LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110518\
Data File : BG037807.D
Acq On : 5 Nov 2018 17:47
Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-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-BG101818.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 | 5.179 | 316 | 322 | 333 | rVB | 28066 | 49621 | 1.29% | 0.247% |
| 2 | 5.638 | 392 | 400 | 413 | rBV | 428851 | 722085 | 18.76% | 3.592% |
| 3 | 7.236 | 665 | 672 | 684 | rBV | 287472 | 528872 | 13.74% | 2.631% |
| 4 | 7.618 | 730 | 737 | 746 | rBV | 782051 | 1406341 | 36.53% | 6.995% |
| 5 | 8.094 | 811 | 818 | 826 | rBV | 195730 | 345830 | 8.98% | 1.720% |
| 6 | 8.417 | 865 | 873 | 883 | rBV | 736791 | 1325858 | 34.44% | 6.595% |
| 7 | 9.269 | 1009 | 1018 | 1031 | rBV | 619656 | 1187485 | 30.84% | 5.907% |
| 8 | 10.914 | 1288 | 1298 | 1307 | rBV | 297904 | 545292 | 14.16% | 2.712% |
| 9 | 13.352 | 1705 | 1713 | 1724 | rBV | 1859304 | 3000360 | 77.93% | 14.924% |
| 10 | 14.169 | 1846 | 1852 | 1859 | rBV | 39729 | 62200 | 1.62% | 0.309% |
| 11 | 14.727 | 1940 | 1947 | 1956 | rBV2 | 474804 | 813070 | 21.12% | 4.044% |
| 12 | 15.955 | 2149 | 2156 | 2163 | rBV2 | 27791 | 46917 | 1.22% | 0.233% |
| 13 | 16.213 | 2193 | 2200 | 2211 | rBV | 1226442 | 1950768 | 50.67% | 9.703% |
| 14 | 16.307 | 2211 | 2216 | 2226 | rVB | 87955 | 160180 | 4.16% | 0.797% |
| 15 | 17.477 | 2407 | 2415 | 2427 | rBV2 | 574507 | 952864 | 24.75% | 4.740% |
| 16 | 18.205 | 2533 | 2539 | 2550 | rBV5 | 19960 | 43646 | 1.13% | 0.217% |
| 17 | 18.329 | 2555 | 2560 | 2571 | rBV3 | 65513 | 118278 | 3.07% | 0.588% |
| 18 | 19.598 | 2772 | 2776 | 2783 | rBV2 | 23019 | 39363 | 1.02% | 0.196% |
| 19 | 20.074 | 2851 | 2857 | 2874 | rBV | 2864331 | 3850088 | 100.00% | 19.150% |
| 20 | 21.754 | 3137 | 3143 | 3161 | rBV2 | 511323 | 967028 | 25.12% | 4.810% |
| 21 | 23.235 | 3390 | 3395 | 3402 | rVB | 32941 | 59684 | 1.55% | 0.297% |
| 22 | 23.434 | 3421 | 3429 | 3439 | rBV | 443929 | 911718 | 23.68% | 4.535% |
| 23 | 24.063 | 3529 | 3536 | 3542 | rVB2 | 33637 | 72868 | 1.89% | 0.362% |
| 24 | 25.085 | 3695 | 3710 | 3726 | rBV2 | 212541 | 847818 | 22.02% | 4.217% |
| 25 | 26.202 | 3889 | 3900 | 3910 | rBV5 | 28794 | 96179 | 2.50% | 0.478% |

Sum of corrected areas: 20104413

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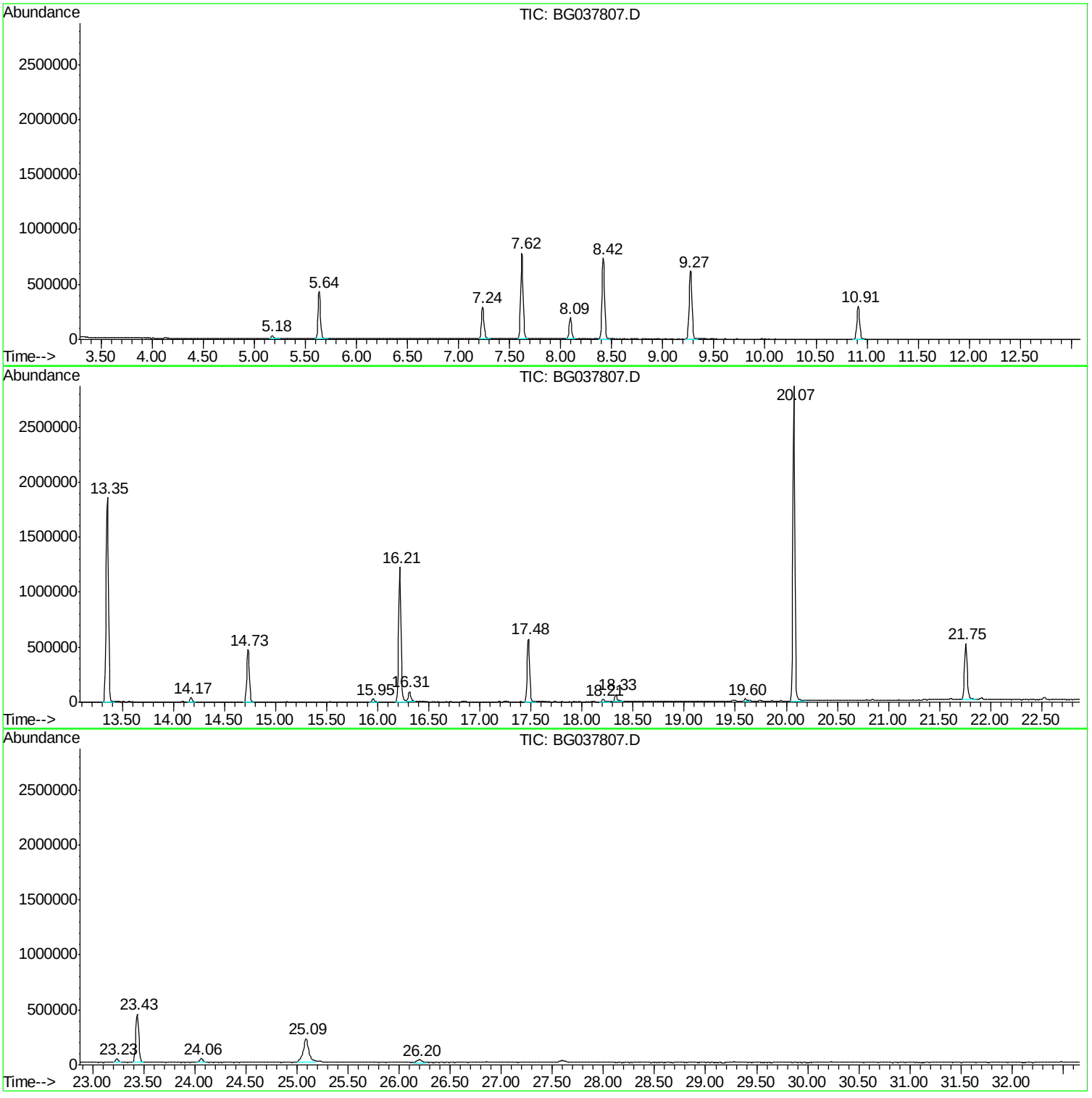
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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\BG110518\
Data File : BG037807.D
Acq On : 5 Nov 2018 17:47
Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

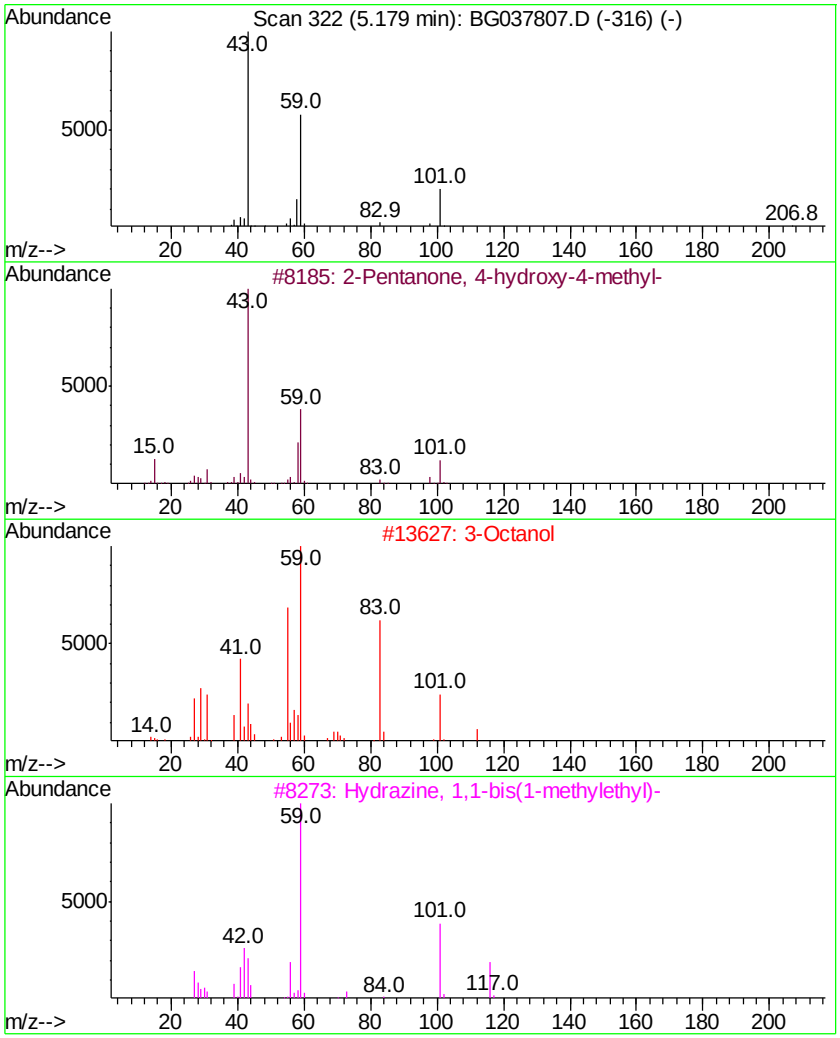
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

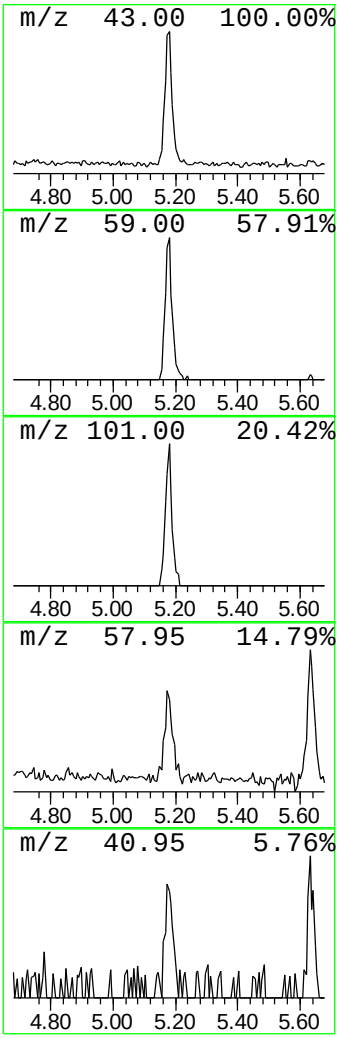
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 2.87 ng | 49621 | 1,4-Dichlorobenzene-d4 | 8.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 39 |
| 2 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 38 |
| 3 | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 28 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 25 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110518\
Data File : BG037807.D
Acq On : 5 Nov 2018 17:47
Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

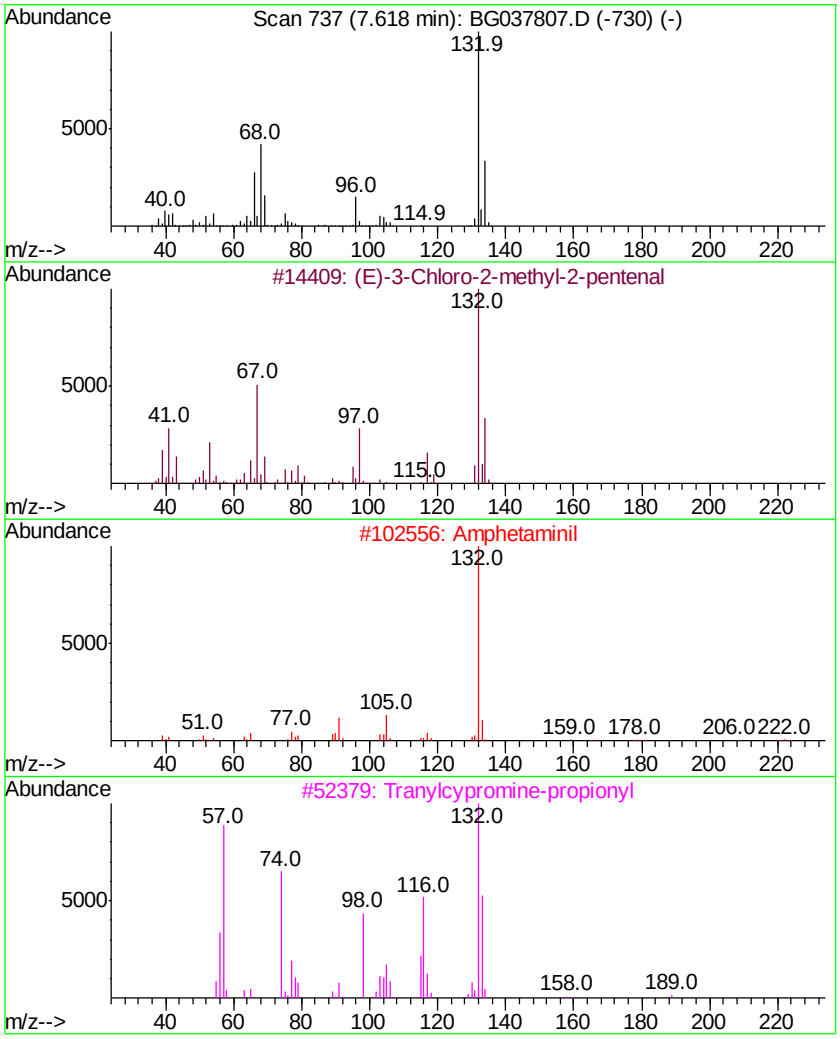
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

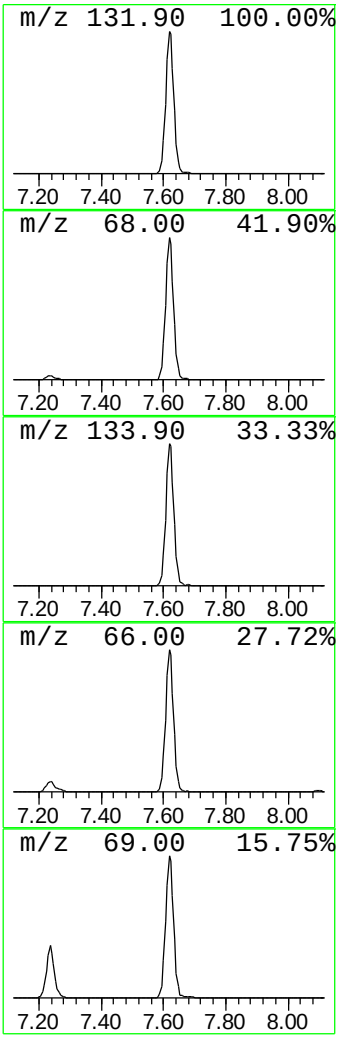
**********

Peak Number 2 unknown7.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.62 | 81.33 ng | 1406340 | 1,4-Dichlorobenzene-d4 | 8.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 2 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | N-(-phenylisopropyl)benzaldimine | 223 | C16H17N | 1000379-01-3 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110518\
Data File : BG037807.D
Acq On : 5 Nov 2018 17:47
Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

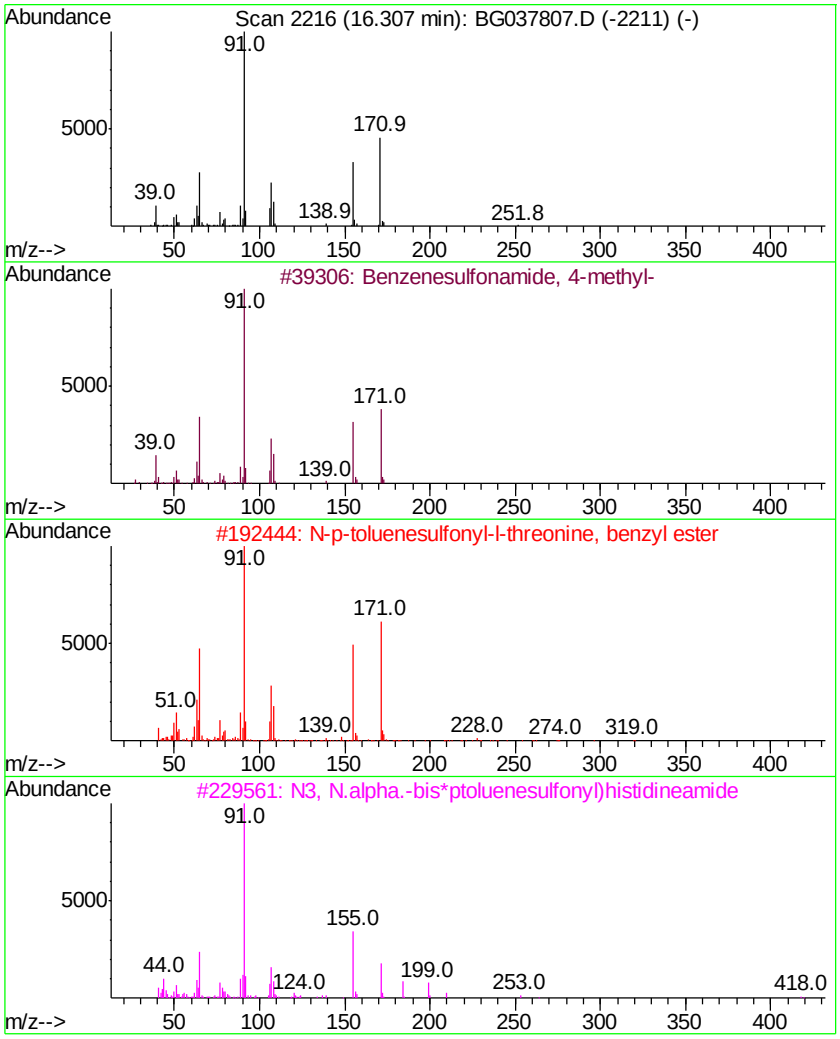
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

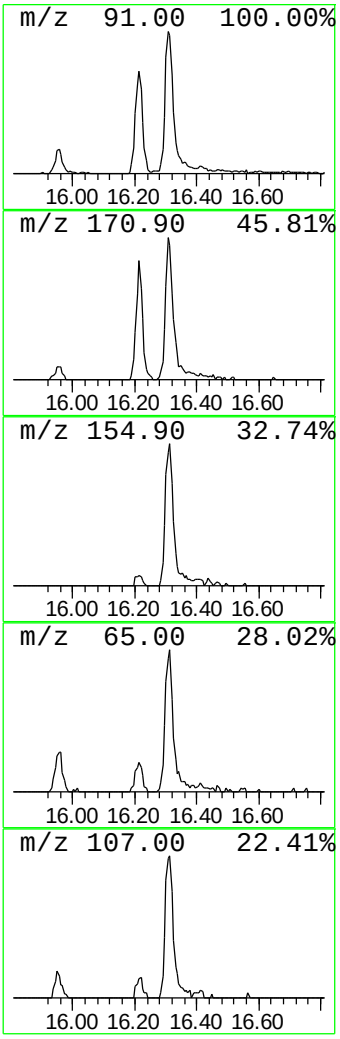
**********

Peak Number 4 Benzenesulfonamide, 4-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.31 | 3.36 ng | 160180 | Phenanthrene-d10 | 17.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfonamide, 4-methyl- | 171 | C7H9NO2S | 000070-55-3 | 98 |
| 2 | N-p-toluenesulfonyl-l-threonine,... | 363 | C18H21NO5S | 1000130-34-4 | 90 |
| 3 | N3, N.alpha.-bis*ptoluenesulfony... | 462 | C20H22N4O5S2 | 1000130-21-9 | 64 |
| 4 | O-p-toluenesulfonyll-N-acetylser... | 315 | C13H17NO6S | 1000126-44-8 | 58 |
| 5 | N-Sulfinyl-p-toluenesulfonamide | 217 | C7H7NO3S2 | 004104-47-6 | 43 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110518\
Data File : BG037807.D
Acq On : 5 Nov 2018 17:47
Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

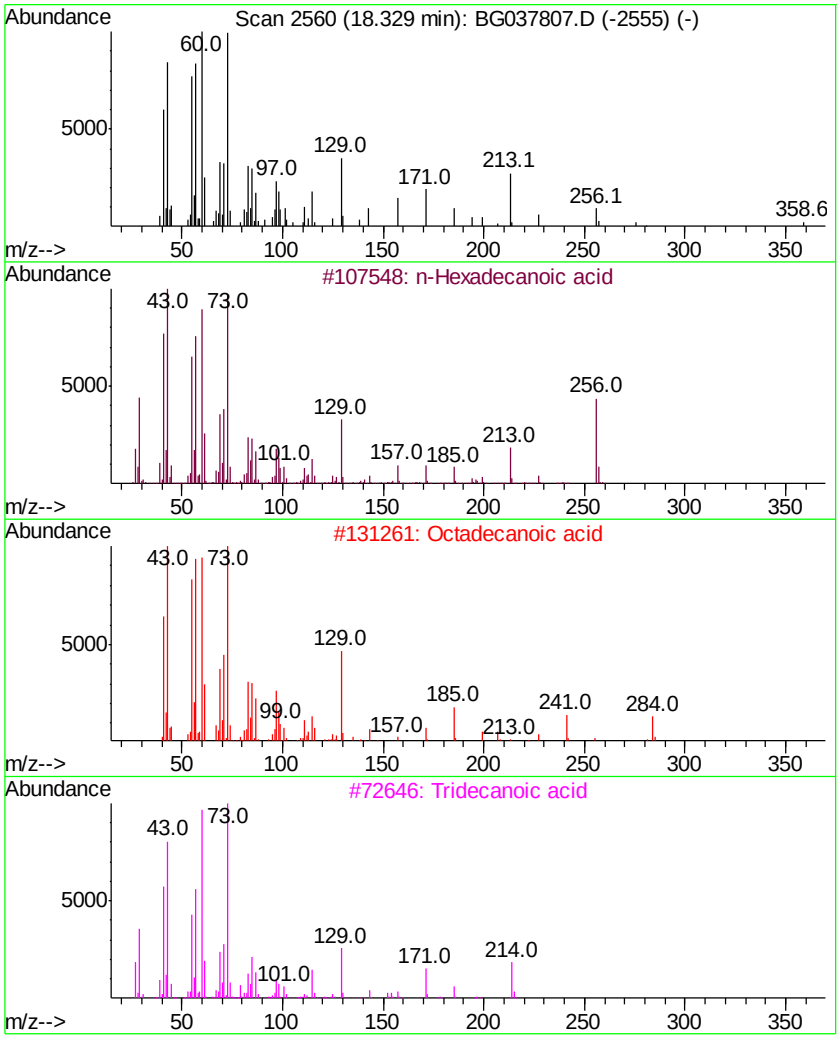
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

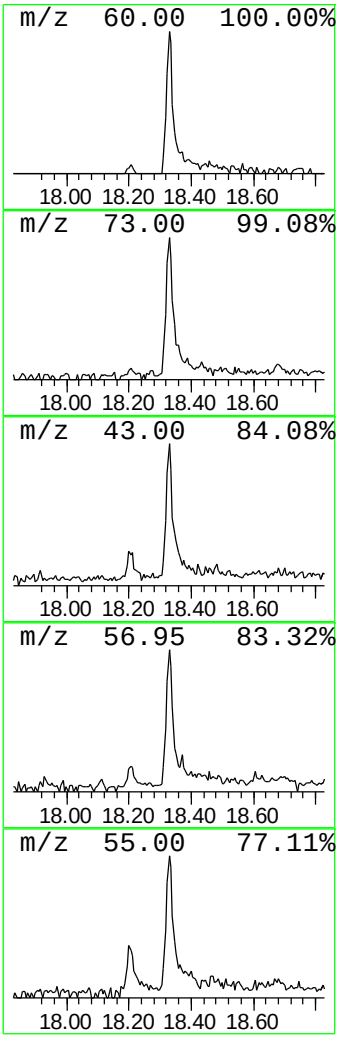
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.33 | 2.48 ng | 118278 | Phenanthrene-d10 | 17.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 76 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |



# Library Search Compound Report

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Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

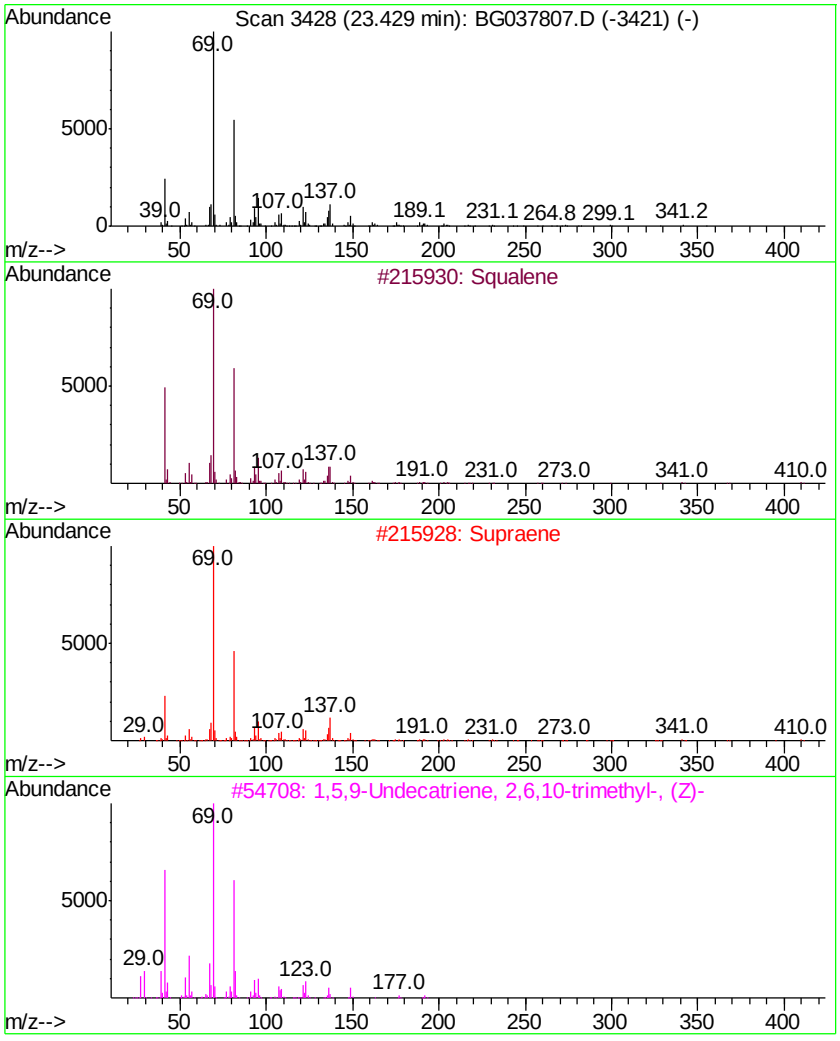
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

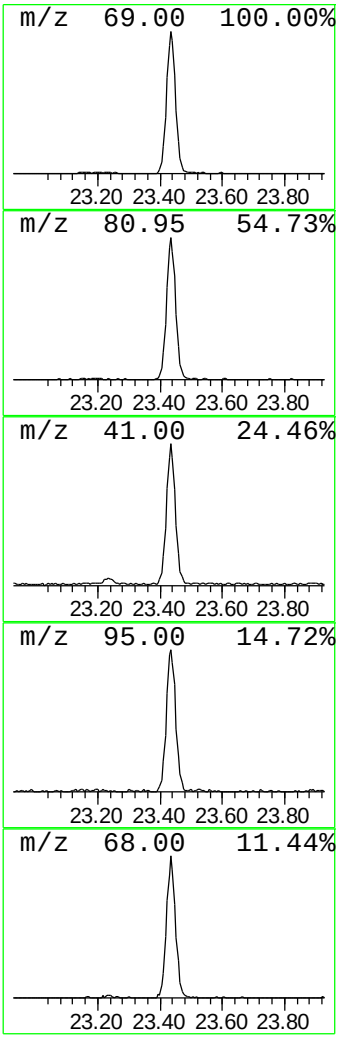
**********

Peak Number 6 Squalene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.43 | 21.51 ng | 911718 | Perylene-d12 | 25.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 3 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 86 |
| 4 | Trideca-1,7,11-triene-1,1-dicarb... | 270 | C18H26N2 | 1000161-46-0 | 50 |
| 5 | 1,5-Heptadiene, 3,4-dimethyl- | 124 | C9H16 | 1000061-77-9 | 50 |



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Operator : JU/SJ
Sample : J5769-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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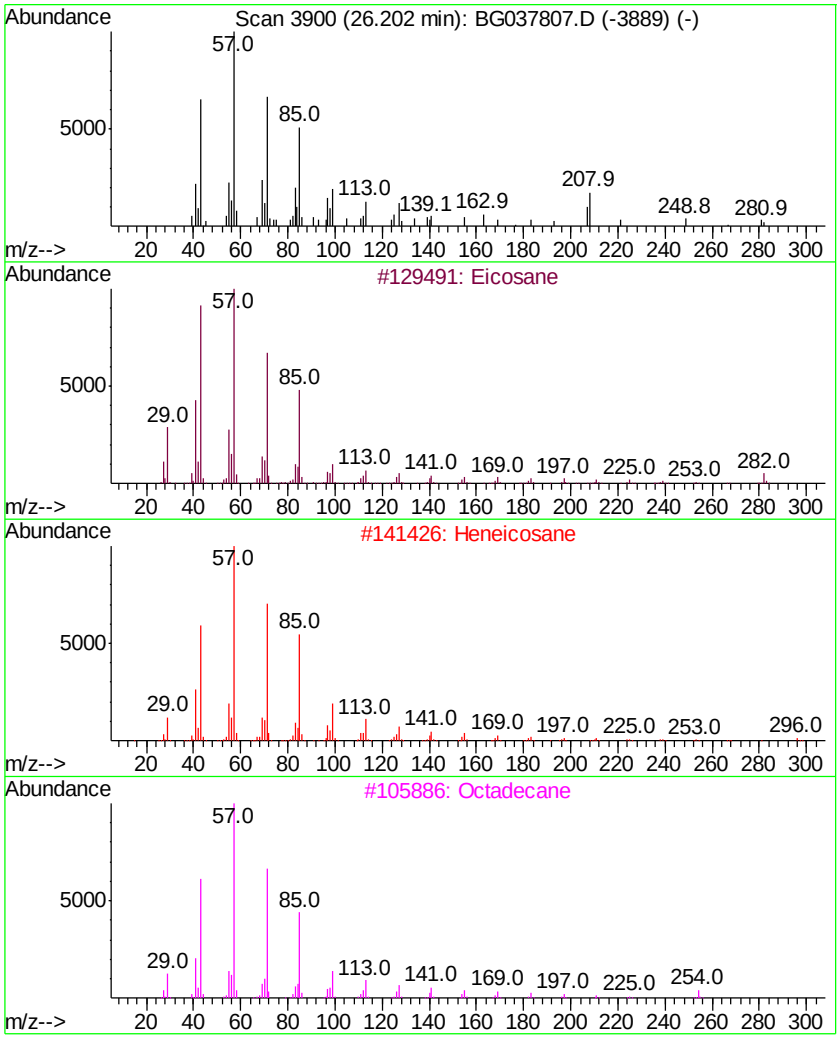
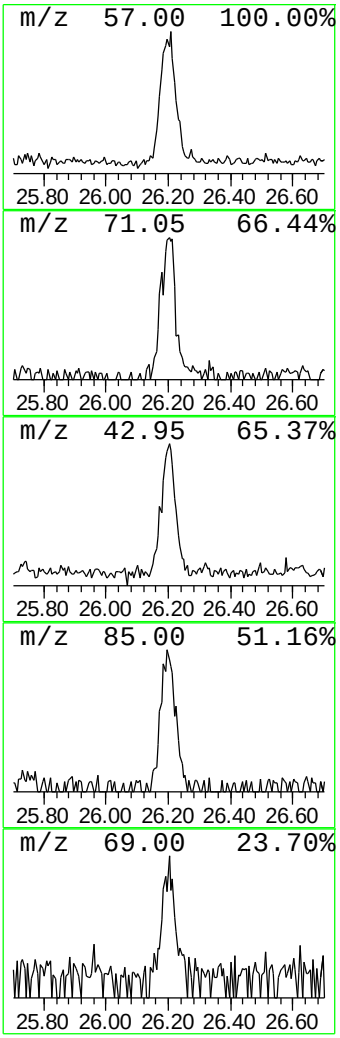
**********

Peak Number 7 Eicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 26.20 | 2.27 ng | 96179 | Perylene-d12 | 25.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 81 |
| 3 | Octadecane | 254 | C18H38 | 000593-45-3 | 74 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 68 |
| 5 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 68 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110518\
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Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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... | 5.18 | 2.9 | ng | 49621 | 1 | 8.09 | 345830 | 20.0 |
| unknown7.62 | 7.62 | 81.3 | ng | 1406340 | 1 | 8.09 | 345830 | 20.0 |
| Benzenesulfonamid... | 16.31 | 3.4 | ng | 160180 | 4 | 17.48 | 952864 | 20.0 |
| n-Hexadecanoic acid | 18.33 | 2.5 | ng | 118278 | 4 | 17.48 | 952864 | 20.0 |
| Squalene | 23.43 | 21.5 | ng | 911718 | 6 | 25.09 | 847818 | 20.0 |
| Eicosane | 26.20 | 2.3 | ng | 96179 | 6 | 25.09 | 847818 | 20.0 |