LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111218\
Data File : BG037949.D
Acq On : 12 Nov 2018 18:05
Operator : JU/SJ
Sample : J5901-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
S-E

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 | 5.173 | 315 | 321 | 329 | rBV | 51671 | 86093 | 2.18% | 0.391% |
| 2 | 5.632 | 391 | 399 | 411 | rBV | 1025008 | 1715990 | 43.38% | 7.801% |
| 3 | 7.236 | 664 | 672 | 684 | rBV | 1089010 | 2117504 | 53.53% | 9.627% |
| 4 | 7.618 | 729 | 737 | 749 | rBV | 1049018 | 1860098 | 47.02% | 8.457% |
| 5 | 8.088 | 810 | 817 | 825 | rBV | 175784 | 318264 | 8.05% | 1.447% |
| 6 | 8.411 | 864 | 872 | 880 | rBV | 764540 | 1386178 | 35.04% | 6.302% |
| 7 | 9.269 | 1009 | 1018 | 1032 | rBV | 684737 | 1276703 | 32.27% | 5.804% |
| 8 | 10.908 | 1289 | 1297 | 1306 | rBV | 270964 | 500382 | 12.65% | 2.275% |
| 9 | 13.346 | 1704 | 1712 | 1722 | rBV | 1956374 | 3109362 | 78.60% | 14.136% |
| 10 | 14.169 | 1841 | 1852 | 1859 | rBV | 219176 | 328388 | 8.30% | 1.493% |
| 11 | 14.727 | 1937 | 1947 | 1958 | rBV2 | 433871 | 745797 | 18.85% | 3.391% |
| 12 | 16.213 | 2193 | 2200 | 2217 | rBV | 1286932 | 2083089 | 52.66% | 9.470% |
| 13 | 17.471 | 2408 | 2414 | 2426 | rBV2 | 543168 | 838869 | 21.21% | 3.814% |
| 14 | 18.323 | 2555 | 2559 | 2569 | rBV | 54952 | 101299 | 2.56% | 0.461% |
| 15 | 19.815 | 2809 | 2813 | 2825 | rVB10 | 25397 | 44187 | 1.12% | 0.201% |
| 16 | 20.074 | 2850 | 2857 | 2871 | rBV | 2822882 | 3955847 | 100.00% | 17.985% |
| 17 | 21.754 | 3136 | 3143 | 3156 | rBV2 | 430494 | 809916 | 20.47% | 3.682% |
| 18 | 24.051 | 3528 | 3534 | 3543 | rVB4 | 20723 | 50708 | 1.28% | 0.231% |
| 19 | 25.080 | 3694 | 3709 | 3723 | rBV2 | 179575 | 667031 | 16.86% | 3.033% |

Sum of corrected areas: 21995705

LSC Report - Integrated Chromatogram

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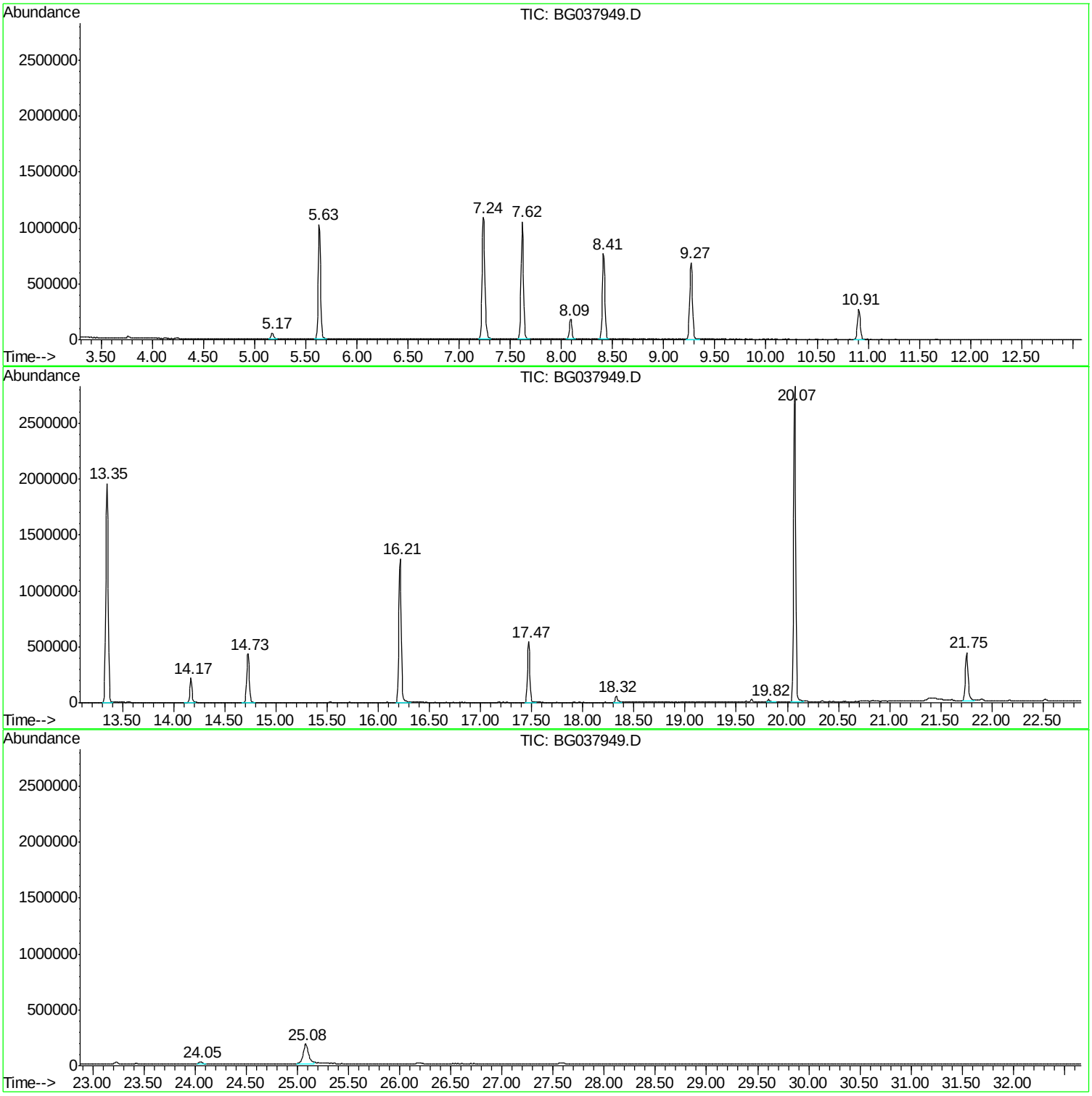
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
S-E

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\BG111218\
Data File : BG037949.D
Acq On : 12 Nov 2018 18:05
Operator : JU/SJ
Sample : J5901-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
S-E

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

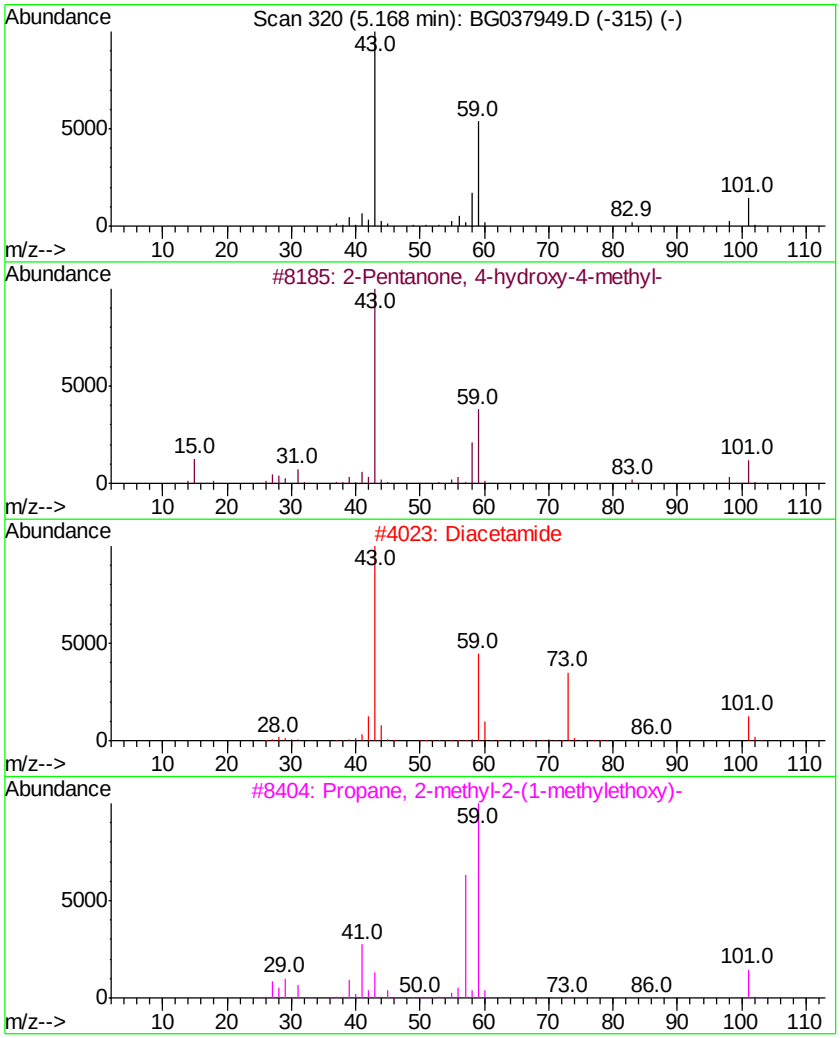
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

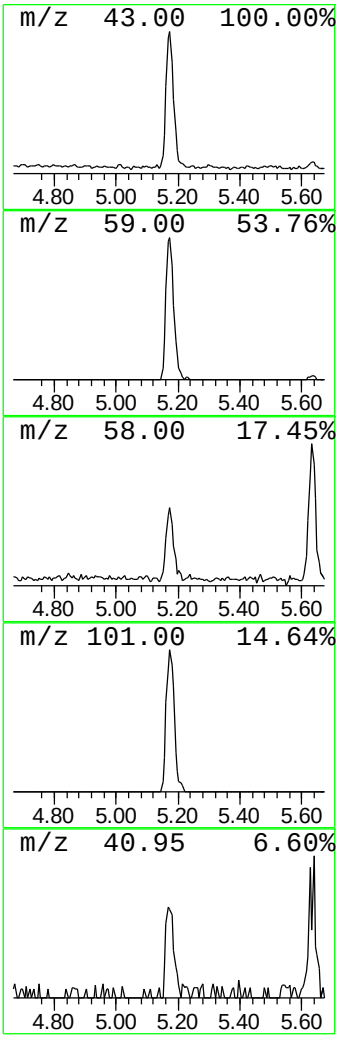
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 5.41 ng | 86093 | 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 | 56 |
| 2 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 36 |
| 3 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 9 |
| 5 | Propane, 2-ethoxy-2-methyl- | 102 | C6H14O | 000637-92-3 | 9 |



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ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
S-E

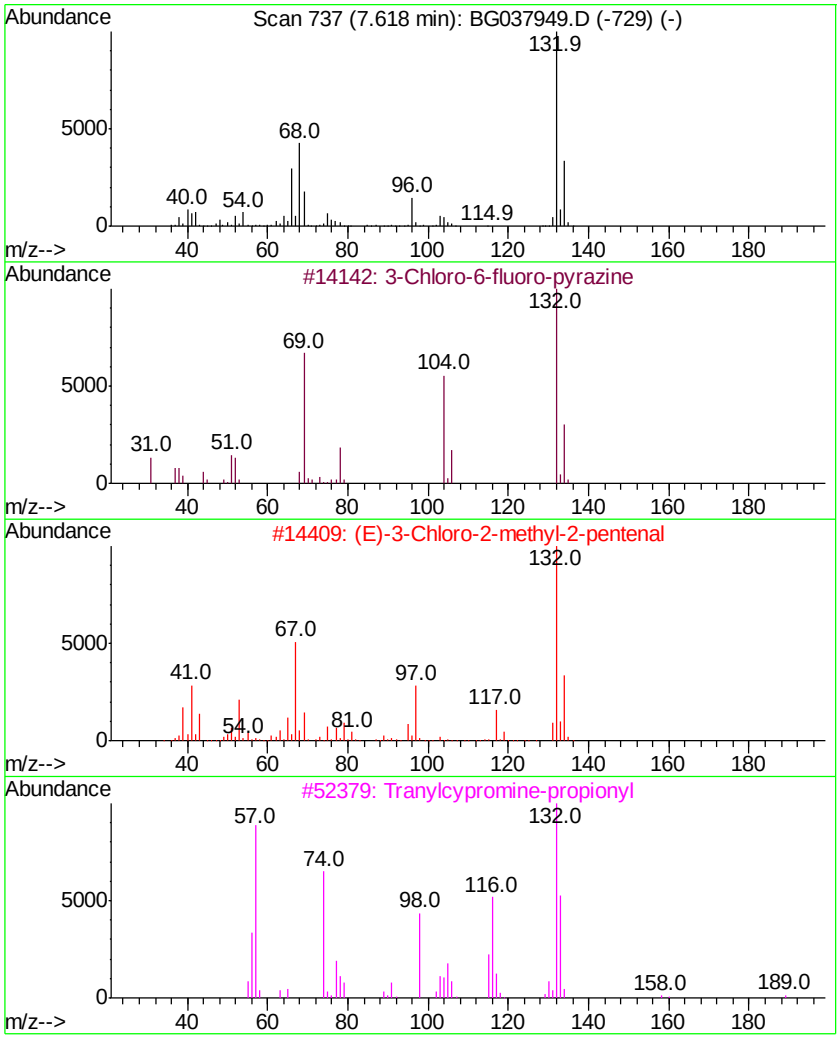
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

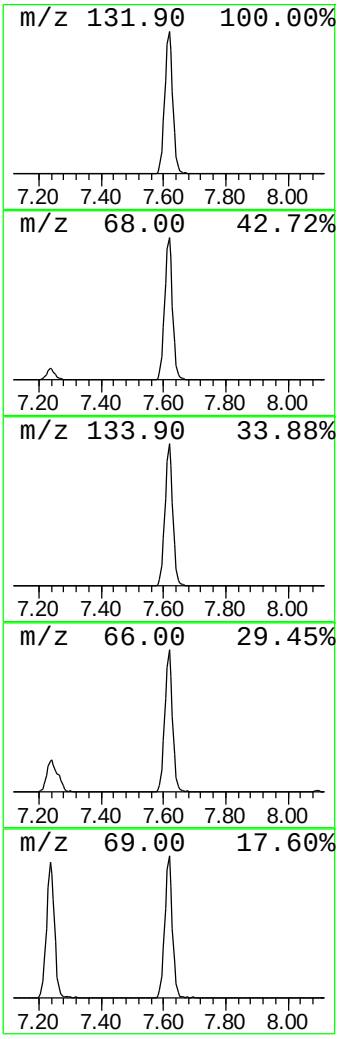
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 unknown7.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.62 | 116.89 ng | 1860100 | 1,4-Dichlorobenzene-d4 | 8.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



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Operator : JU/SJ
Sample : J5901-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
S-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
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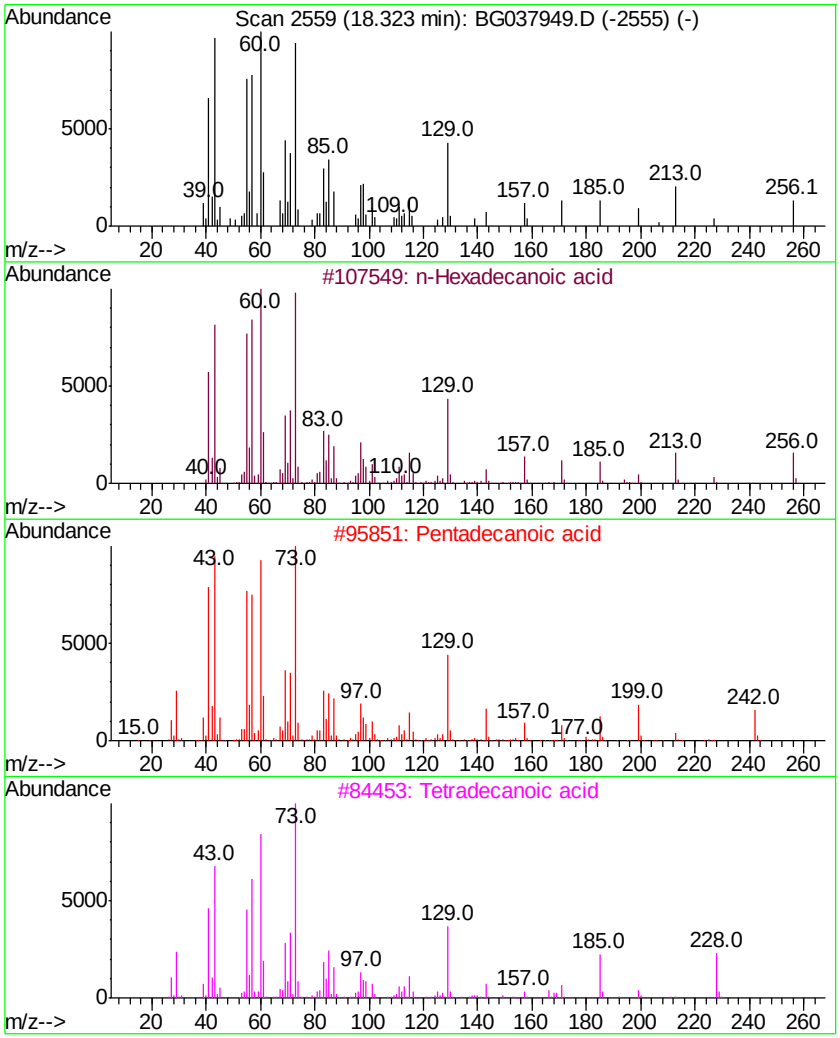
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

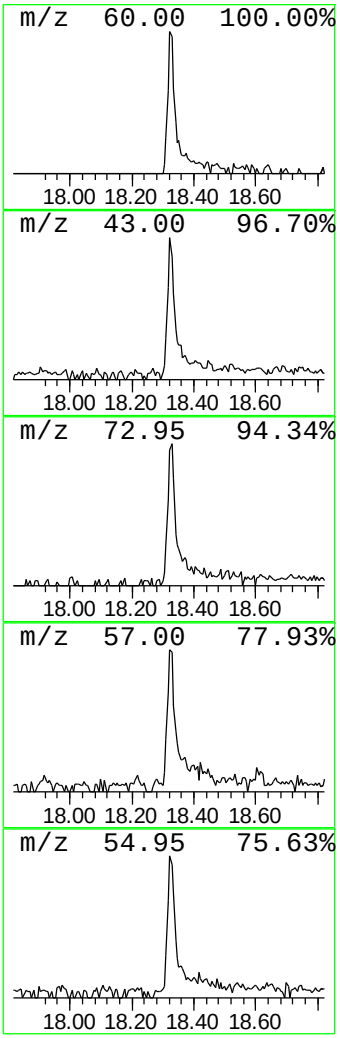
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.32 | 2.42 ng | 101299 | Phenanthrene-d10 | 17.47 |

| 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 | 68 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 49 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 43 |



Tentatively Identified Compound (LSC) summary

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BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name | RT | EstConc | Units | Response | Internal Standard # | RT | Resp | Conc |
|---|---|---|---|---|---|---|---|---|
| 2-Pentanone, 4-hy... | 5.17 | 5.4 | ng | 86093 | 1 | 8.09 | 318264 | 20.0 |
| unknown7.62 | 7.62 | 116.9 | ng | 1860100 | 1 | 8.09 | 318264 | 20.0 |
| n-Hexadecanoic acid | 18.32 | 2.4 | ng | 101299 | 4 | 17.47 | 838869 | 20.0 |