LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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 | 3.176 | 9 | 15 | 28 | rVB | 129906 | 257594 | 11.54% | 1.840% |
| 2 | 5.115 | 339 | 345 | 356 | rBV | 114008 | 186560 | 8.35% | 1.333% |
| 3 | 5.609 | 421 | 429 | 445 | rBV | 553258 | 969177 | 43.40% | 6.924% |
| 4 | 7.213 | 695 | 702 | 717 | rBV | 572488 | 1117317 | 50.03% | 7.983% |
| 5 | 7.559 | 753 | 761 | 772 | rBV | 612765 | 1108802 | 49.65% | 7.922% |
| 6 | 8.006 | 830 | 837 | 845 | rBV | 120098 | 211850 | 9.49% | 1.514% |
| 7 | 8.329 | 884 | 892 | 902 | rBV | 446580 | 808519 | 36.21% | 5.776% |
| 8 | 9.169 | 1027 | 1035 | 1047 | rBV | 323979 | 646860 | 28.97% | 4.621% |
| 9 | 10.814 | 1307 | 1315 | 1326 | rBV | 134014 | 269679 | 12.08% | 1.927% |
| 10 | 13.258 | 1724 | 1731 | 1746 | rBV | 903909 | 1442022 | 64.58% | 10.302% |
| 11 | 14.087 | 1865 | 1872 | 1884 | rBV | 77634 | 137376 | 6.15% | 0.981% |
| 12 | 14.539 | 1943 | 1949 | 1957 | rVB2 | 42299 | 75664 | 3.39% | 0.541% |
| 13 | 14.639 | 1959 | 1966 | 1976 | rBV | 240140 | 411221 | 18.41% | 2.938% |
| 14 | 15.021 | 2026 | 2031 | 2035 | rBV2 | 19368 | 28382 | 1.27% | 0.203% |
| 15 | 15.444 | 2098 | 2103 | 2109 | rBV | 18113 | 29130 | 1.30% | 0.208% |
| 16 | 16.132 | 2213 | 2220 | 2234 | rBV | 867397 | 1454694 | 65.14% | 10.393% |
| 17 | 16.678 | 2308 | 2313 | 2319 | rBV2 | 21923 | 32108 | 1.44% | 0.229% |
| 18 | 17.289 | 2412 | 2417 | 2422 | rBV5 | 13088 | 31211 | 1.40% | 0.223% |
| 19 | 17.383 | 2427 | 2433 | 2449 | rVV | 294461 | 513915 | 23.01% | 3.672% |
| 20 | 17.501 | 2449 | 2453 | 2459 | rVB3 | 31738 | 45634 | 2.04% | 0.326% |
| 21 | 17.565 | 2459 | 2464 | 2469 | rBV3 | 38488 | 54304 | 2.43% | 0.388% |
| 22 | 18.276 | 2581 | 2585 | 2593 | rBV2 | 52540 | 96733 | 4.33% | 0.691% |
| 23 | 19.992 | 2872 | 2877 | 2888 | rVB | 1663922 | 2233084 | 100.00% | 15.954% |
| 24 | 20.744 | 3001 | 3005 | 3009 | rBV | 242356 | 287901 | 12.89% | 2.057% |
| 25 | 21.531 | 3136 | 3139 | 3146 | rVB | 113041 | 156843 | 7.02% | 1.121% |
| 26 | 21.649 | 3155 | 3159 | 3177 | rVB | 340918 | 744340 | 33.33% | 5.318% |
| 27 | 24.851 | 3698 | 3704 | 3714 | rVB | 240327 | 646026 | 28.93% | 4.615% |

Sum of corrected areas: 13996946

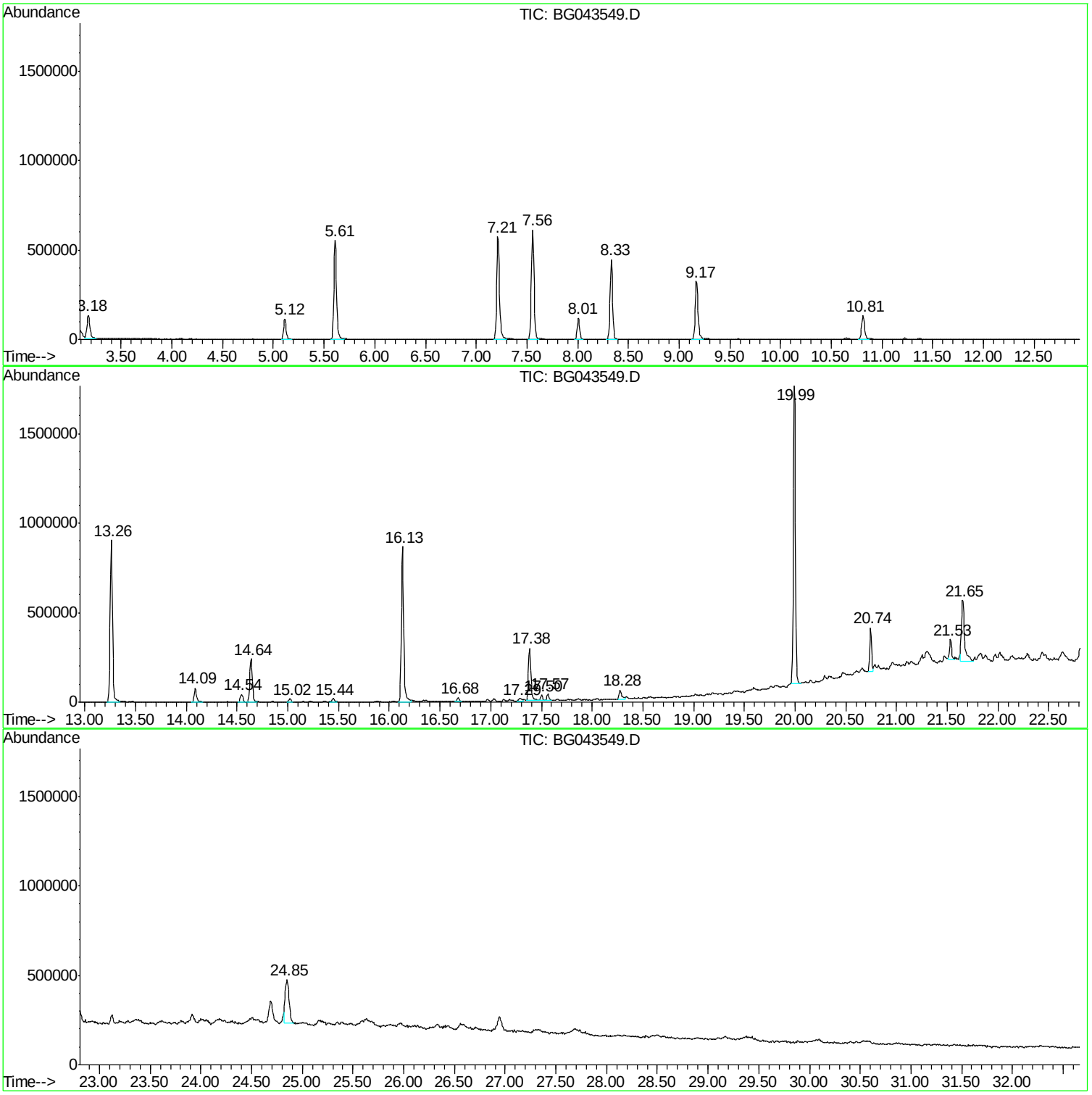
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

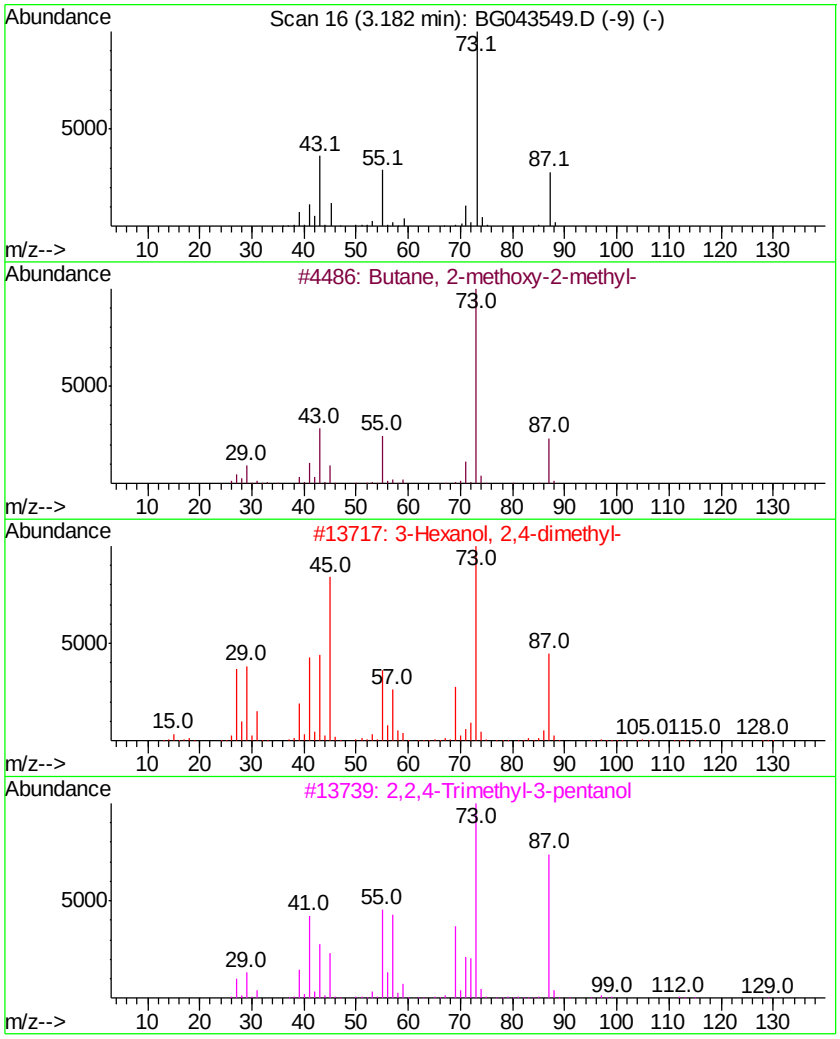
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

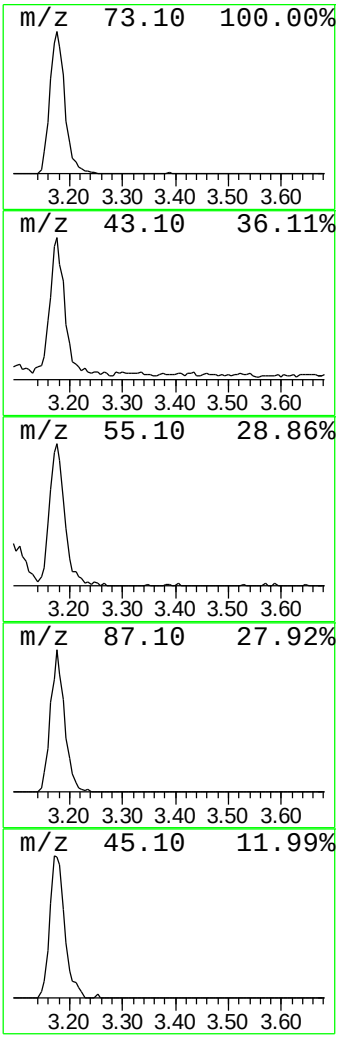
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.18 | 24.32 ng | 257594 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 56 |
| 2 | 3-Hexanol, 2,4-dimethyl- | 130 | C8H18O | 013432-25-2 | 36 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 36 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

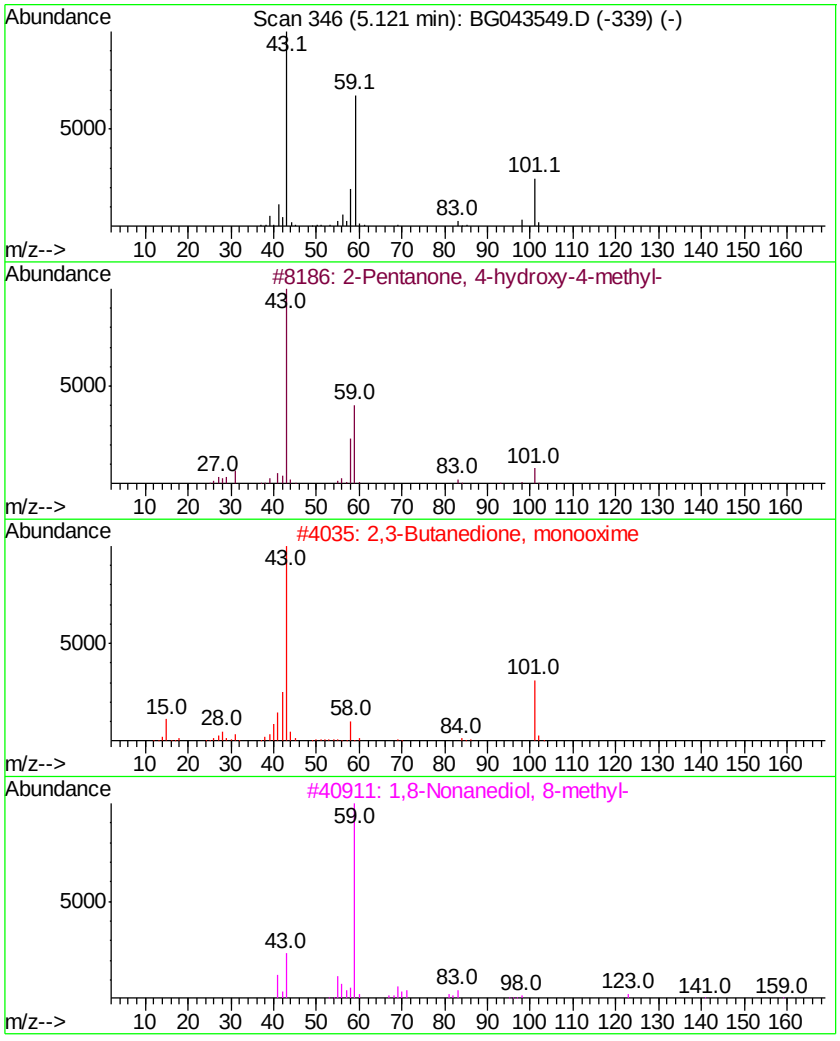
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

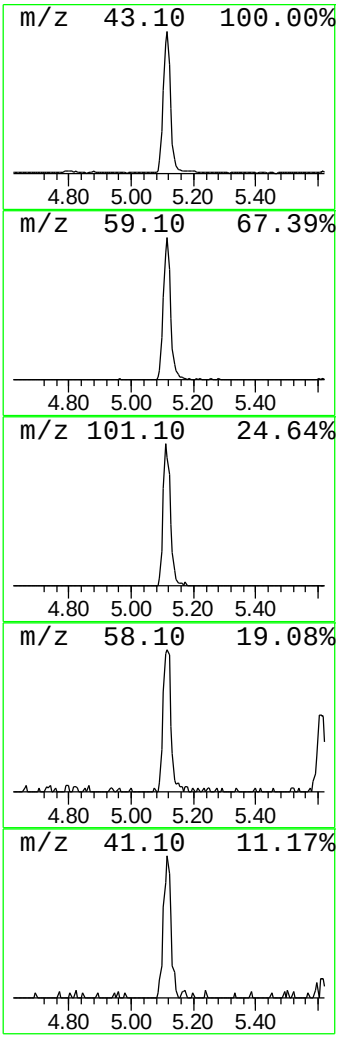
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 17.61 ng | 186560 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 38 |
| 3 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 25 |
| 4 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 23 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

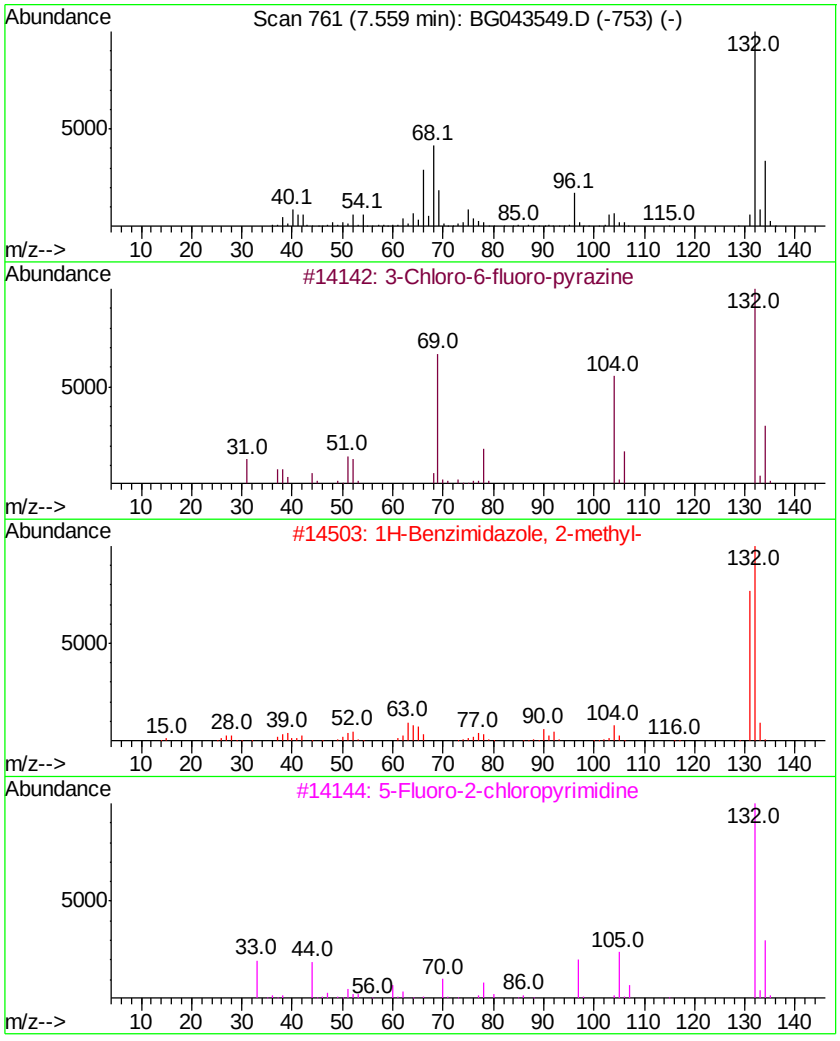
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

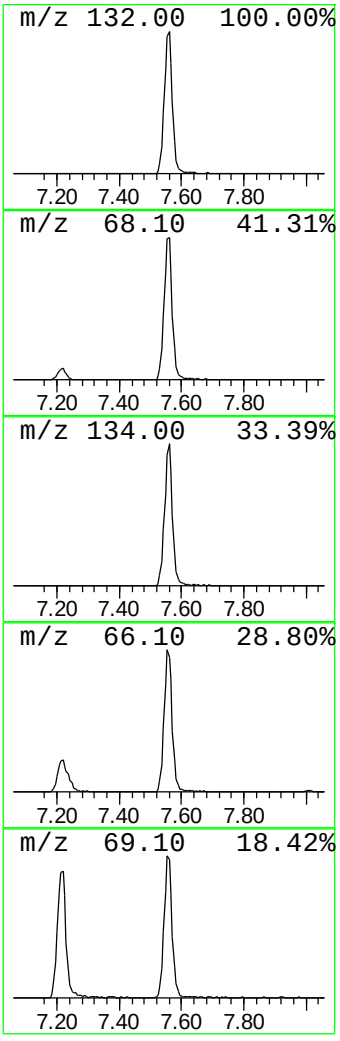
**********

Peak Number 3 unknown7.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.56 | 104.68 ng | 1108800 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

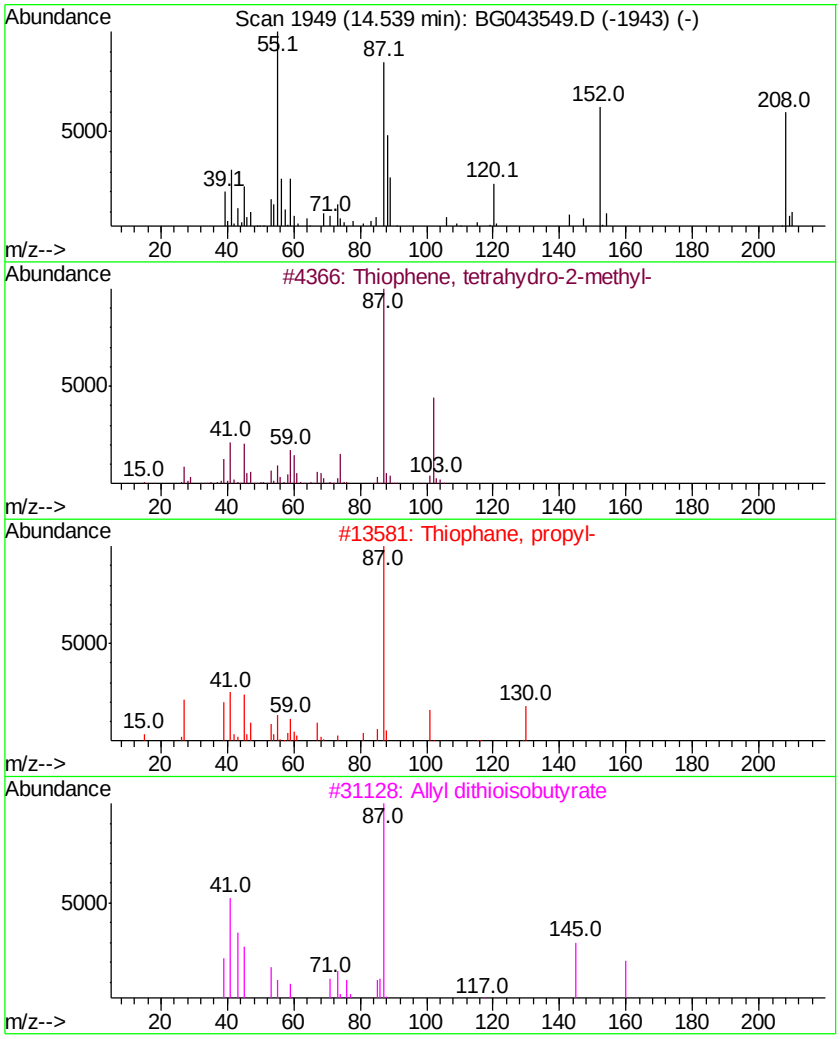
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

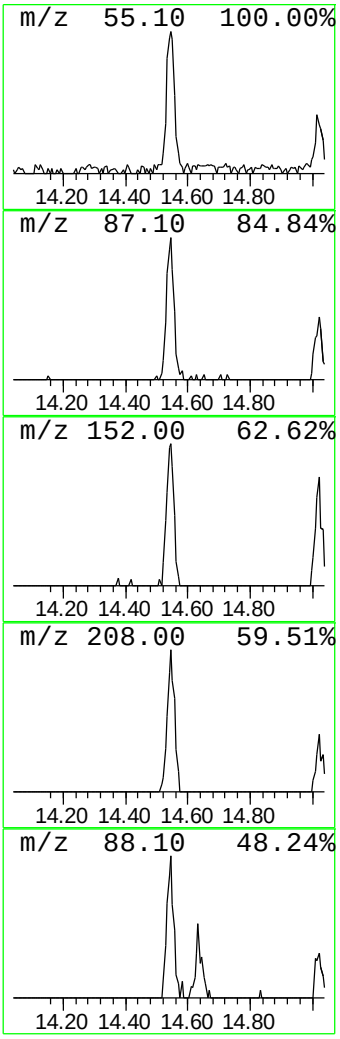
**********

Peak Number 5 unknown14.54 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.54 | 3.68 ng | 75664 | Acenaphthene-d10 | 14.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene, tetrahydro-2-methyl- | 102 | C5H10S | 001795-09-1 | 27 |
| 2 | Thiophane, propyl- | 130 | C7H14S | 001551-34-4 | 22 |
| 3 | Allyl dithioisobutyrate | 160 | C7H12S2 | 063881-54-9 | 14 |
| 4 | .alpha.-D-Xylofuranoside, methyl... | 178 | C7H14O5 | 032469-86-6 | 14 |
| 5 | 2-O-Methyl-d-xylose | 164 | C6H12O5 | 1000130-01-3 | 14 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

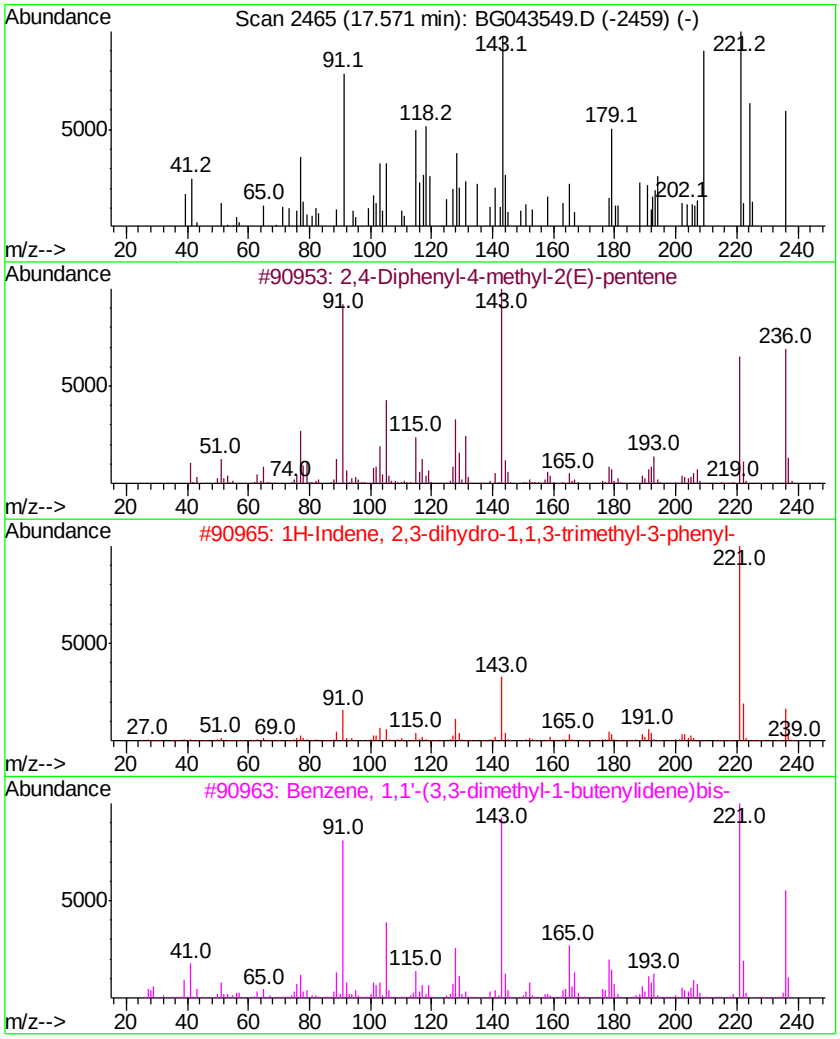
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

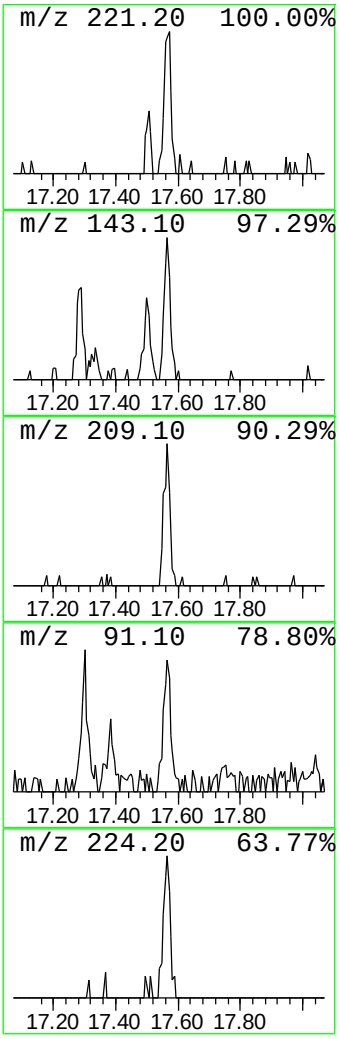
**********

Peak Number 6 unknown17.57 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.57 | 2.11 ng | 54304 | Phenanthrene-d10 | 17.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4-Diphenyl-4-methyl-2(E)-pentene | 236 | C18H20 | 022768-22-5 | 38 |
| 2 | 1H-Indene, 2,3-dihydro-1,1,3-tri... | 236 | C18H20 | 003910-35-8 | 38 |
| 3 | Benzene, 1,1'-(3,3-dimethyl-1-bu... | 236 | C18H20 | 023586-64-3 | 35 |
| 4 | Benzoic acid, 4-[(trimethylsilyl... | 224 | C11H16O3Si | 027739-17-9 | 25 |
| 5 | 1,8-Naphthyridine, 1,2,3,4,4a,5,... | 224 | C13H24N2O | 069340-71-2 | 20 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

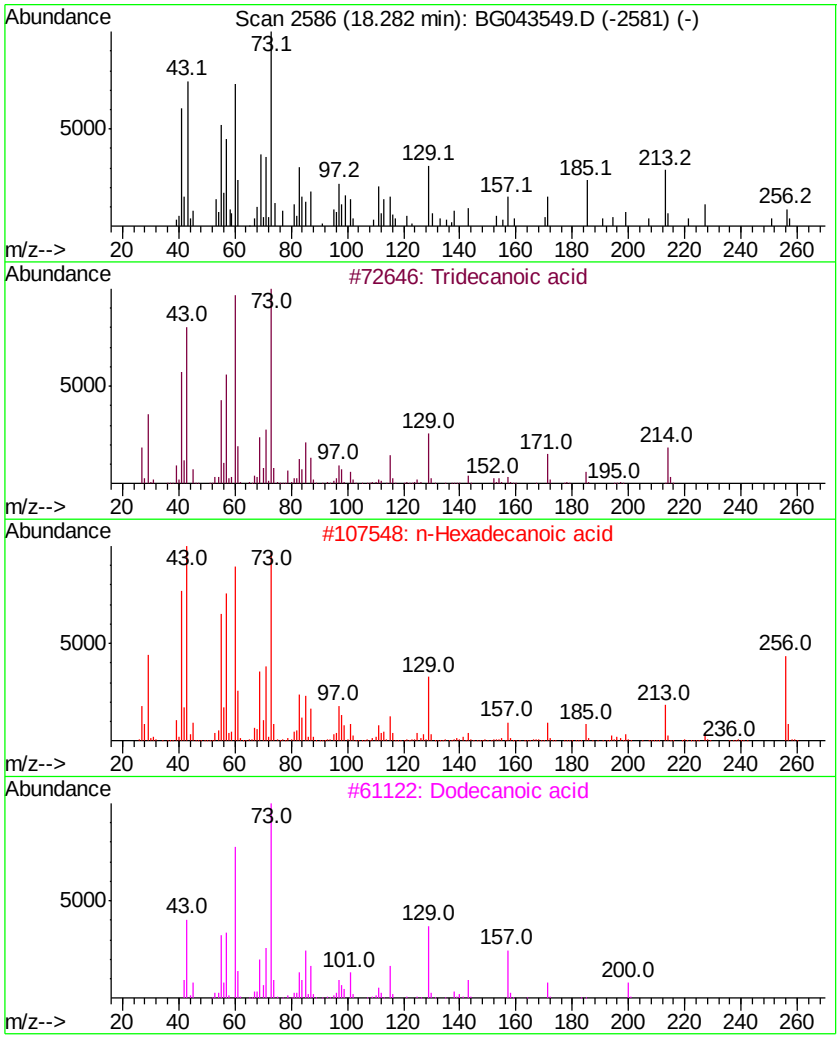
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

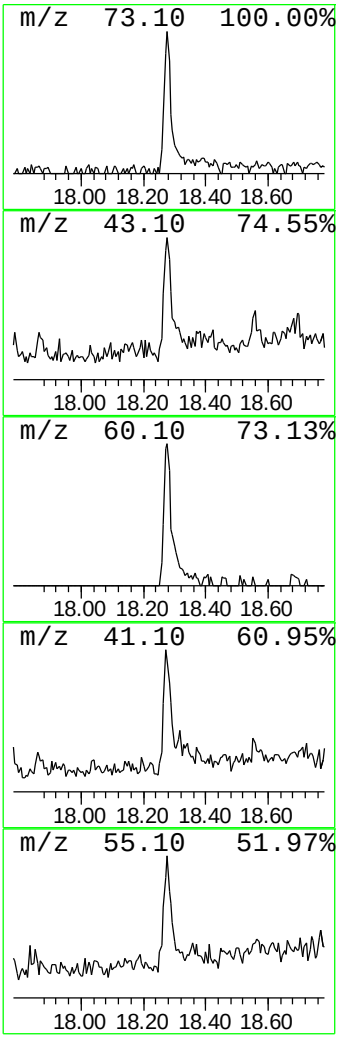
**********

Peak Number 7 Tridecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.28 | 3.76 ng | 96733 | Phenanthrene-d10 | 17.38 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 86 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 81 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 58 |



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Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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

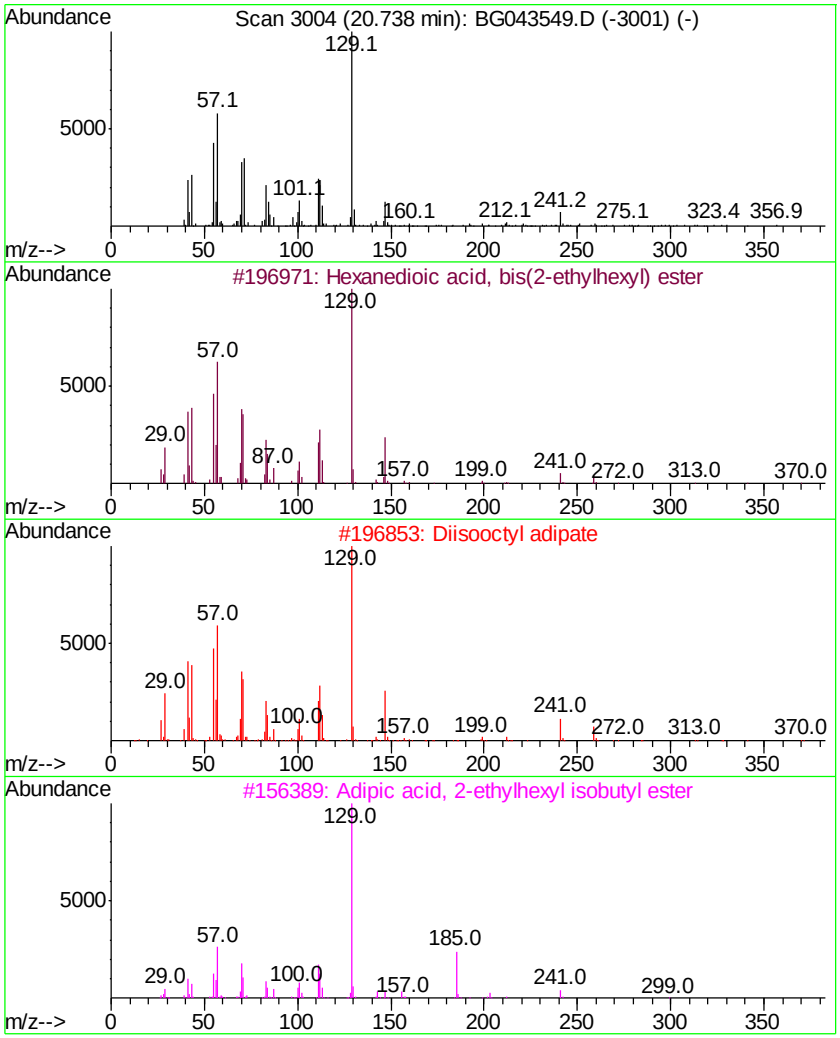
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

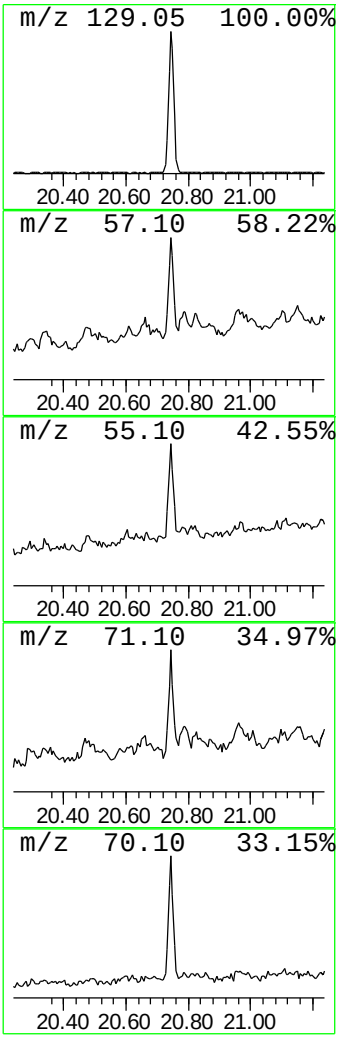
**********

Peak Number 8 Hexanedioic acid, bis(2-eth... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.74 | 7.74 ng | 287901 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1 | 87 |
| 2 | Diisooctyl adipate | 370 | C22H42O4 | 001330-86-5 | 86 |
| 3 | Adipic acid, 2-ethylhexyl isobut... | 314 | C18H34O4 | 1000324-48-0 | 47 |
| 4 | Hexanedioic acid, dioctyl ester | 370 | C22H42O4 | 000123-79-5 | 46 |
| 5 | Adipic acid, cyclohexyl octyl ester | 340 | C20H36O4 | 1000324-26-3 | 43 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110719\
Data File : BG043549.D
Acq On : 7 Nov 2019 21:26
Operator : JU
Sample : K5723-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 10-A

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... | 3.18 | 24.3 | ng | 257594 | 1 | 8.01 | 211850 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 17.6 | ng | 186560 | 1 | 8.01 | 211850 | 20.0 |
| unknown7.56 | 7.56 | 104.7 | ng | 1108800 | 1 | 8.01 | 211850 | 20.0 |
| unknown14.54 | 14.54 | 3.7 | ng | 75664 | 3 | 14.64 | 411221 | 20.0 |
| unknown17.57 | 17.57 | 2.1 | ng | 54304 | 4 | 17.38 | 513915 | 20.0 |
| Tridecanoic acid | 18.28 | 3.8 | ng | 96733 | 4 | 17.38 | 513915 | 20.0 |
| Hexanedioic acid,... | 20.74 | 7.7 | ng | 287901 | 5 | 21.65 | 744340 | 20.0 |