LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045031.D
Acq On : 30 Sep 2021 06:59
Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Title : SW846 8260

Signal : TIC: VU045031.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.629 | 390 | 401 | 420 | rBV | 33578 | 58187 | 1.68% | 0.365% |
| 2 | 3.047 | 519 | 531 | 546 | rVB | 22069 | 41582 | 1.20% | 0.261% |
| 3 | 5.292 | 1213 | 1229 | 1242 | rBV | 173316 | 367245 | 10.59% | 2.306% |
| 4 | 5.375 | 1242 | 1255 | 1275 | rVB | 306393 | 627243 | 18.09% | 3.938% |
| 5 | 5.703 | 1341 | 1357 | 1376 | rBV2 | 213997 | 434778 | 12.54% | 2.730% |
| 6 | 5.915 | 1410 | 1423 | 1442 | rBV2 | 20432 | 41557 | 1.20% | 0.261% |
| 7 | 6.253 | 1515 | 1528 | 1578 | rVB | 475770 | 963952 | 27.80% | 6.052% |
| 8 | 6.931 | 1719 | 1739 | 1755 | rVB2 | 21095 | 60332 | 1.74% | 0.379% |
| 9 | 7.044 | 1759 | 1774 | 1806 | rBV | 1333360 | 2304150 | 66.46% | 14.467% |
| 10 | 7.742 | 1977 | 1991 | 2002 | rBV | 224327 | 372005 | 10.73% | 2.336% |
| 11 | 7.902 | 2022 | 2041 | 2056 | rBV | 735161 | 1262004 | 36.40% | 7.924% |
| 12 | 8.468 | 2205 | 2217 | 2233 | rBV | 58734 | 95630 | 2.76% | 0.600% |
| 13 | 8.578 | 2233 | 2251 | 2262 | rVV | 145789 | 245213 | 7.07% | 1.540% |
| 14 | 8.732 | 2281 | 2299 | 2317 | rVV | 2265027 | 3466942 | 100.00% | 21.768% |
| 15 | 8.838 | 2318 | 2332 | 2353 | rVB | 179105 | 304466 | 8.78% | 1.912% |
| 16 | 9.214 | 2432 | 2449 | 2484 | rBV | 1410115 | 2176136 | 62.77% | 13.663% |
| 17 | 9.420 | 2502 | 2513 | 2537 | rVB | 696046 | 1132756 | 32.67% | 7.112% |
| 18 | 10.076 | 2707 | 2717 | 2739 | rBV | 35142 | 55442 | 1.60% | 0.348% |
| 19 | 10.635 | 2878 | 2891 | 2915 | rBV | 545152 | 856293 | 24.70% | 5.376% |
| 20 | 11.816 | 3244 | 3258 | 3275 | rBV | 669176 | 1061158 | 30.61% | 6.663% |

Sum of corrected areas: 15927071

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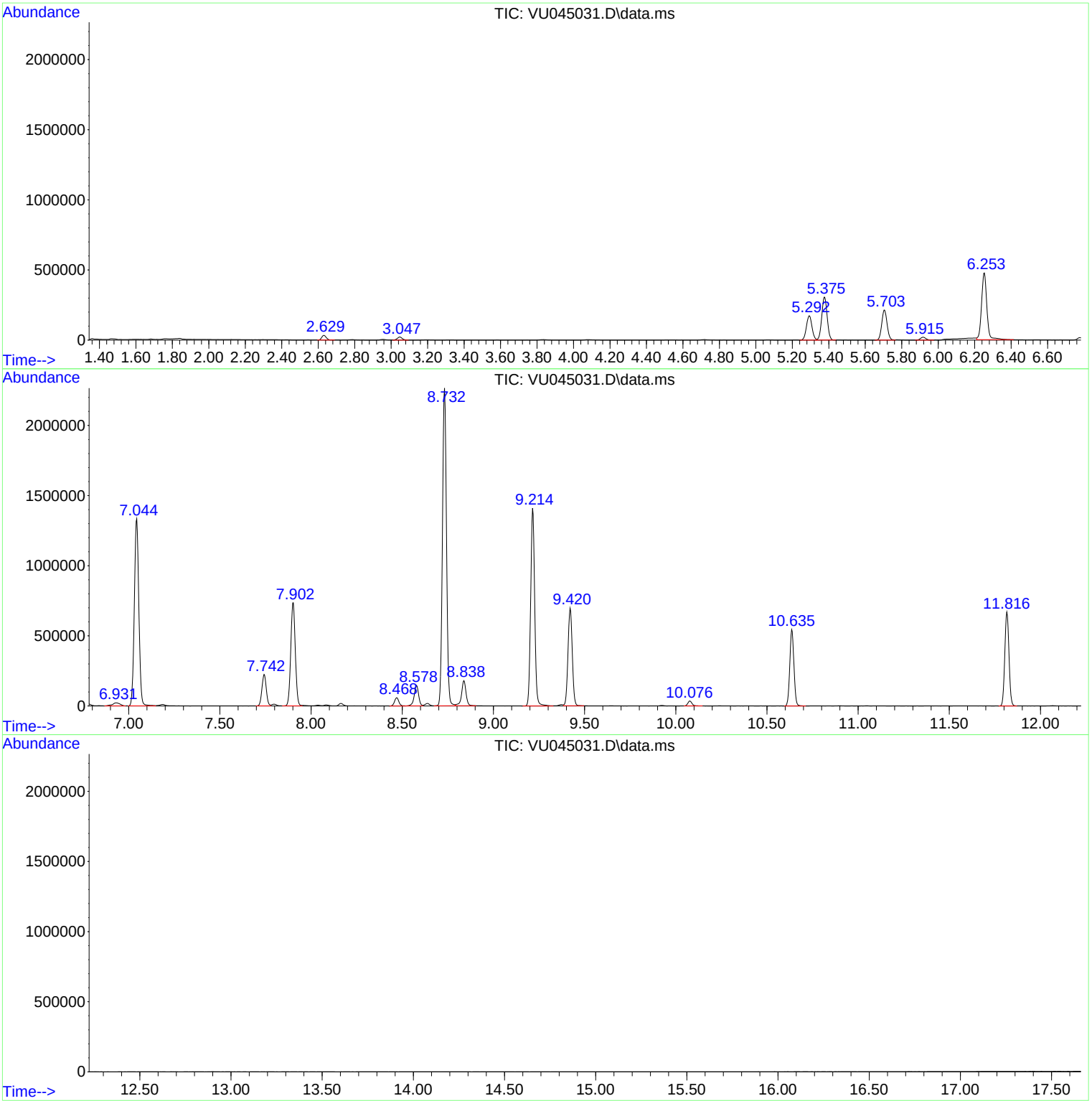
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
RP-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045031.D
Acq On : 30 Sep 2021 06:59
Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

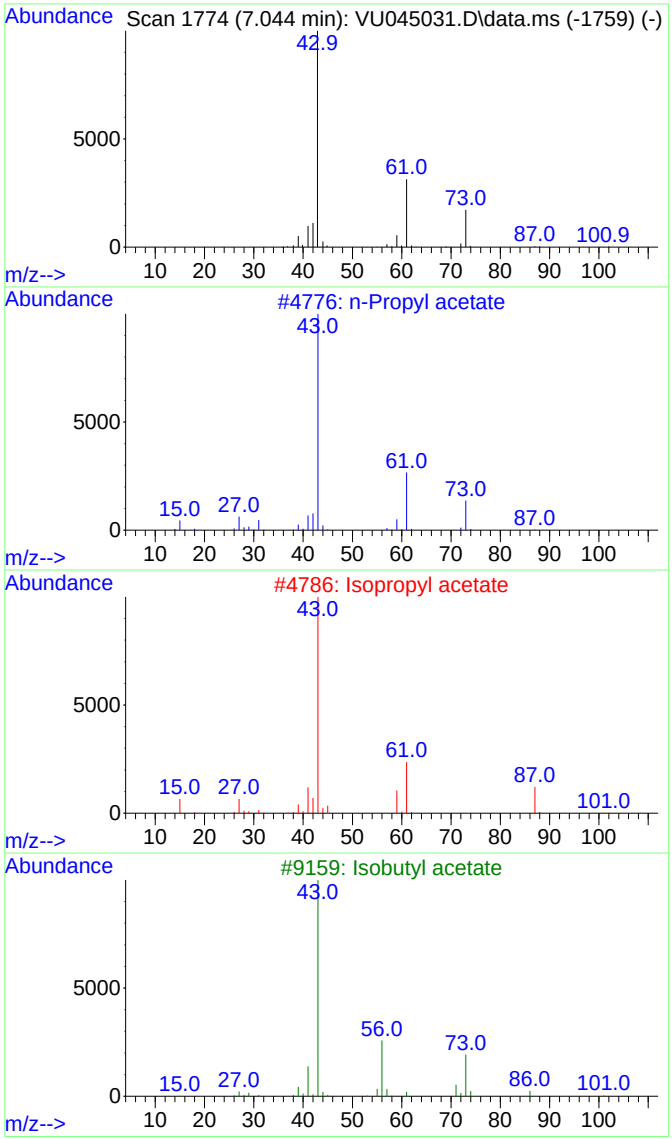
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

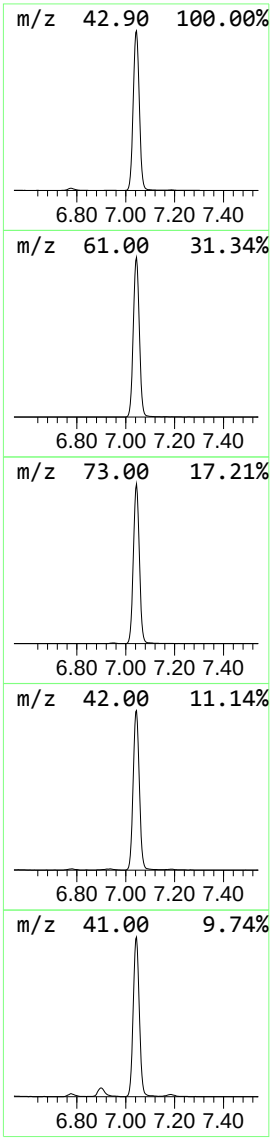
**********

Peak Number 1 n-Propyl acetate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.044 | 119.52 ug/l | 2304150 | 1,4-Difluorobenzene | 6.253 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Propyl acetate | 102 | C5H10O2 | 000109-60-4 | 83 |
| 2 | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 36 |
| 3 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 9 |
| 4 | Propanal, 2,3-dihydroxy-, (S)- | 90 | C3H6O3 | 000497-09-6 | 9 |
| 5 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 7 |



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Data File : VU045031.D
Acq On : 30 Sep 2021 06:59
Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

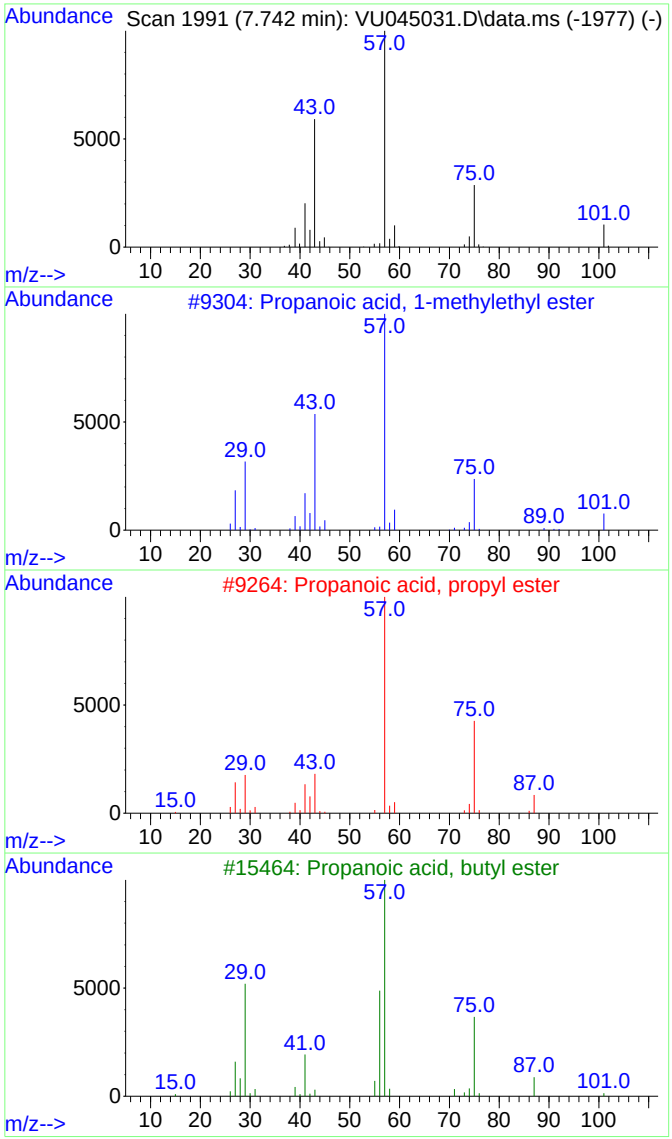
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

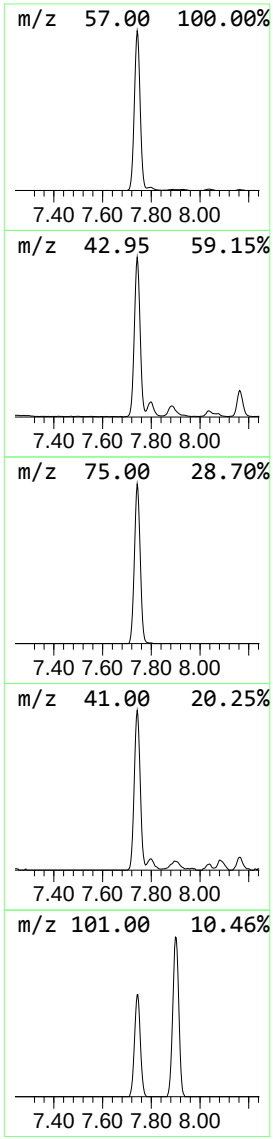
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.742 | 19.30 ug/l | 372005 | 1,4-Difluorobenzene | 6.253 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2 | 000637-78-5 | 90 |
| 2 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 50 |
| 3 | Propanoic acid, butyl ester | 130 | C7H14O2 | 000590-01-2 | 28 |
| 4 | Propane, 1-(1-methylethoxy)- | 102 | C6H14O | 000627-08-7 | 23 |
| 5 | 1,3-Dioxane, 4-methyl- | 102 | C5H10O2 | 001120-97-4 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045031.D
Acq On : 30 Sep 2021 06:59
Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
RP-COMP-3

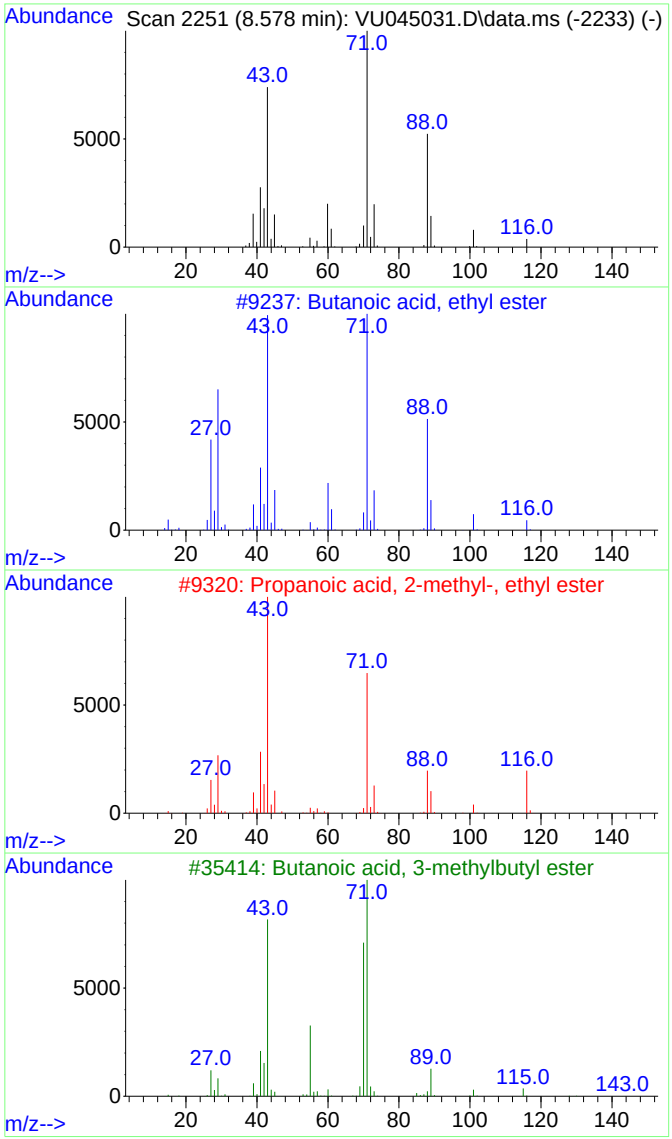
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

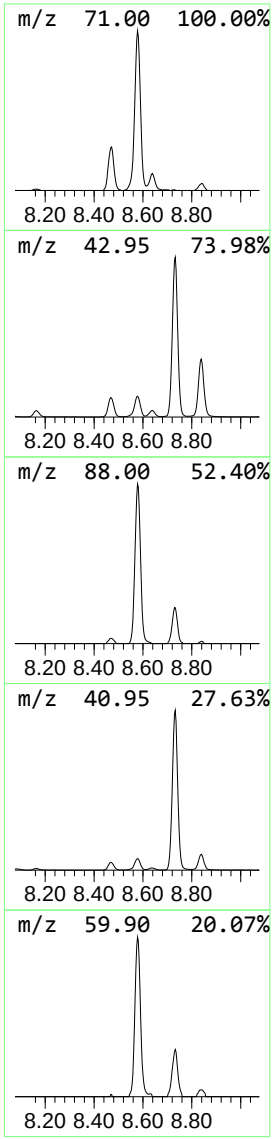
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.578 | 10.82 ug/l | 245213 | Chlorobenzene-d5 | 9.420 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, ethyl ester | 116 | C6H12O2 | 000105-54-4 | 97 |
| 2 | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2 | 000097-62-1 | 42 |
| 3 | Butanoic acid, 3-methylbutyl ester | 158 | C9H18O2 | 000106-27-4 | 38 |
| 4 | Butanoic acid, propyl ester | 130 | C7H14O2 | 000105-66-8 | 38 |
| 5 | 3-Mercaptohexyl butanoate | 204 | C10H20O2S | 136954-21-7 | 37 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045031.D
Acq On : 30 Sep 2021 06:59
Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

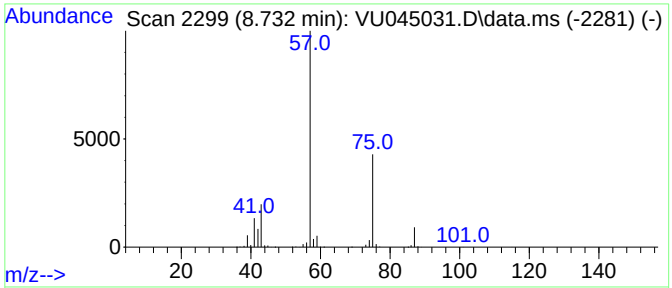
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

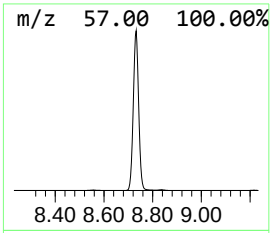
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

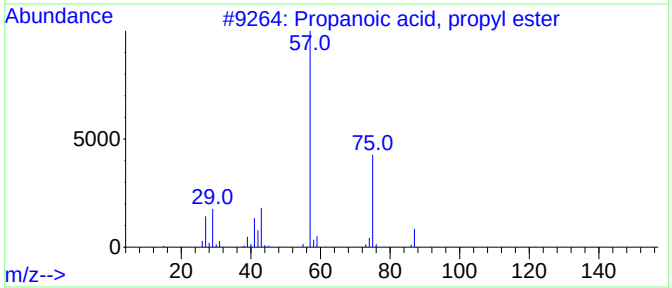
**********
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

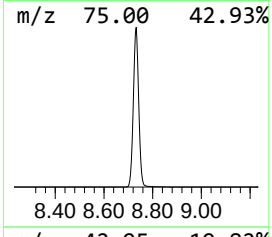
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.732 | 153.03 ug/l | 3466940 | Chlorobenzene-d5 | 9.420 |

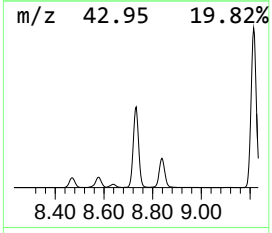
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 83 |
| 2 | Propanoic acid, butyl ester | 130 | C7H14O2 | 000590-01-2 | 28 |
| 3 | di-tert-Butyl dicarbonate | 218 | C10H18O5 | 024424-99-5 | 9 |
| 4 | 2-(Isobutoxymethyl)oxirane | 130 | C7H14O2 | 003814-55-9 | 9 |
| 5 | Isobutyl ether | 130 | C8H18O | 000628-55-7 | 9 |

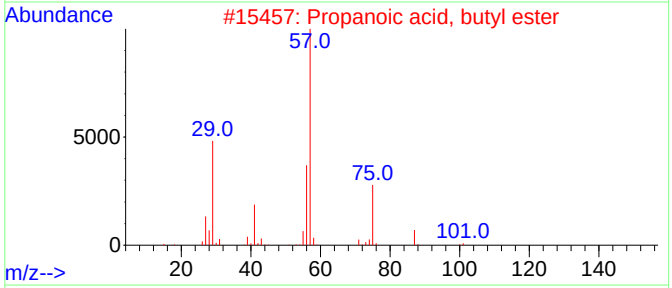


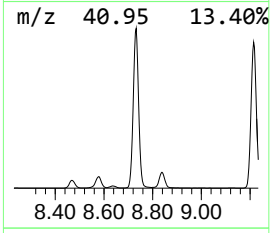



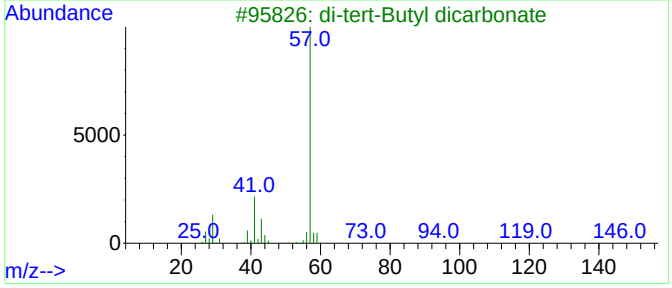



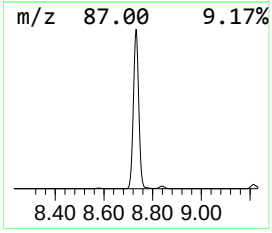



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ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

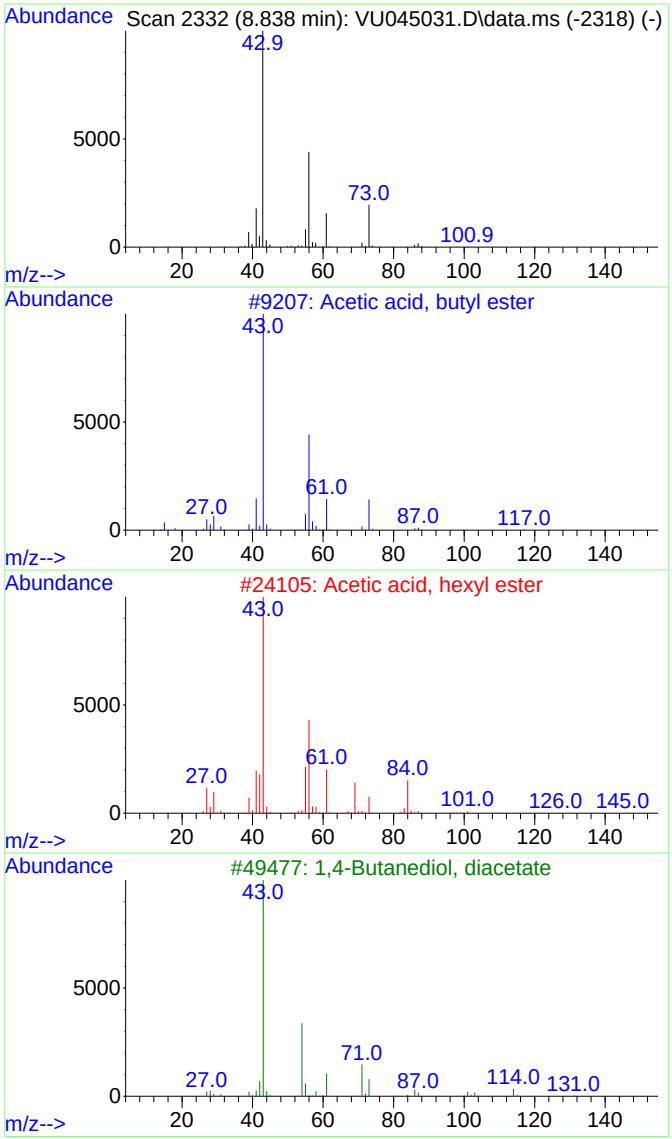
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

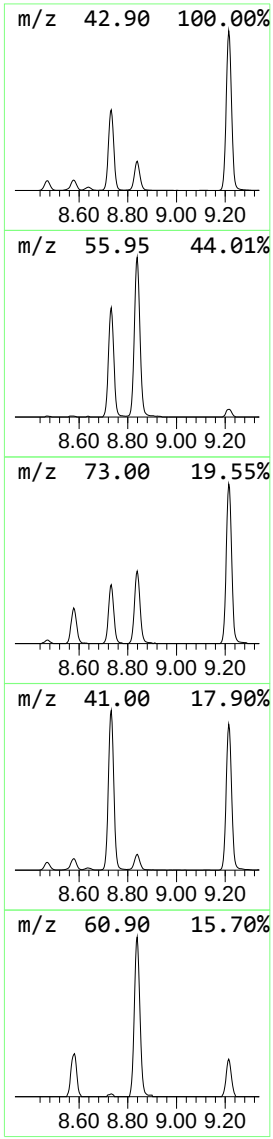
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.838 | 13.44 ug/l | 304466 | Chlorobenzene-d5 | 9.420 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid, butyl ester | 116 | C6H12O2 | 000123-86-4 | 78 |
| 2 | Acetic acid, hexyl ester | 144 | C8H16O2 | 000142-92-7 | 33 |
| 3 | 1,4-Butanediol, diacetate | 174 | C8H14O4 | 000628-67-1 | 12 |
| 4 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |



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Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

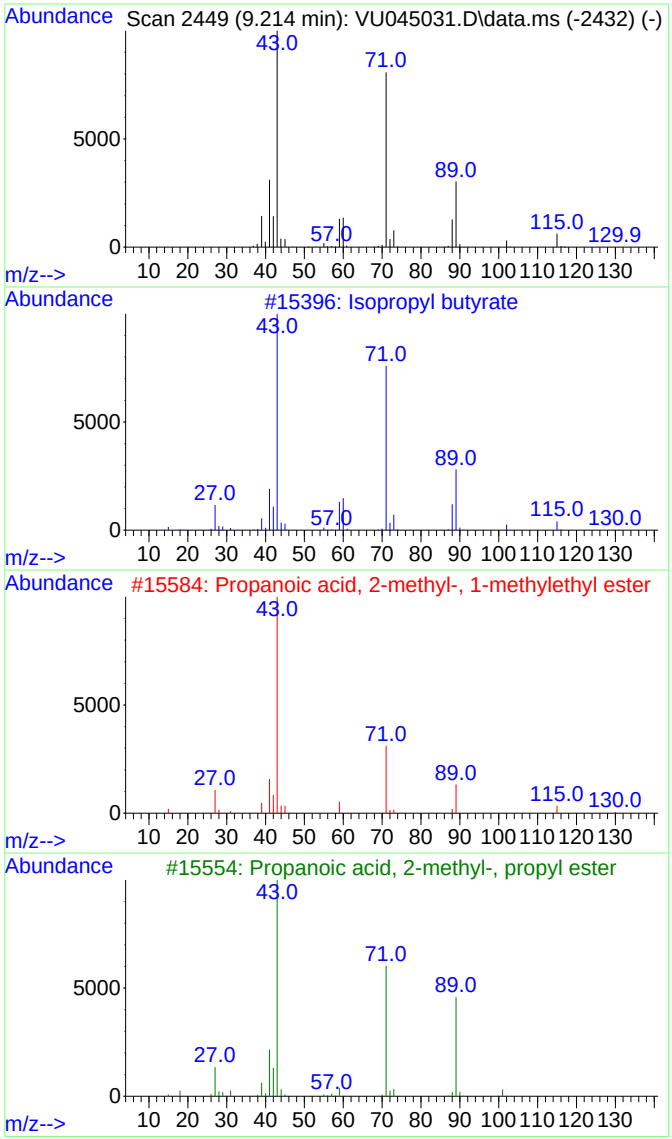
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

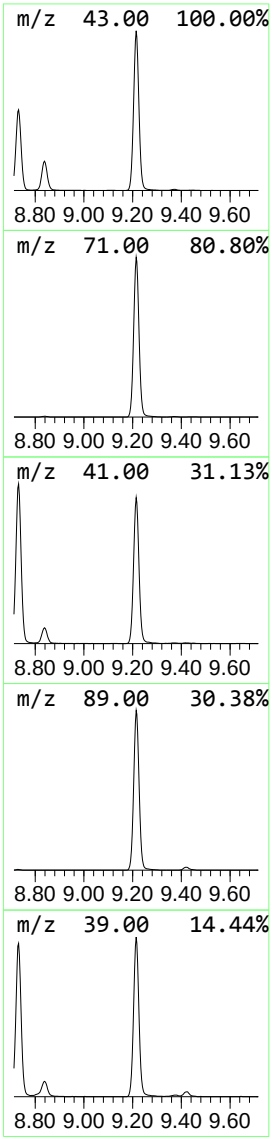
**********

Peak Number 6 Isopropyl butyrate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.214 | 96.05 ug/l | 2176140 | Chlorobenzene-d5 | 9.420 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isopropyl butyrate | 130 | C7H14O2 | 000638-11-9 | 91 |
| 2 | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 78 |
| 3 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 72 |
| 4 | Ethylene glycol Formate Isobutyrate | 160 | C7H12O4 | 1000458-48-0 | 64 |
| 5 | Butanoic acid, pentyl ester | 158 | C9H18O2 | 000540-18-1 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
Data File : VU045031.D
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Operator : SY/MD
Sample : M3971-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** RP-COMP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| n-Propyl acetate | 7.044 | 119.5 | ug/l | 2304150 | 2 | 6.253 | 963952 | 50.0 |
| Propanoic acid,... | 7.742 | 19.3 | ug/l | 372005 | 2 | 6.253 | 963952 | 50.0 |
| Butanoic acid, ... | 8.578 | 10.8 | ug/l | 245213 | 3 | 9.420 | 1132760 | 50.0 |
| Propanoic acid,... | 8.732 | 153.0 | ug/l | 3466940 | 3 | 9.420 | 1132760 | 50.0 |
| Acetic acid, bu... | 8.838 | 13.4 | ug/l | 304466 | 3 | 9.420 | 1132760 | 50.0 |
| Isopropyl butyrate | 9.214 | 96.1 | ug/l | 2176140 | 3 | 9.420 | 1132760 | 50.0 |