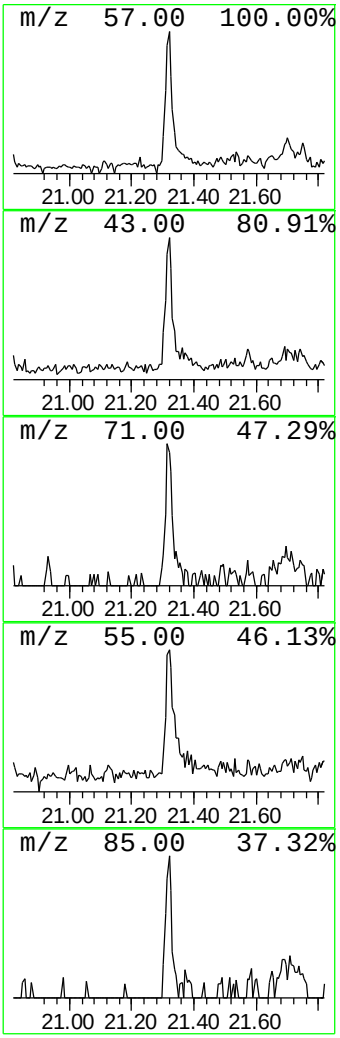
**********

Peak Number 5 1-Octadecanesulphonyl chloride Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.32 | 2.43 ng | 45386 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Octadecanesulphonyl chloride | 352 | C18H37ClO2S | 1000342-70-4 | 80 |
| 2 | 1-Decanol, 2-octyl- | 270 | C18H38O | 045235-48-1 | 80 |
| 3 | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 74 |
| 4 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 64 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 53 |



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Operator : JU/SJ
Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** P001-SS002-1824-01

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

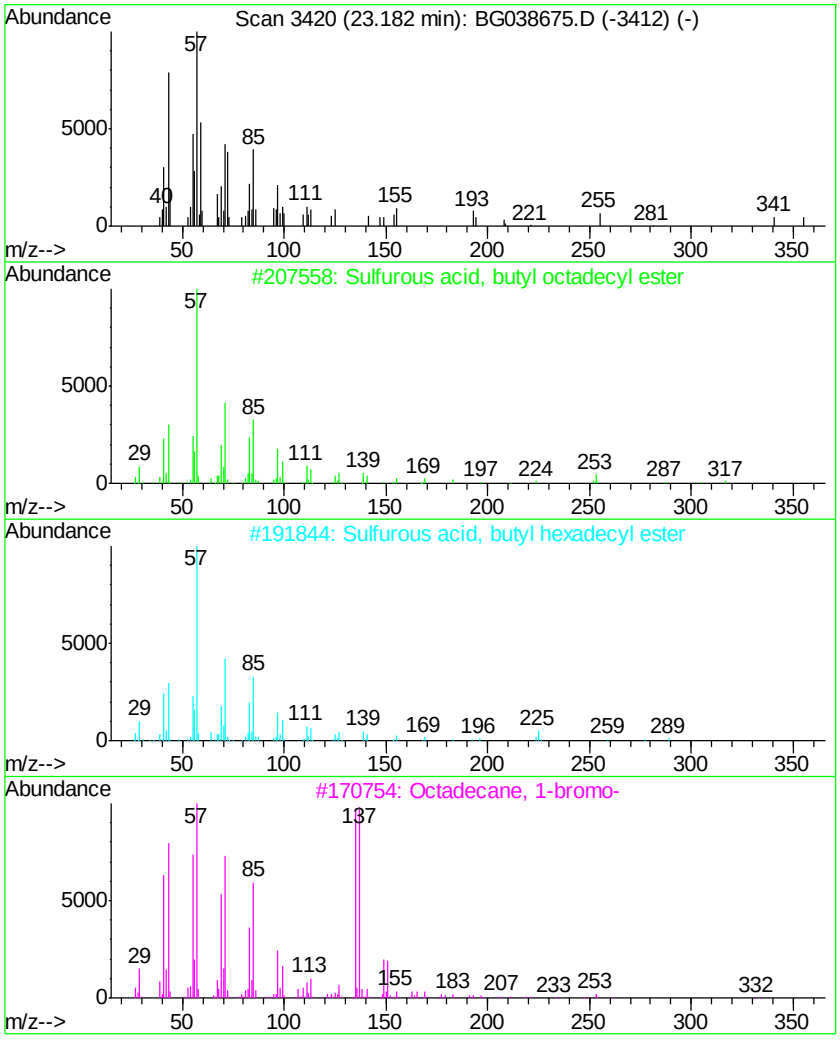
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

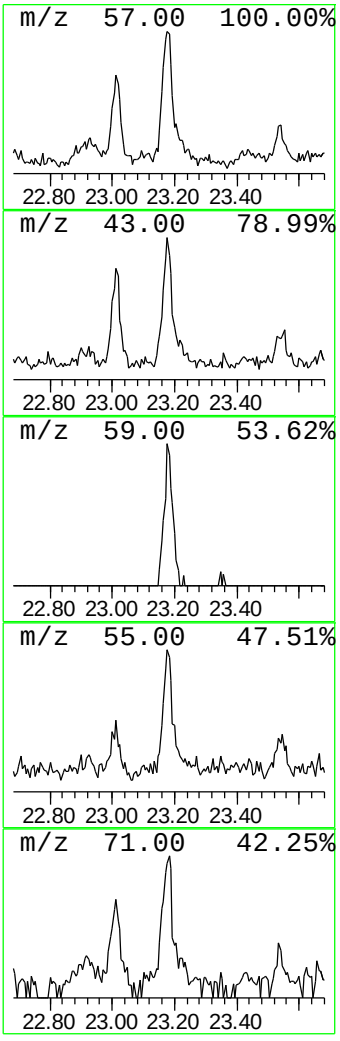
**********

Peak Number 6 unknown23.18 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.18 | 3.59 ng | 66995 | Chrysene-d12 | 21.72 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, butyl octadecyl ... | 390 | C22H46O3S | 1000309-18-5 | 46 |
| 2 | Sulfurous acid, butyl hexadecyl ... | 362 | C20H42O3S | 1000309-18-3 | 38 |
| 3 | Octadecane, 1-bromo- | 332 | C18H37Br | 000112-89-0 | 38 |
| 4 | 2-methyltetracosane | 352 | C25H52 | 1000376-72-6 | 38 |
| 5 | 1-Bromodocosane | 388 | C22H45Br | 006938-66-5 | 35 |



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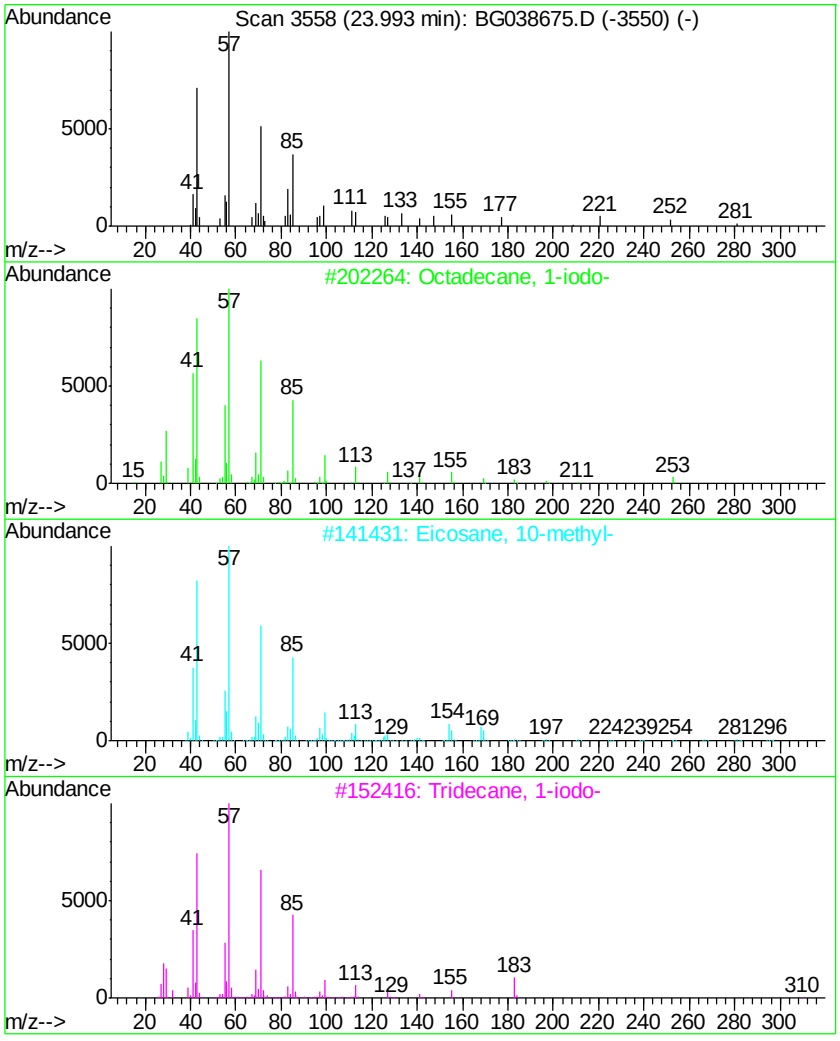
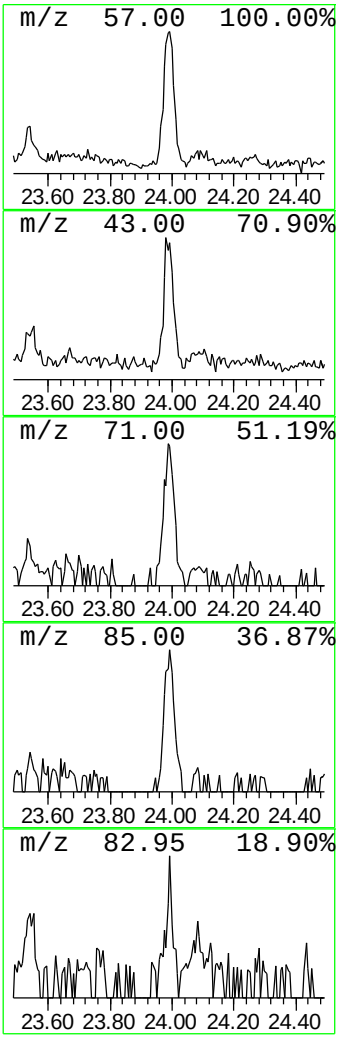
**********

Peak Number 7 Octadecane, 1-iodo- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.99 | 2.17 ng | 39327 | Perylene-d12 | 25.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 72 |
| 2 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 72 |
| 3 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 72 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 64 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 64 |



Tentatively Identified Compound (LSC) summary

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Sample : J6379-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
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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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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.14 | 6.5 | ng | 40524 | 1 | 8.06 | 124883 | 20.0 |
| unknown7.59 | 7.59 | 125.5 | ng | 783312 | 1 | 8.06 | 124883 | 20.0 |
| n-Hexadecanoic acid | 18.30 | 2.9 | ng | 49923 | 4 | 17.44 | 342708 | 20.0 |
| 1-Octadecanesulph... | 21.32 | 2.4 | ng | 45386 | 5 | 21.72 | 373370 | 20.0 |
| unknown23.18 | 23.18 | 3.6 | ng | 66995 | 5 | 21.72 | 373370 | 20.0 |
| Octadecane, 1-iodo- | 23.99 | 2.2 | ng | 39327 | 6 | 25.02 | 361685 | 20.0 |