LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043729.D
Acq On : 20 Nov 2019 15:54
Operator : JU
Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

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-BG102119.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 | 3.146 | 6 | 10 | 19 | rVB | 80371 | 117259 | 4.48% | 0.956% |
| 2 | 5.091 | 333 | 341 | 353 | rBV | 98861 | 161320 | 6.16% | 1.315% |
| 3 | 5.579 | 417 | 424 | 436 | rBV | 496288 | 847014 | 32.34% | 6.902% |
| 4 | 7.183 | 690 | 697 | 707 | rBV | 502105 | 963728 | 36.80% | 7.853% |
| 5 | 7.529 | 748 | 756 | 767 | rBV | 529934 | 958974 | 36.62% | 7.815% |
| 6 | 7.988 | 827 | 834 | 842 | rBV2 | 96160 | 161011 | 6.15% | 1.312% |
| 7 | 8.311 | 881 | 889 | 908 | rBV | 392022 | 717846 | 27.41% | 5.850% |
| 8 | 9.151 | 1025 | 1032 | 1045 | rBV | 264213 | 550733 | 21.03% | 4.488% |
| 9 | 10.796 | 1304 | 1312 | 1331 | rBV | 84968 | 207511 | 7.92% | 1.691% |
| 10 | 13.240 | 1721 | 1728 | 1752 | rBV | 809585 | 1384006 | 52.85% | 11.278% |
| 11 | 14.081 | 1865 | 1871 | 1881 | rBV3 | 36582 | 84396 | 3.22% | 0.688% |
| 12 | 14.621 | 1957 | 1963 | 1974 | rBV | 174333 | 306230 | 11.69% | 2.495% |
| 13 | 16.113 | 2210 | 2217 | 2234 | rBV | 707379 | 1252869 | 47.84% | 10.210% |
| 14 | 17.371 | 2424 | 2431 | 2447 | rBV | 215569 | 414103 | 15.81% | 3.375% |
| 15 | 17.488 | 2447 | 2451 | 2458 | rVB6 | 17283 | 32298 | 1.23% | 0.263% |
| 16 | 18.258 | 2578 | 2582 | 2592 | rBV2 | 28647 | 60171 | 2.30% | 0.490% |
| 17 | 19.980 | 2868 | 2875 | 2890 | rBV | 1847204 | 2618734 | 100.00% | 21.340% |
| 18 | 21.290 | 3090 | 3098 | 3099 | rBV6 | 14908 | 26809 | 1.02% | 0.218% |
| 19 | 21.631 | 3150 | 3156 | 3172 | rBV | 273292 | 524921 | 20.04% | 4.278% |
| 20 | 22.400 | 3282 | 3287 | 3292 | rBV3 | 19452 | 33409 | 1.28% | 0.272% |
| 21 | 23.088 | 3397 | 3404 | 3411 | rBV4 | 24628 | 50870 | 1.94% | 0.415% |
| 22 | 23.276 | 3428 | 3436 | 3442 | rBV2 | 36716 | 71179 | 2.72% | 0.580% |
| 23 | 23.869 | 3531 | 3537 | 3545 | rBV2 | 28769 | 58484 | 2.23% | 0.477% |
| 24 | 24.803 | 3686 | 3696 | 3714 | rBV2 | 192167 | 602708 | 23.02% | 4.911% |
| 25 | 25.902 | 3875 | 3883 | 3884 | rBV5 | 18712 | 34904 | 1.33% | 0.284% |
| 26 | 27.230 | 4099 | 4109 | 4114 | rBV9 | 9755 | 29893 | 1.14% | 0.244% |

Sum of corrected areas: 12271380

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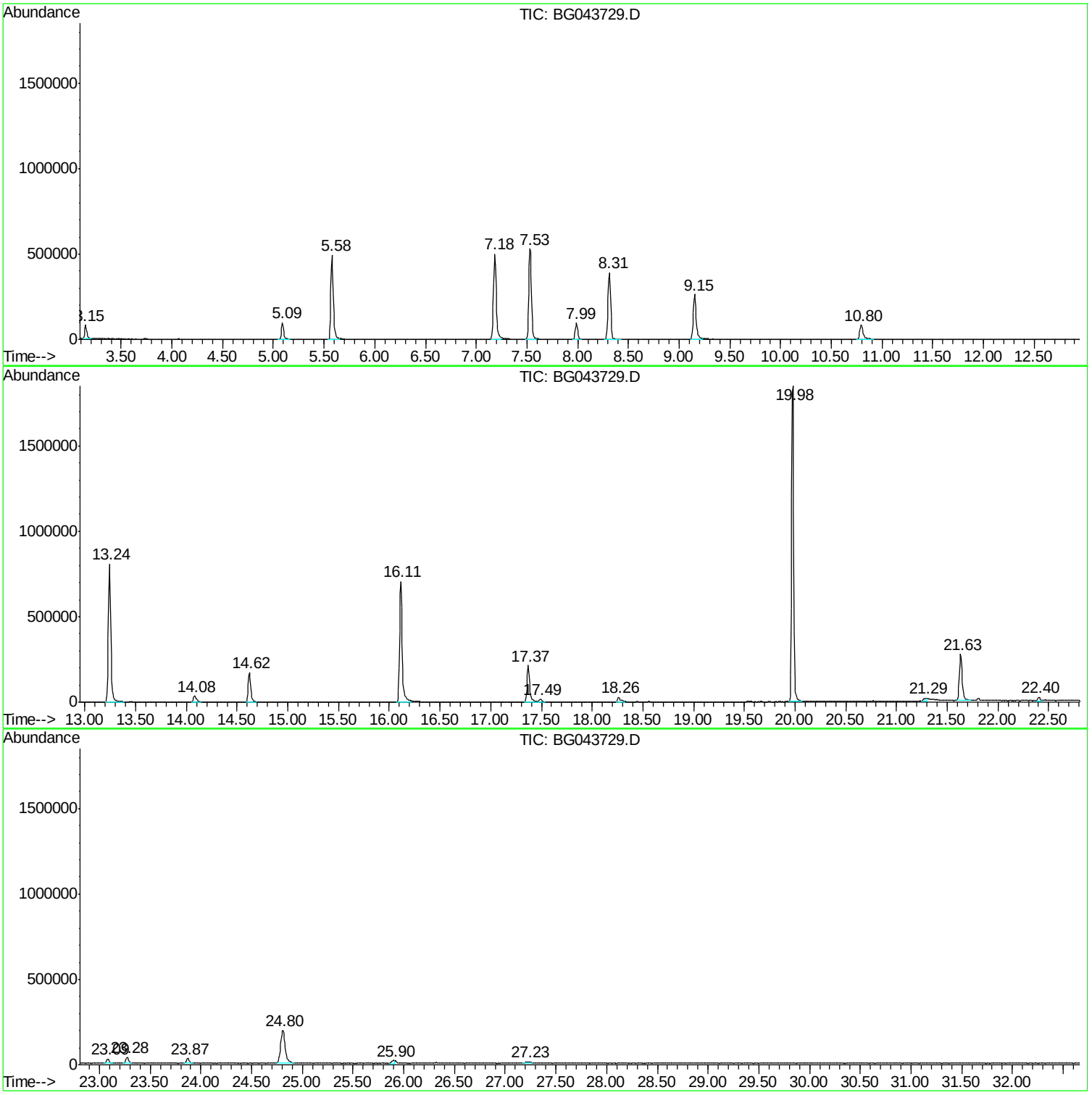
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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\BG112019\
Data File : BG043729.D
Acq On : 20 Nov 2019 15:54
Operator : JU
Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

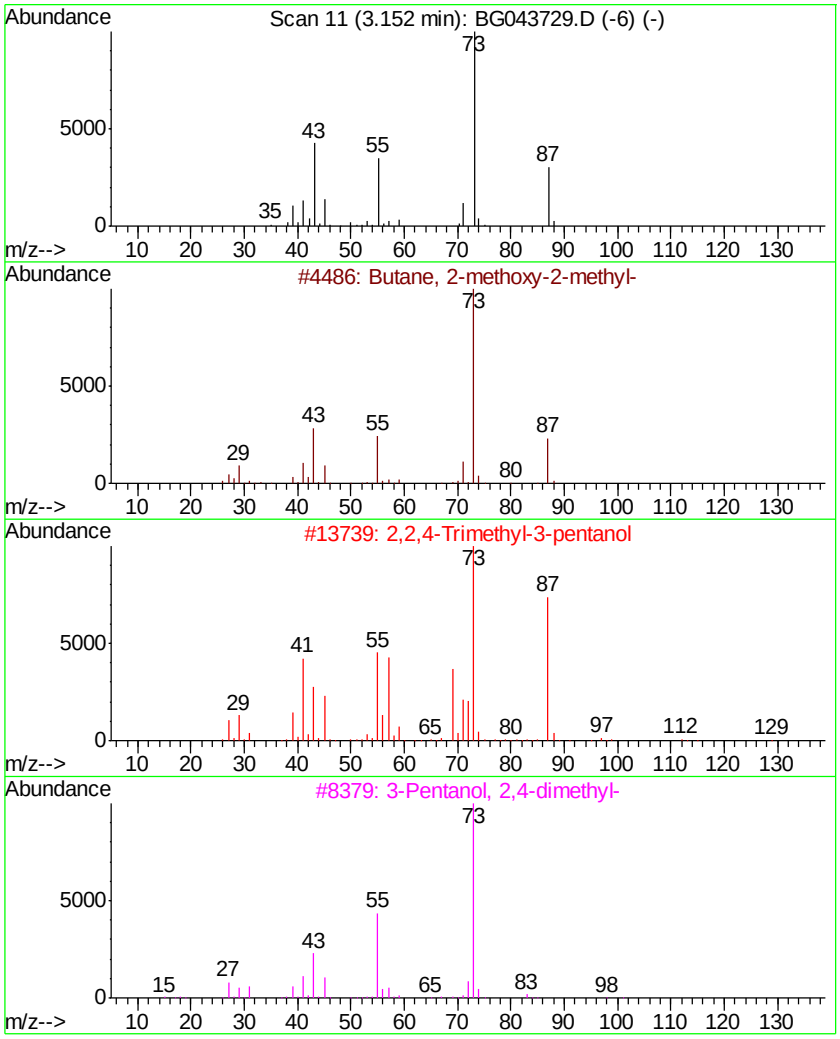
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

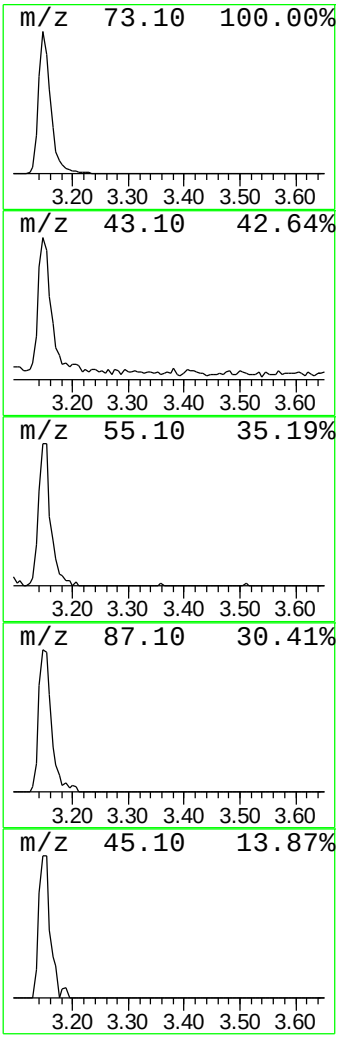
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.15 | 14.57 ng | 117259 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 37 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 17 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043729.D
Acq On : 20 Nov 2019 15:54
Operator : JU
Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

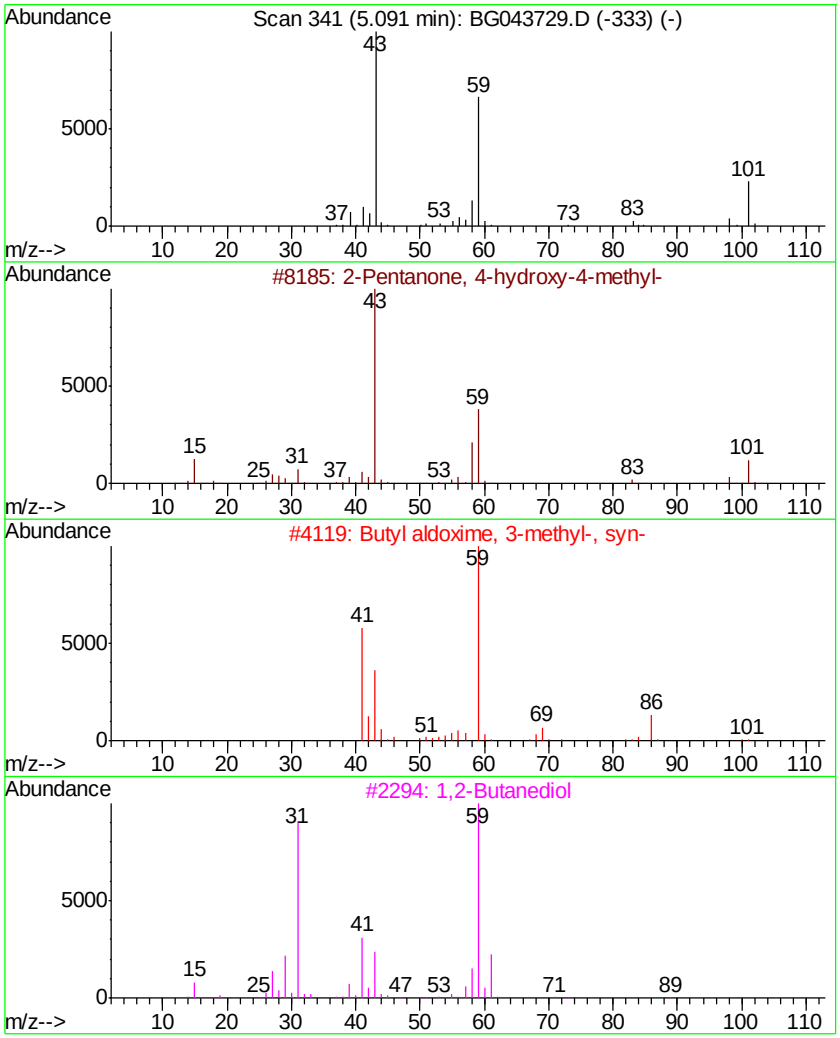
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

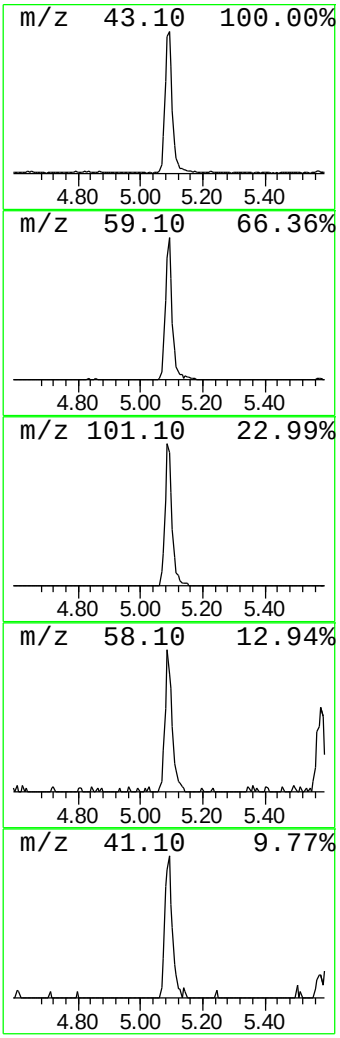
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 20.04 ng | 161320 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 25 |
| 3 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 25 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 25 |
| 5 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 23 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043729.D
Acq On : 20 Nov 2019 15:54
Operator : JU
Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

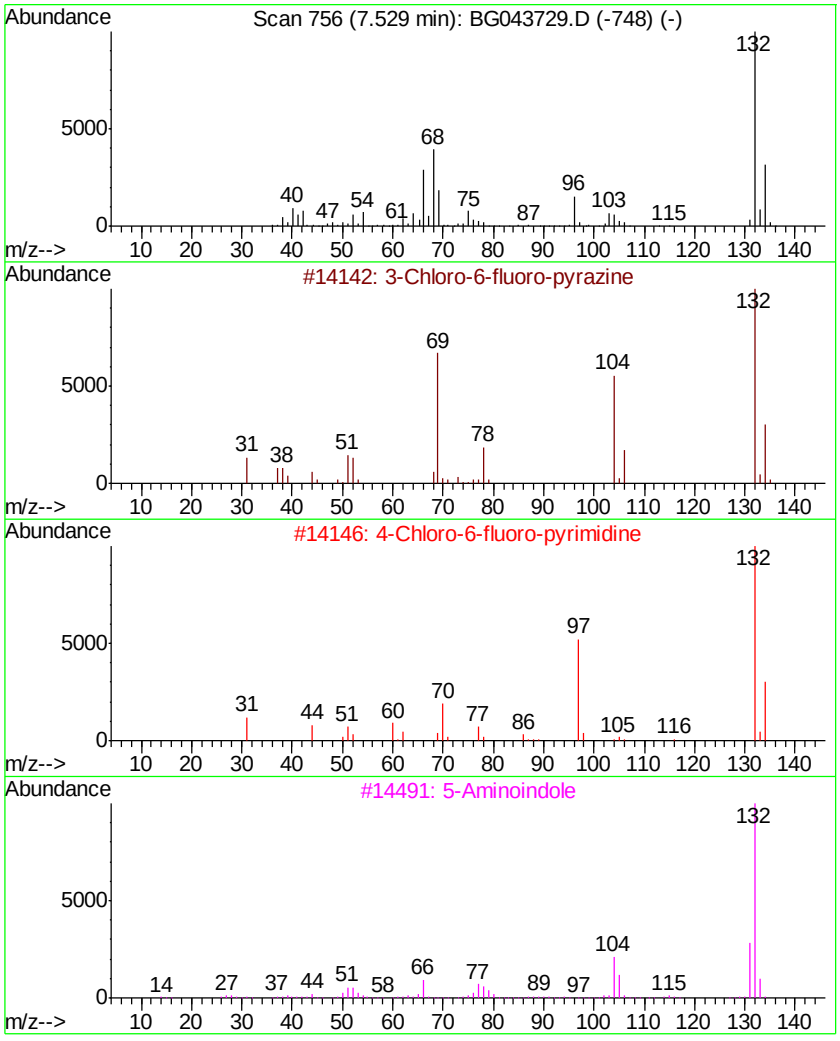
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

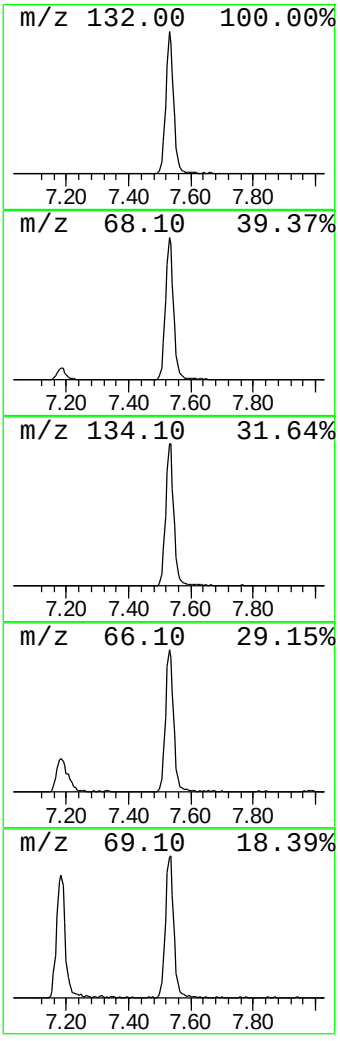
**********

Peak Number 3 unknown7.53 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.53 | 119.12 ng | 958974 | 1,4-Dichlorobenzene-d4 | 7.99 |

| 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 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 5 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 22 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112019\
Data File : BG043729.D
Acq On : 20 Nov 2019 15:54
Operator : JU
Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

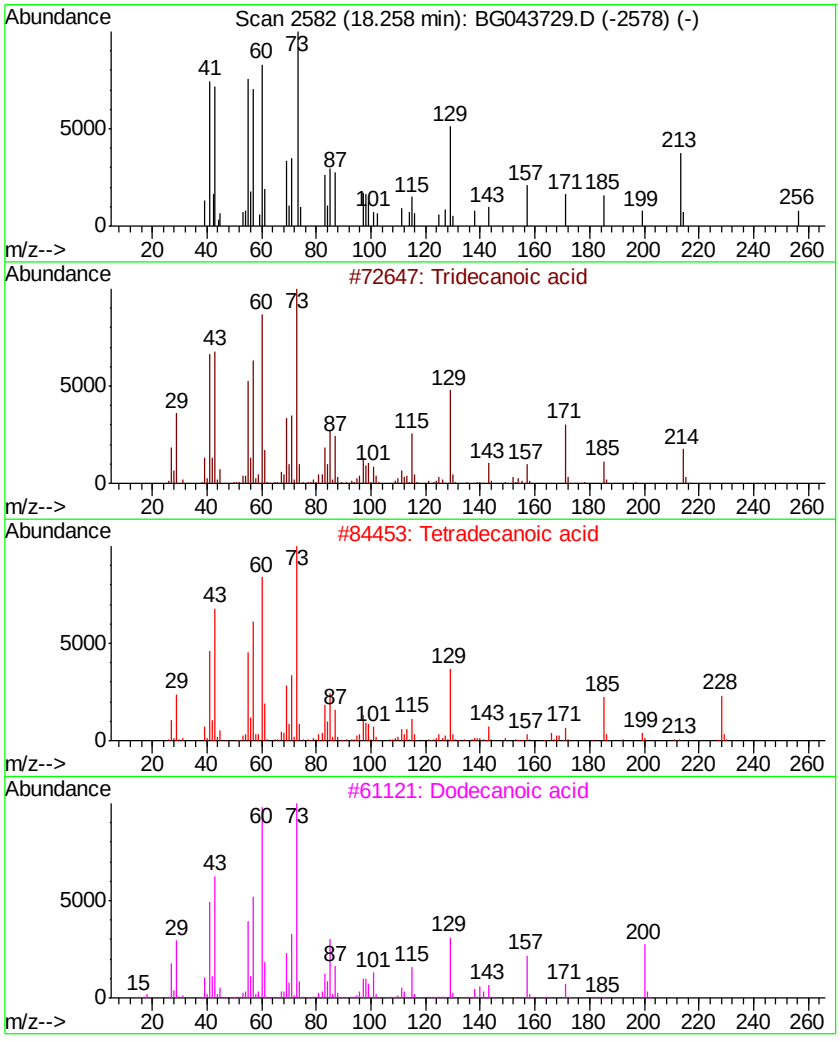
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

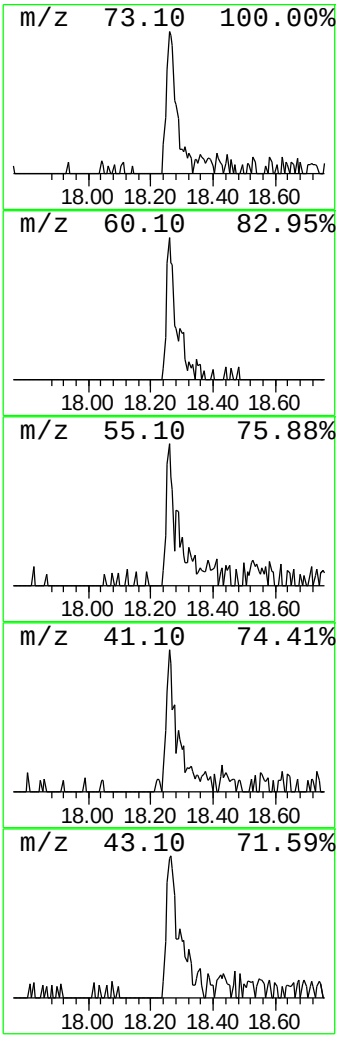
**********

Peak Number 5 Tridecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.26 | 2.91 ng | 60171 | Phenanthrene-d10 | 17.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 91 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 59 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 53 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 50 |



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Sample : K5904-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 1-(16-18)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

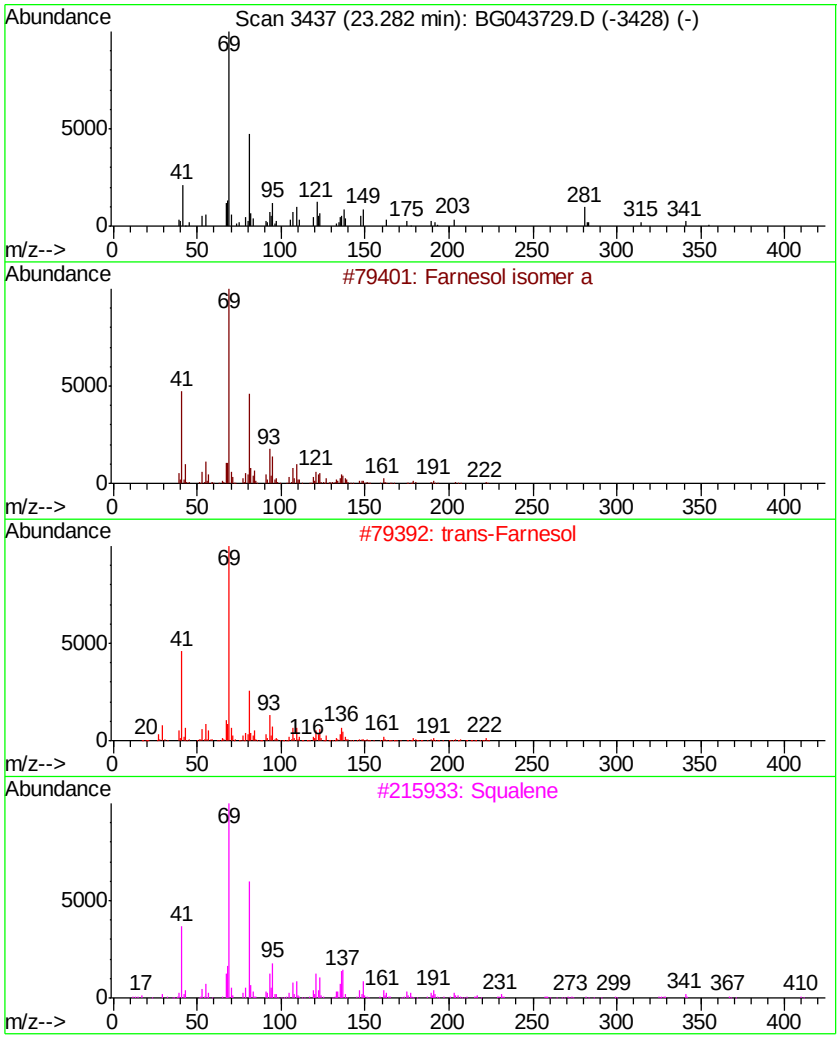
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

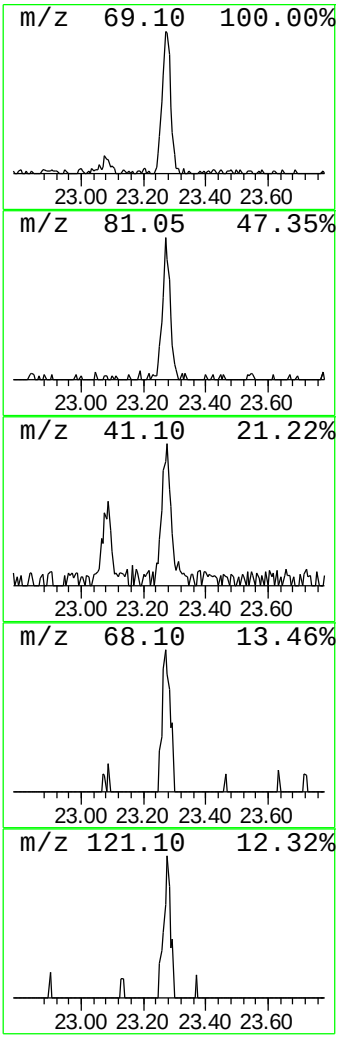
**********

Peak Number 6 Farnesol isomer a Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.28 | 2.36 ng | 71179 | Perylene-d12 | 24.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Farnesol isomer a | 222 | C15H26O | 1000108-92-4 | 90 |
| 2 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 87 |
| 3 | Squalene | 410 | C30H50 | 000111-02-4 | 86 |
| 4 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0 | 86 |
| 5 | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66 | 000502-62-5 | 78 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG112019\
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Misc :
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**Instrument :** BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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... | 3.15 | 14.6 | ng | 117259 | 1 | 7.99 | 161011 | 20.0 |
| 2-Pentanone, 4-hy... | 5.09 | 20.0 | ng | 161320 | 1 | 7.99 | 161011 | 20.0 |
| unknown7.53 | 7.53 | 119.1 | ng | 958974 | 1 | 7.99 | 161011 | 20.0 |
| Tridecanoic acid | 18.26 | 2.9 | ng | 60171 | 4 | 17.37 | 414103 | 20.0 |
| Farnesol isomer a | 23.28 | 2.4 | ng | 71179 | 6 | 24.81 | 602708 | 20.0 |