# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110519\
Data File : BG043505.D
Acq On : 5 Nov 2019 13:20
Operator : JU
Sample : PB124540TB
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

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 | 3.205 | 12 | 20 | 32 | rVB | 579326 | 1121133 | 32.20% | 7.128% |
| 2 | 3.487 | 63 | 68 | 76 | rVB | 99267 | 123616 | 3.55% | 0.786% |
| 3 | 4.627 | 258 | 262 | 268 | rBV | 28445 | 39398 | 1.13% | 0.250% |
| 4 | 5.085 | 334 | 340 | 342 | rBV | 36337 | 52361 | 1.50% | 0.333% |
| 5 | 5.120 | 342 | 346 | 354 | rVB | 106060 | 165337 | 4.75% | 1.051% |
| 6 | 5.602 | 421 | 428 | 441 | rBV | 519518 | 899197 | 25.82% | 5.717% |
| 7 | 7.200 | 692 | 700 | 712 | rBV | 477612 | 928874 | 26.67% | 5.906% |
| 8 | 7.553 | 752 | 760 | 771 | rBV | 577872 | 1024918 | 29.43% | 6.517% |
| 9 | 8.011 | 830 | 838 | 847 | rBV | 123346 | 215902 | 6.20% | 1.373% |
| 10 | 8.334 | 886 | 893 | 905 | rBV | 404163 | 732172 | 21.03% | 4.655% |
| 11 | 9.175 | 1026 | 1036 | 1050 | rBV | 285850 | 585987 | 16.83% | 3.726% |
| 12 | 10.820 | 1308 | 1316 | 1325 | rBV | 119374 | 253225 | 7.27% | 1.610% |
| 13 | 13.264 | 1725 | 1732 | 1745 | rBV | 843221 | 1434445 | 41.19% | 9.120% |
| 14 | 14.098 | 1869 | 1874 | 1887 | rVB2 | 18936 | 44071 | 1.27% | 0.280% |
| 15 | 14.639 | 1958 | 1966 | 1979 | rBV | 233038 | 401652 | 11.53% | 2.554% |
| 16 | 16.131 | 2214 | 2220 | 2240 | rBV | 777701 | 1468040 | 42.16% | 9.334% |
| 17 | 17.388 | 2428 | 2434 | 2445 | rBV | 310518 | 548544 | 15.75% | 3.488% |
| 18 | 19.997 | 2872 | 2878 | 2896 | rBV | 2491278 | 3482194 | 100.00% | 22.140% |
| 19 | 21.302 | 3096 | 3100 | 3108 | rBV6 | 44739 | 112792 | 3.24% | 0.717% |
| 20 | 21.378 | 3109 | 3113 | 3124 | rVB2 | 34567 | 77978 | 2.24% | 0.496% |
| 21 | 21.654 | 3153 | 3160 | 3174 | rBV | 424232 | 803966 | 23.09% | 5.112% |
| 22 | 22.441 | 3290 | 3294 | 3299 | rBV2 | 33683 | 47440 | 1.36% | 0.302% |
| 23 | 23.123 | 3405 | 3410 | 3417 | rBV2 | 38769 | 70879 | 2.04% | 0.451% |
| 24 | 23.916 | 3541 | 3545 | 3555 | rVB3 | 37742 | 81691 | 2.35% | 0.519% |
| 25 | 24.856 | 3694 | 3705 | 3717 | rBV2 | 303836 | 896182 | 25.74% | 5.698% |
| 26 | 25.972 | 3888 | 3895 | 3904 | rVB6 | 27808 | 78809 | 2.26% | 0.501% |
| 27 | 27.306 | 4115 | 4122 | 4129 | rBV6 | 12003 | 37044 | 1.06% | 0.236% |

Sum of corrected areas: 15727847

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Misc :
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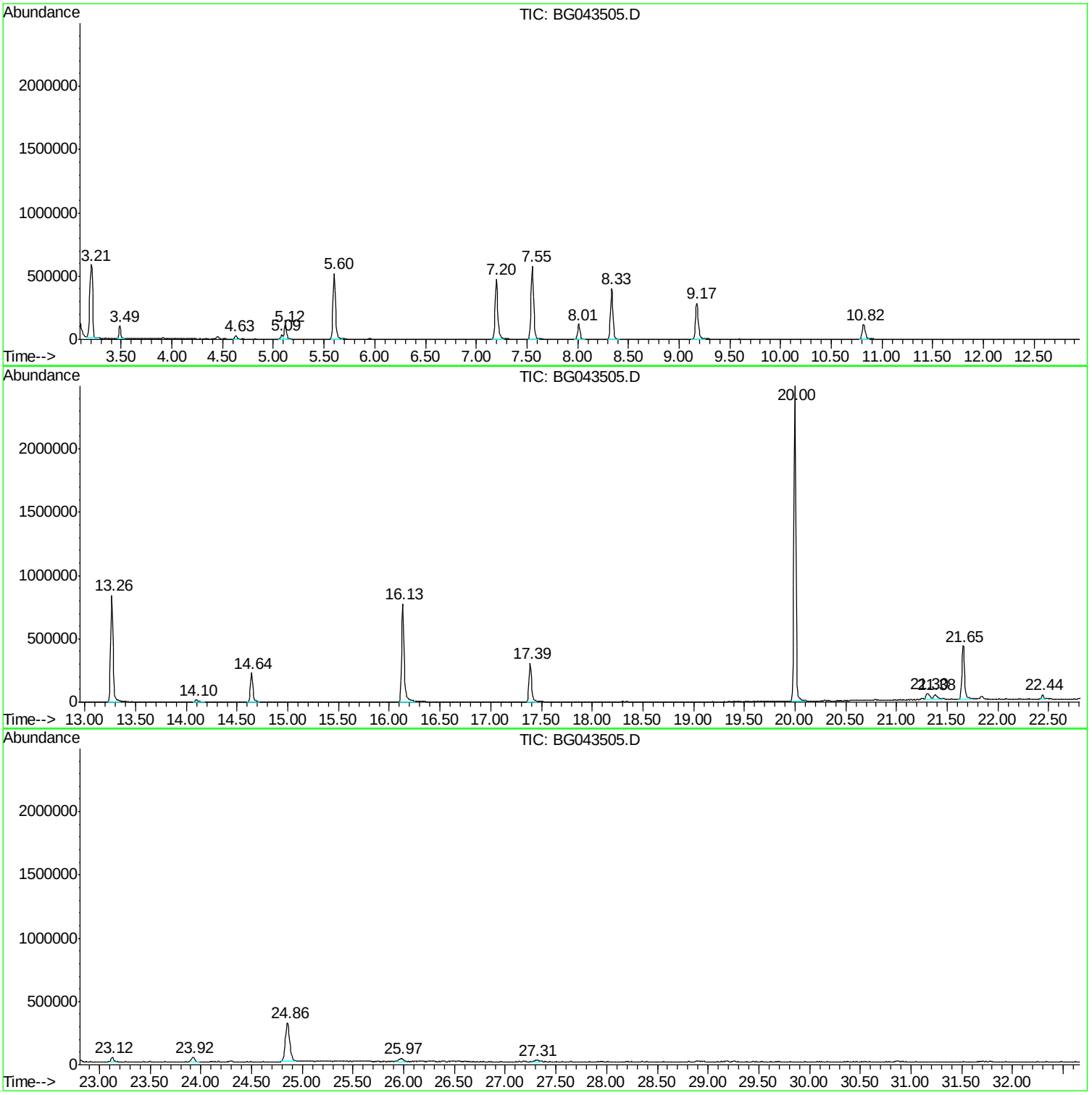
**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

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

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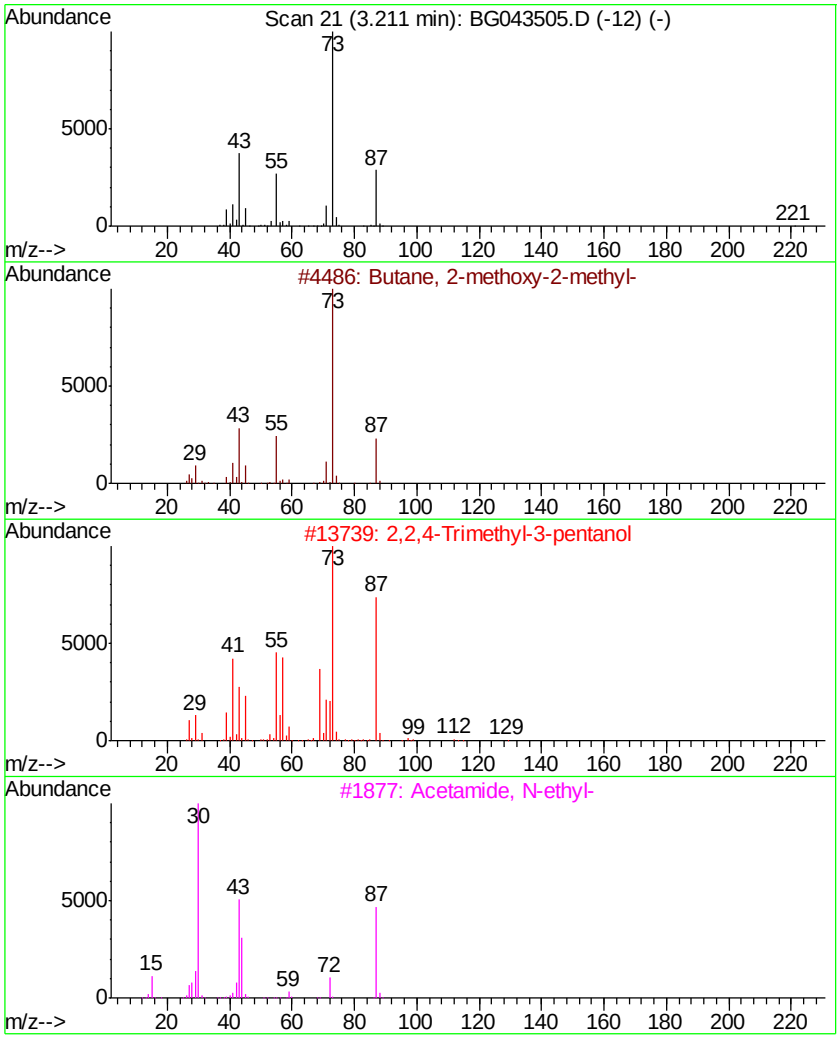
TIC Integration Parameters: LSCINT.P

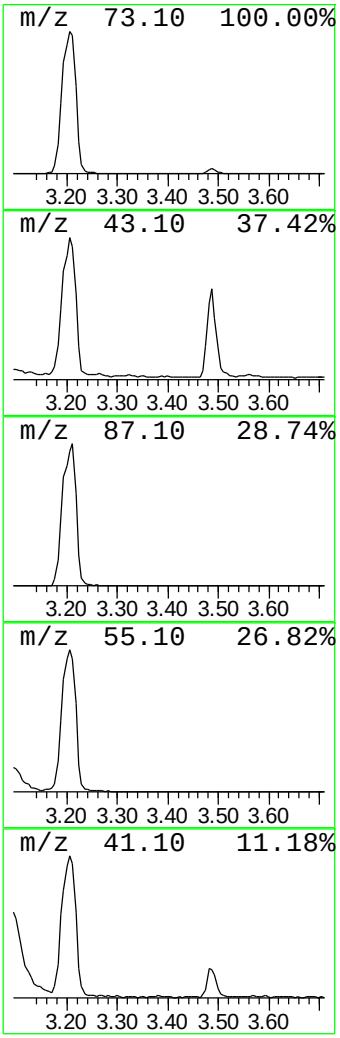
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.21 | 103.86 ng | 1121130 | 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 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



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ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

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

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TIC Integration Parameters: LSCINT.P

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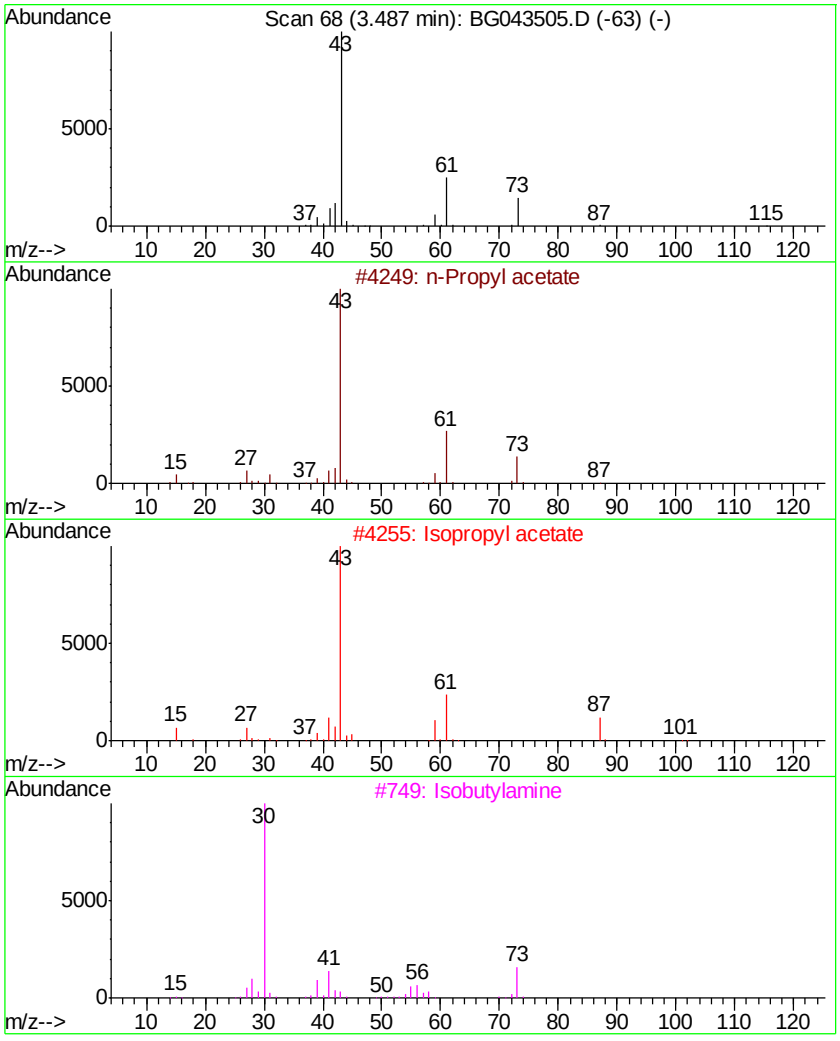
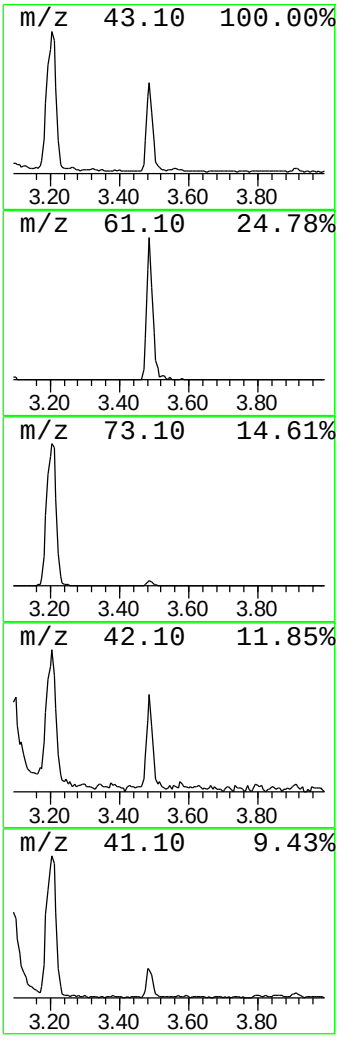
Peak Number 2 n-Propyl acetate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.49 | 11.45 ng | 123616 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Propyl acetate | 102 | C5H10O2 | 000109-60-4 | 78 |
| 2 | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 36 |
| 3 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |
| 4 | 1-Pentanol, 5-chloro-, acetate | 164 | C7H13ClO2 | 020395-28-2 | 9 |
| 5 | 1-Butanamine | 73 | C4H11N | 000109-73-9 | 5 |



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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

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

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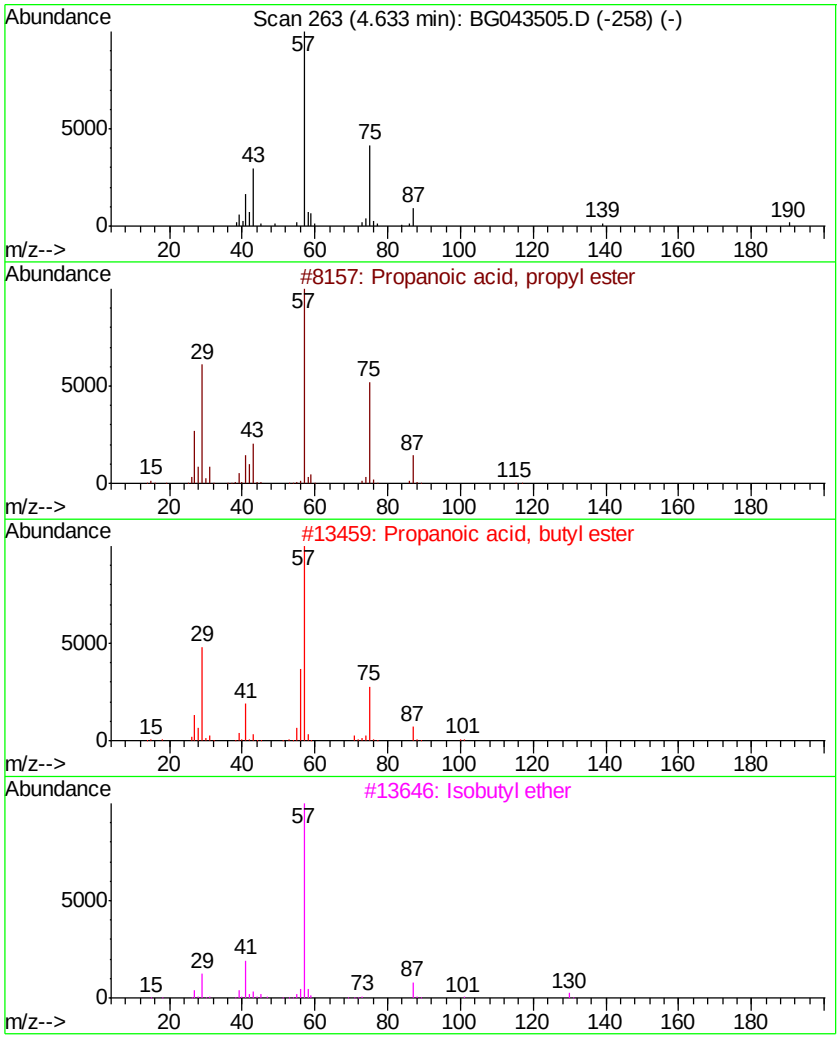
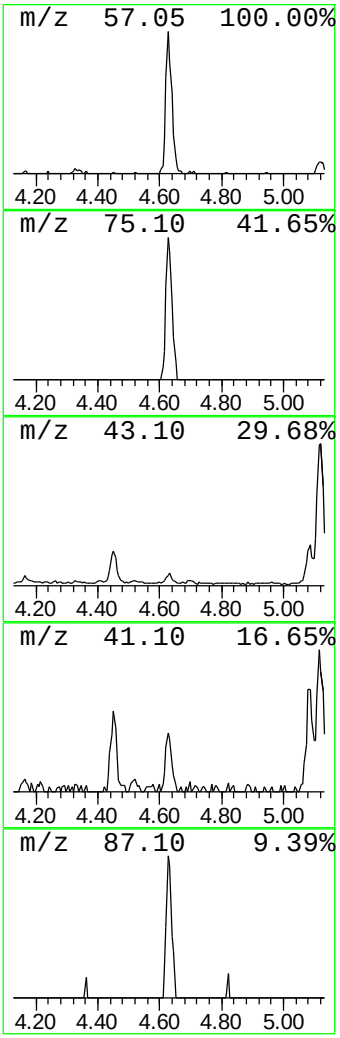
Peak Number 3 Propanoic acid, propyl ester Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.63 | 3.65 ng | 39398 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 78 |
| 2 | Propanoic acid, butyl ester | 130 | C7H14O2 | 000590-01-2 | 38 |
| 3 | Isobutyl ether | 130 | C8H18O | 000628-55-7 | 9 |
| 4 | Azetidine | 57 | C3H7N | 000503-29-7 | 5 |
| 5 | 1-Butanamine, 3-methyl- | 87 | C5H13N | 000107-85-7 | 4 |



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ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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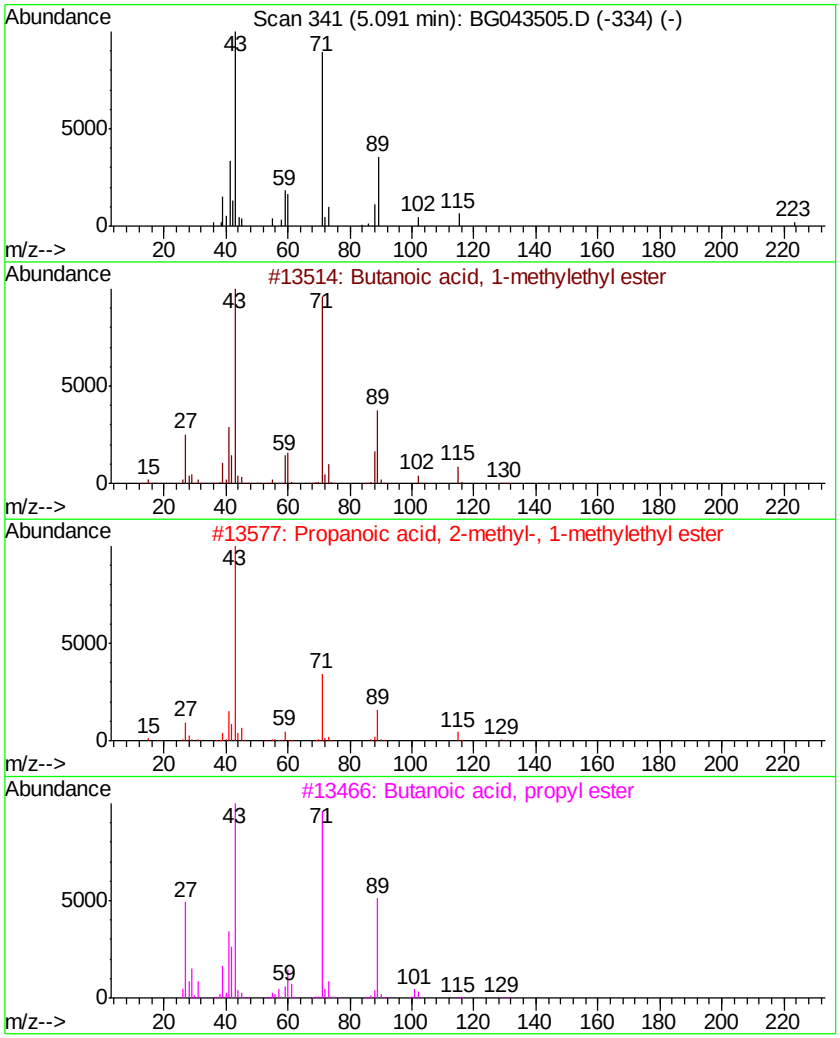
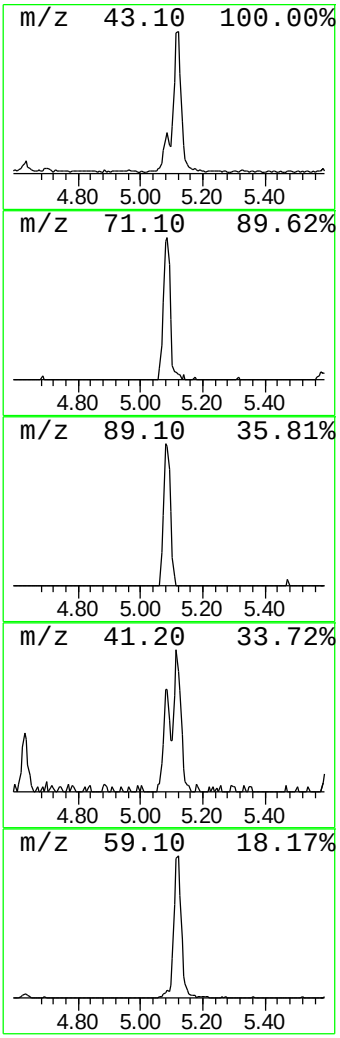
**********

Peak Number 4 Butanoic acid, 1-methylethy... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.09 | 4.85 ng | 52361 | 1,4-Dichlorobenzene-d4 | 8.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, 1-methylethyl ester | 130 | C7H14O2 | 000638-11-9 | 80 |
| 2 | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 59 |
| 3 | Butanoic acid, propyl ester | 130 | C7H14O2 | 000105-66-8 | 53 |
| 4 | Butanoic acid, butyl ester | 144 | C8H16O2 | 000109-21-7 | 42 |
| 5 | 2-Oxovaleric acid, methyl ester | 130 | C6H10O3 | 1000353-27-4 | 37 |



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ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB124540TB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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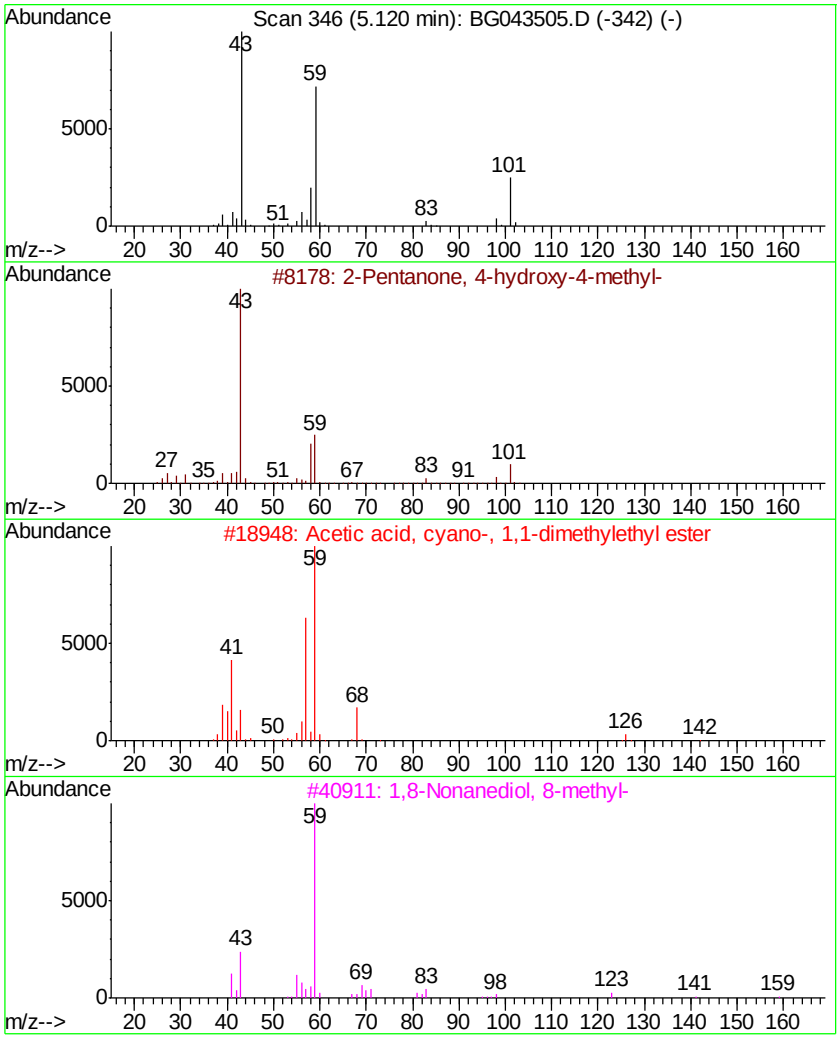
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

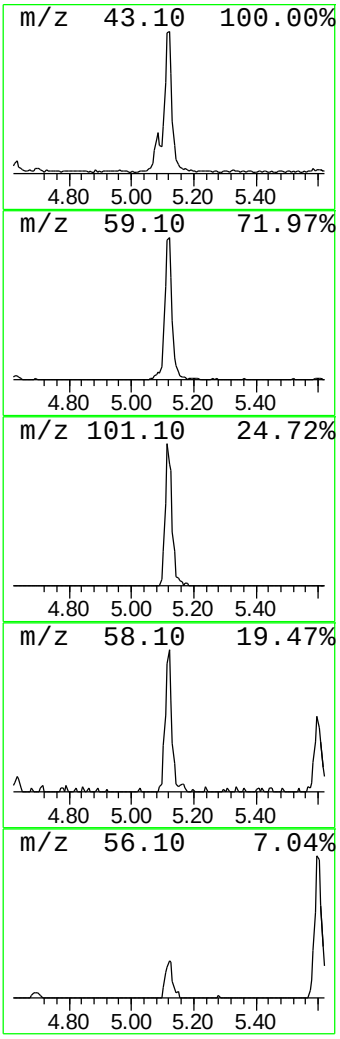
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 15.32 ng | 165337 | 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 | 53 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 17 |
| 4 | 2-Nonanone | 142 | C9H18O | 000821-55-6 | 17 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 10 |



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**Instrument :** BNA_G
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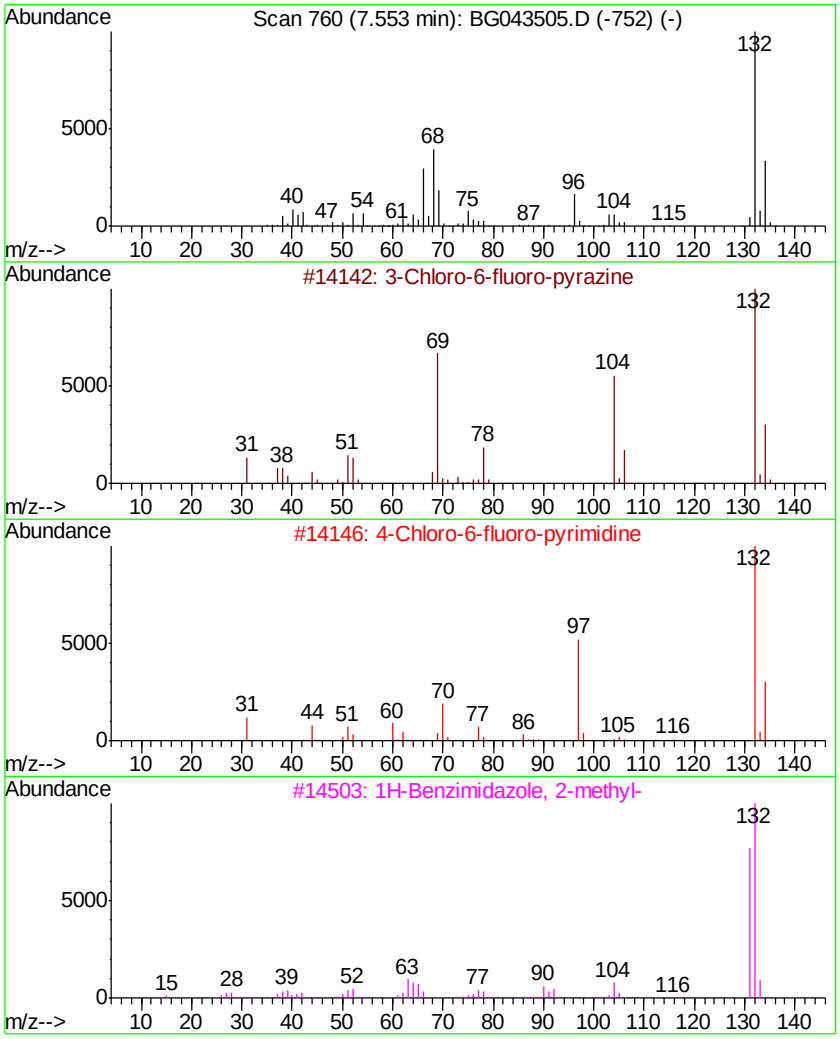
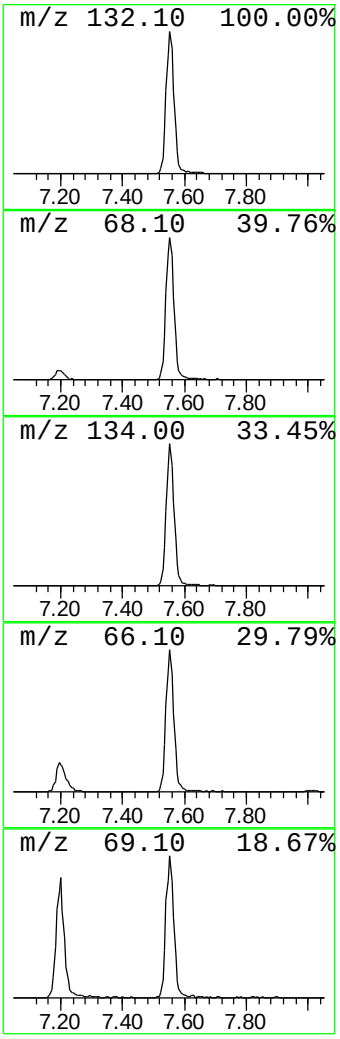
**********

Peak Number 6 unknown7.55 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.55 | 94.94 ng | 1024920 | 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 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 5 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |



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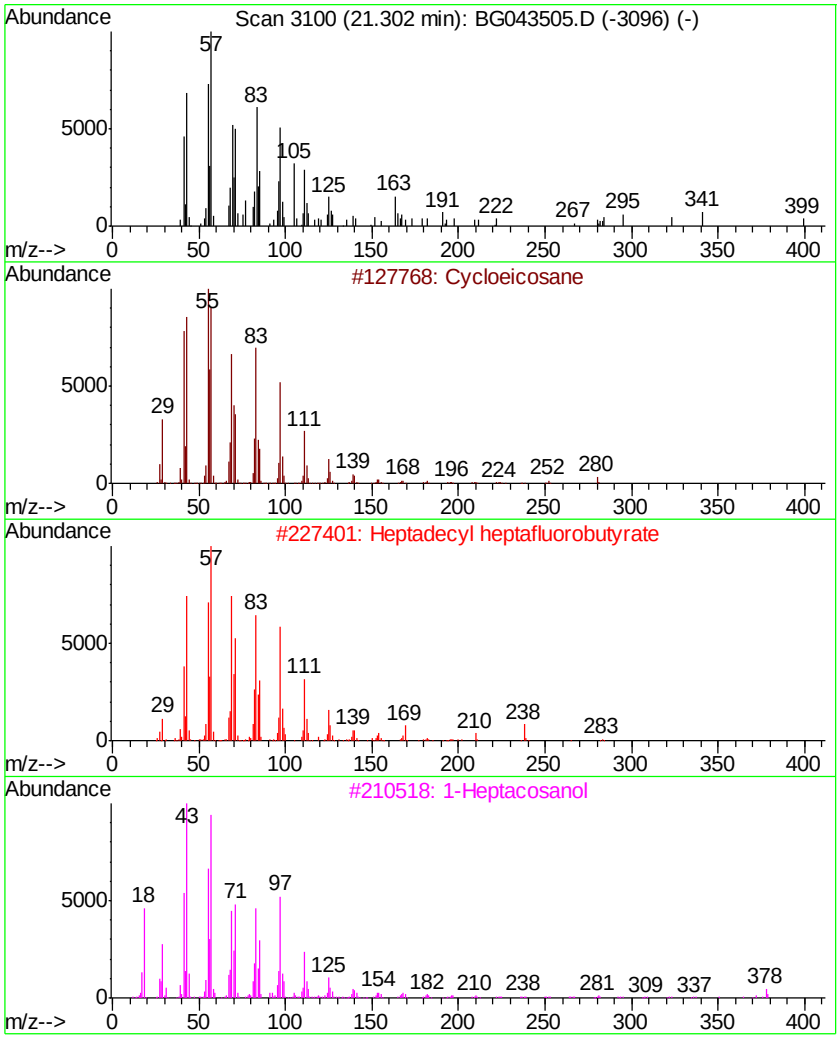
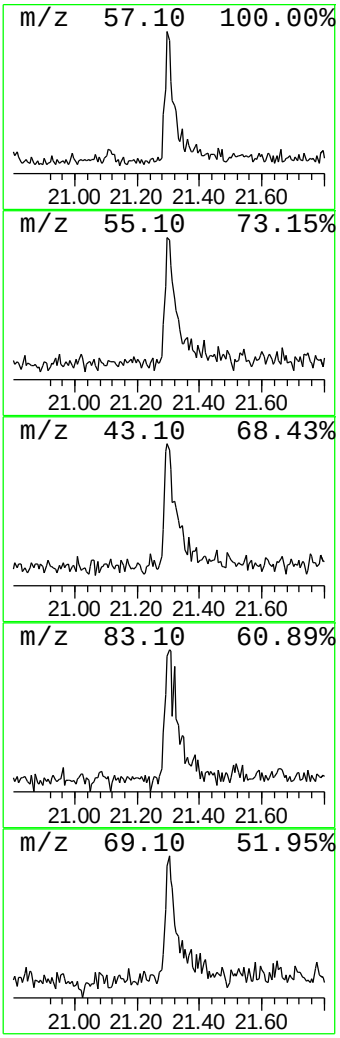
**********

Peak Number 8 Cycloeicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.30 | 2.81 ng | 112792 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 93 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 87 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 87 |
| 4 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 87 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 87 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 3.21 | 103.9 | ng | 1121130 | 1 | 8.01 | 215902 | 20.0 |
| n-Propyl acetate | 3.49 | 11.4 | ng | 123616 | 1 | 8.01 | 215902 | 20.0 |
| Propanoic acid, p... | 4.63 | 3.6 | ng | 39398 | 1 | 8.01 | 215902 | 20.0 |
| Butanoic acid, 1-... | 5.09 | 4.8 | ng | 52361 | 1 | 8.01 | 215902 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 15.3 | ng | 165337 | 1 | 8.01 | 215902 | 20.0 |
| unknown7.55 | 7.55 | 94.9 | ng | 1024920 | 1 | 8.01 | 215902 | 20.0 |
| Cycloeicosane | 21.30 | 2.8 | ng | 112792 | 5 | 21.65 | 803966 | 20.0 |