LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

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:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Title : SW846 8260

Signal : TIC: VN068494.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.563 | 200 | 214 | 264 | rBV3 | 39218143 | 89945824 | 100.00% | 30.108% |
| 2 | 4.090 | 777 | 783 | 788 | rBV2 | 52990583 | 68410991 | 76.06% | 22.900% |
| 3 | 6.616 | 1686 | 1725 | 1775 | rBV | 8114404 | 26486232 | 29.45% | 8.866% |
| 4 | 7.064 | 1869 | 1892 | 1919 | rBV | 955519 | 2631329 | 2.93% | 0.881% |
| 5 | 8.021 | 2226 | 2249 | 2260 | rBV | 586594 | 1379902 | 1.53% | 0.462% |
| 6 | 8.086 | 2261 | 2273 | 2306 | rVB | 1214595 | 2715242 | 3.02% | 0.909% |
| 7 | 8.437 | 2378 | 2404 | 2432 | rBV2 | 532368 | 1320312 | 1.47% | 0.442% |
| 8 | 8.968 | 2585 | 2602 | 2624 | rVB | 1413884 | 2884385 | 3.21% | 0.966% |
| 9 | 10.333 | 3094 | 3111 | 3134 | rBV | 520736 | 967397 | 1.08% | 0.324% |
| 10 | 10.443 | 3134 | 3152 | 3161 | rVV | 2163298 | 4005802 | 4.45% | 1.341% |
| 11 | 10.507 | 3161 | 3176 | 3201 | rVV3 | 36720242 | 67424794 | 74.96% | 22.570% |
| 12 | 11.744 | 3612 | 3637 | 3662 | rBV2 | 2030191 | 5878965 | 6.54% | 1.968% |
| 13 | 11.846 | 3662 | 3675 | 3697 | rVV | 978270 | 1940233 | 2.16% | 0.649% |
| 14 | 11.950 | 3698 | 3714 | 3745 | rVB | 3930771 | 7711950 | 8.57% | 2.581% |
| 15 | 12.283 | 3811 | 3838 | 3859 | rBV | 2197952 | 3983332 | 4.43% | 1.333% |
| 16 | 12.733 | 3994 | 4006 | 4034 | rVB | 1463080 | 2590182 | 2.88% | 0.867% |
| 17 | 12.986 | 4087 | 4100 | 4108 | rBV | 587062 | 1038156 | 1.15% | 0.348% |
| 18 | 13.155 | 4149 | 4163 | 4174 | rBV | 746889 | 1199695 | 1.33% | 0.402% |
| 19 | 13.219 | 4174 | 4187 | 4203 | rVB2 | 559597 | 1102526 | 1.23% | 0.369% |
| 20 | 13.369 | 4224 | 4243 | 4272 | rVB | 930522 | 2099918 | 2.33% | 0.703% |
| 21 | 13.675 | 4343 | 4357 | 4366 | rBV | 1631408 | 3023082 | 3.36% | 1.012% |

Sum of corrected areas: 298740249

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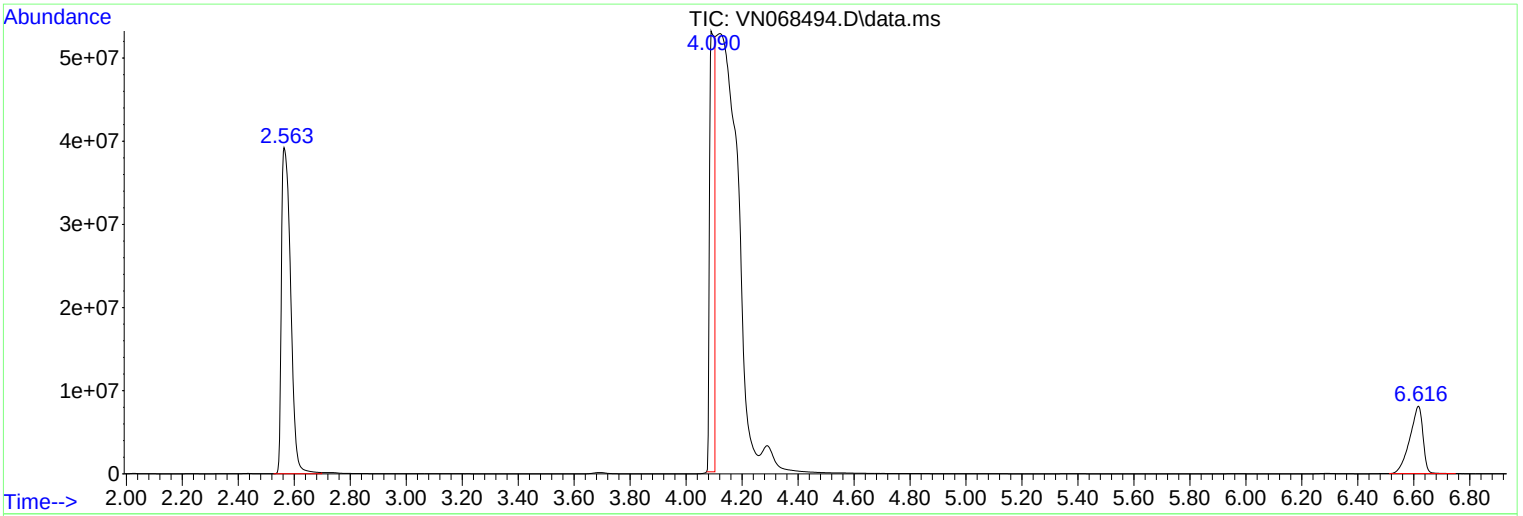
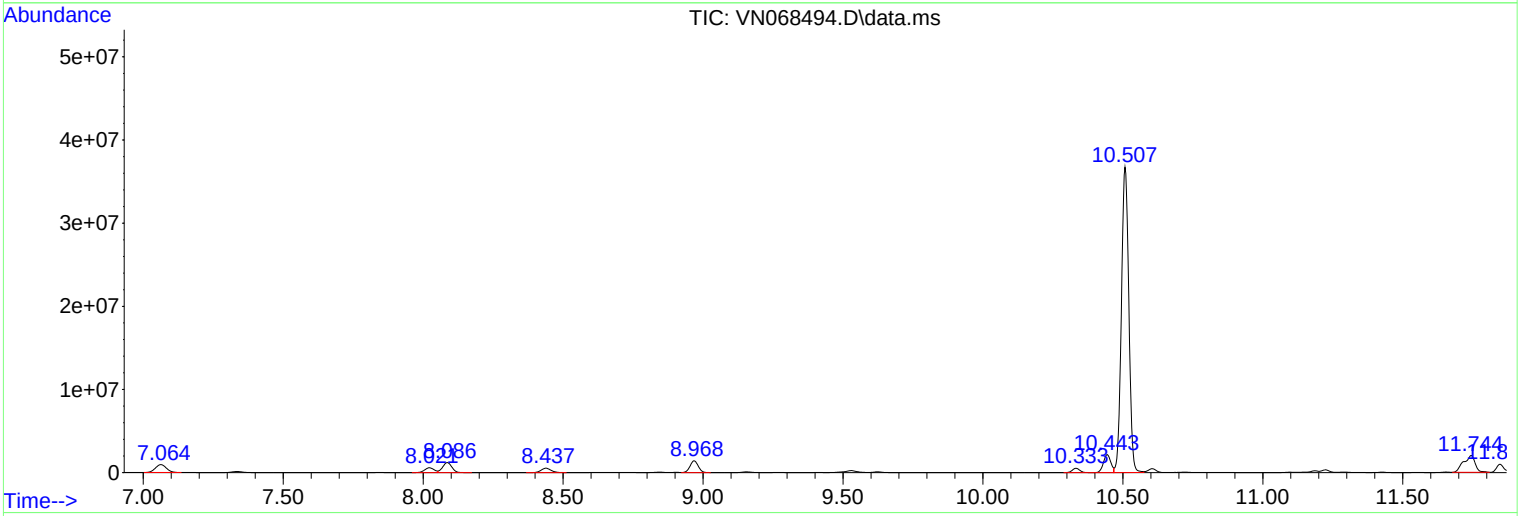
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

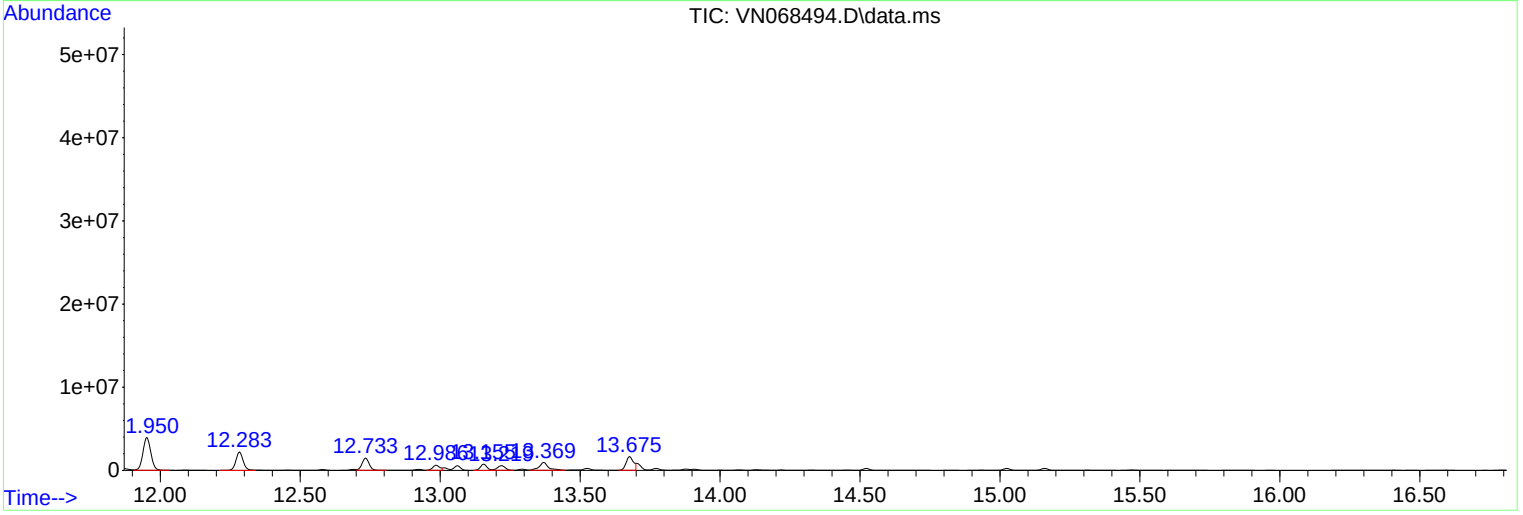
**Instrument :**
MSVOA_N
**ClientSampleId :**
31209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

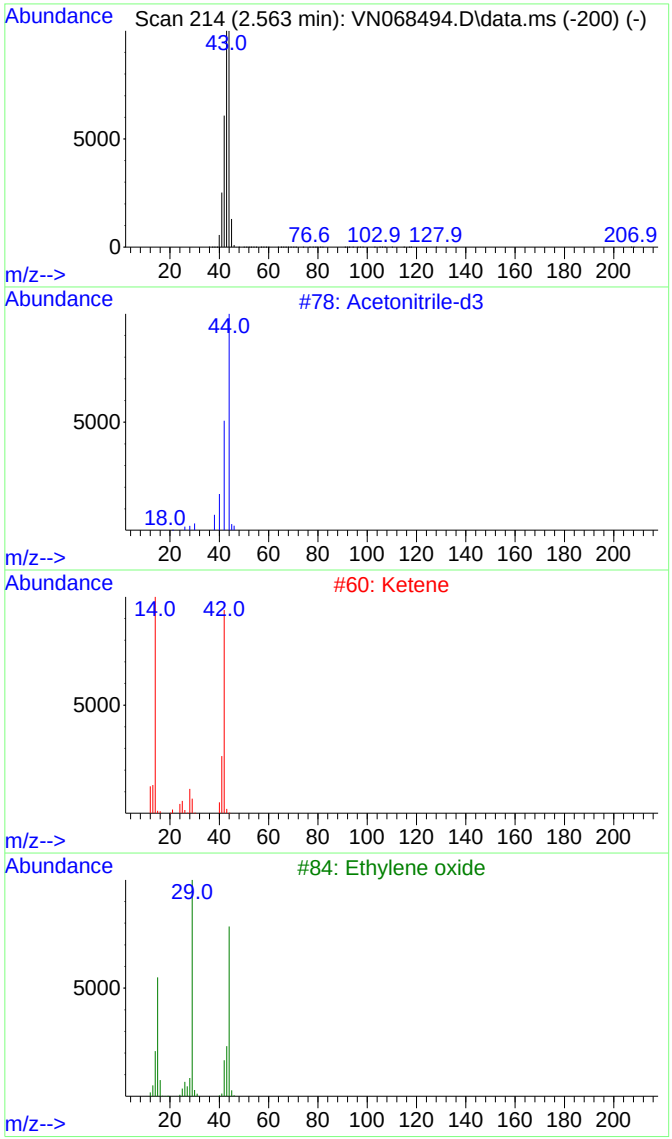
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

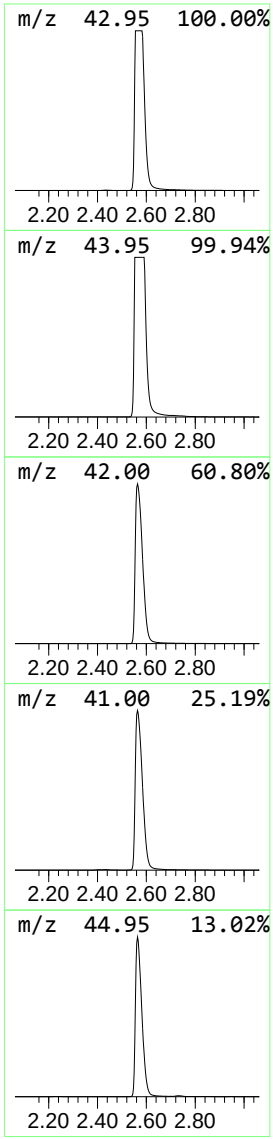
**********

Peak Number 1 unknown2.563 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.563 | 1656.31 ug/l | 89945800 | Pentafluorobenzene | 8.086 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetonitrile-d3 | 44 | C2D3N | 002206-26-0 | 4 |
| 2 | Ketene | 42 | C2H2O | 000463-51-4 | 4 |
| 3 | Ethylene oxide | 44 | C2H4O | 000075-21-8 | 3 |
| 4 | Propane | 44 | C3H8 | 000074-98-6 | 3 |
| 5 | Methane, diazo- | 42 | CH2N2 | 000334-88-3 | 3 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

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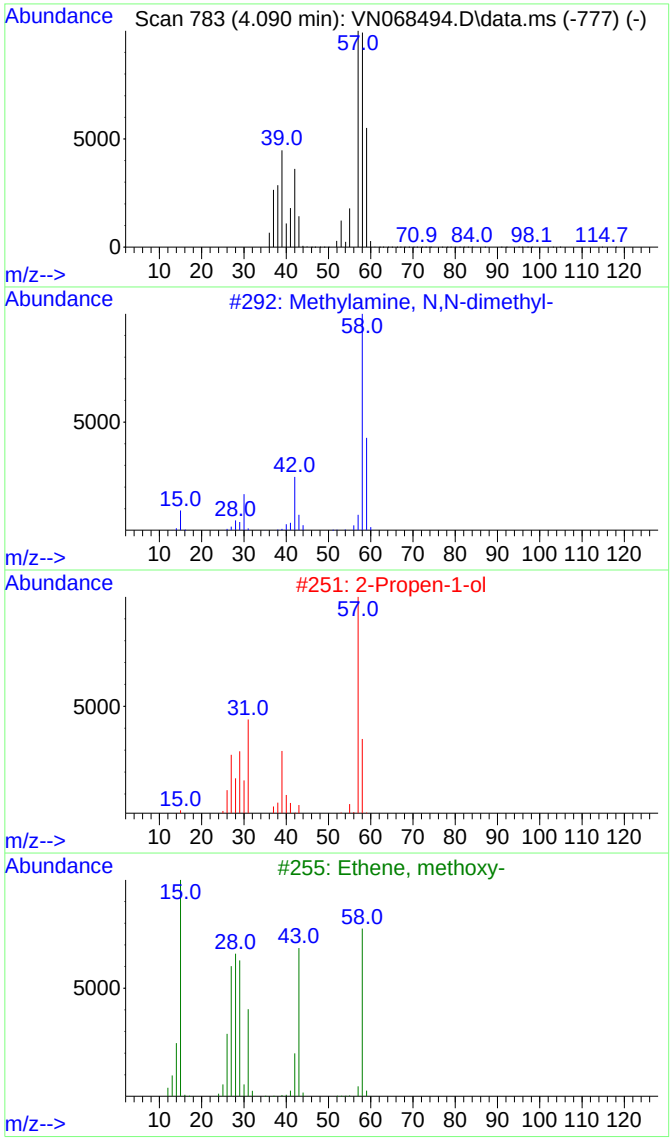
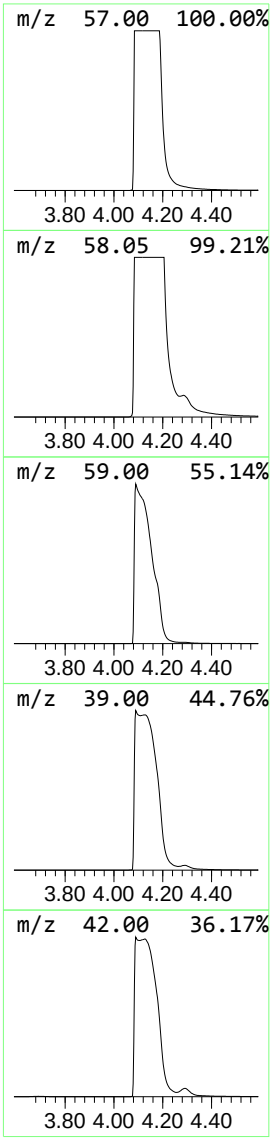
Peak Number 2 unknown4.090 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.090 | 1259.76 ug/l | 68411000 | Pentafluorobenzene | 8.086 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methylamine, N,N-dimethyl- | 59 | C3H9N | 000075-50-3 | 27 |
| 2 | 2-Propen-1-ol | 58 | C3H6O | 000107-18-6 | 7 |
| 3 | Ethene, methoxy- | 58 | C3H6O | 000107-25-5 | 4 |
| 4 | Propanal | 58 | C3H6O | 000123-38-6 | 4 |
| 5 | Diazene, dimethyl- | 58 | C2H6N2 | 000503-28-6 | 3 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
31209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

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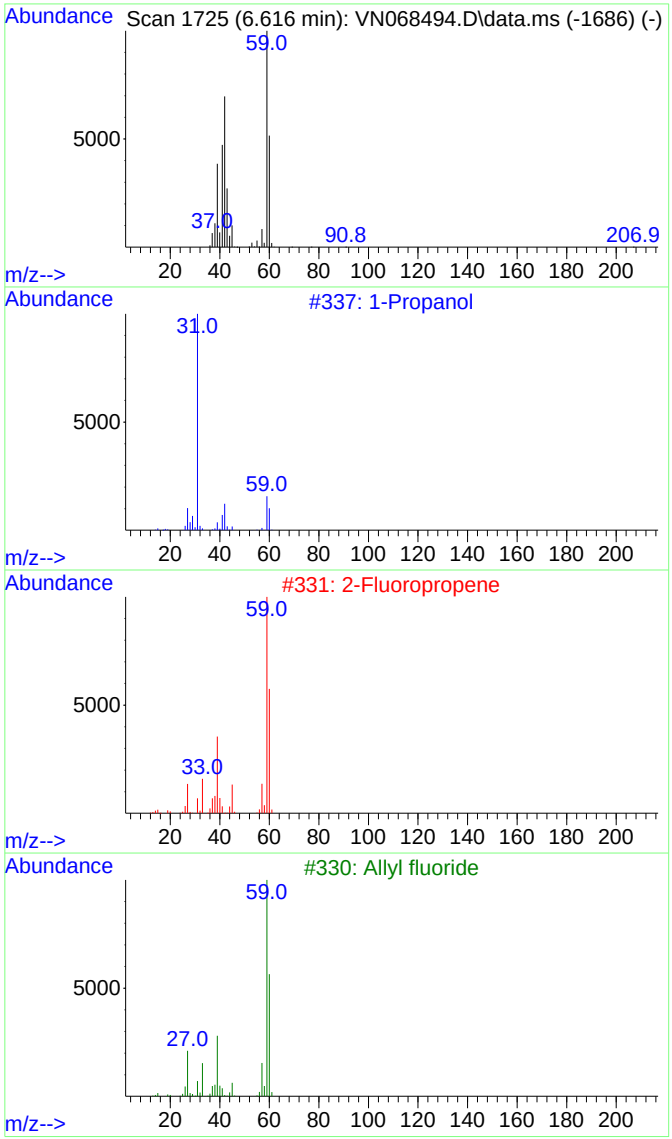
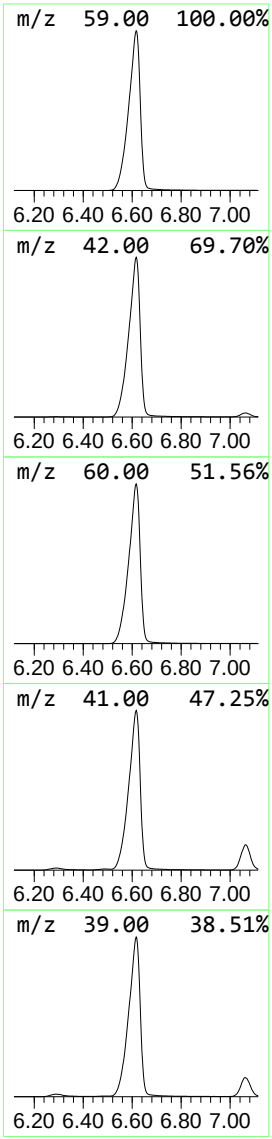
Peak Number 3 1-Propanol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.616 | 487.73 ug/l | 26486200 | Pentafluorobenzene | 8.086 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanol | 60 | C3H8O | 000071-23-8 | 59 |
| 2 | 2-Fluoropropene | 60 | C3H5F | 001184-60-7 | 45 |
| 3 | Allyl fluoride | 60 | C3H5F | 000818-92-8 | 38 |
| 4 | Formamidoxime | 60 | CH4N2O | 000624-82-8 | 22 |
| 5 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 16 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

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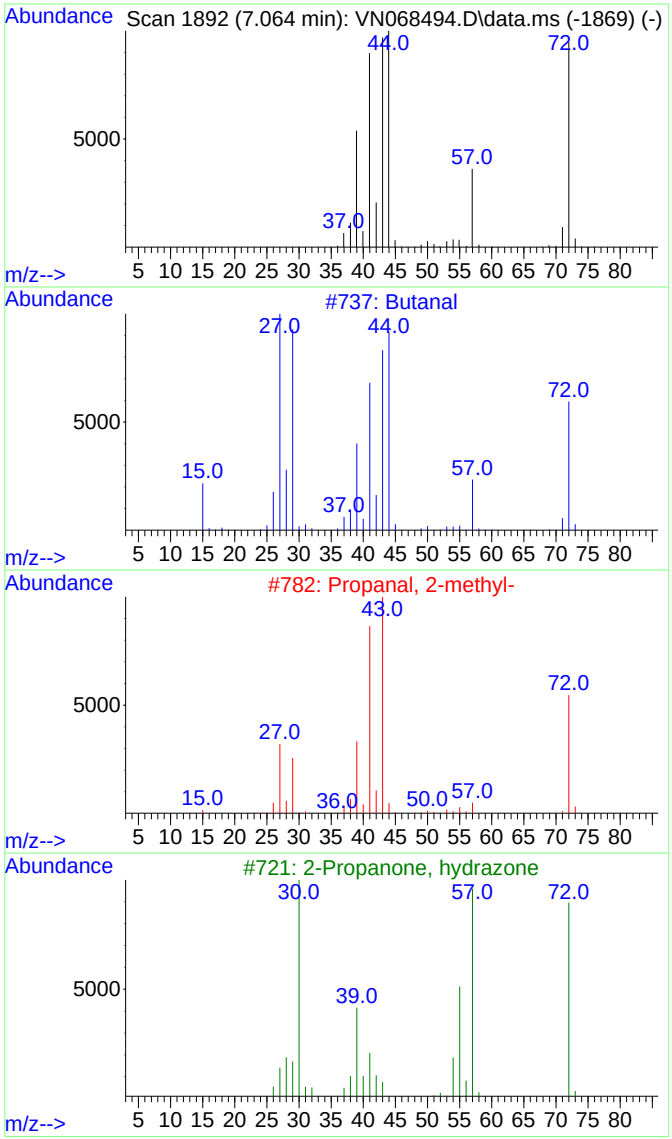
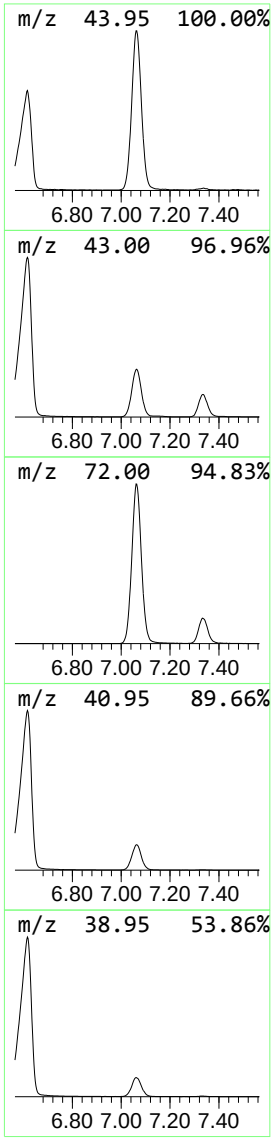
Peak Number 4 Butanal Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.064 | 48.45 ug/l | 2631330 | Pentafluorobenzene | 8.086 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanal | 72 | C4H8O | 000123-72-8 | 80 |
| 2 | Propanal, 2-methyl- | 72 | C4H8O | 000078-84-2 | 43 |
| 3 | 2-Propanone, hydrazone | 72 | C3H8N2 | 005281-20-9 | 38 |
| 4 | 1-Propene, 3-methoxy- | 72 | C4H8O | 000627-40-7 | 37 |
| 5 | Propane | 44 | C3H8 | 000074-98-6 | 35 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068494.D
Acq On : 15 Sep 2021 19:31
Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

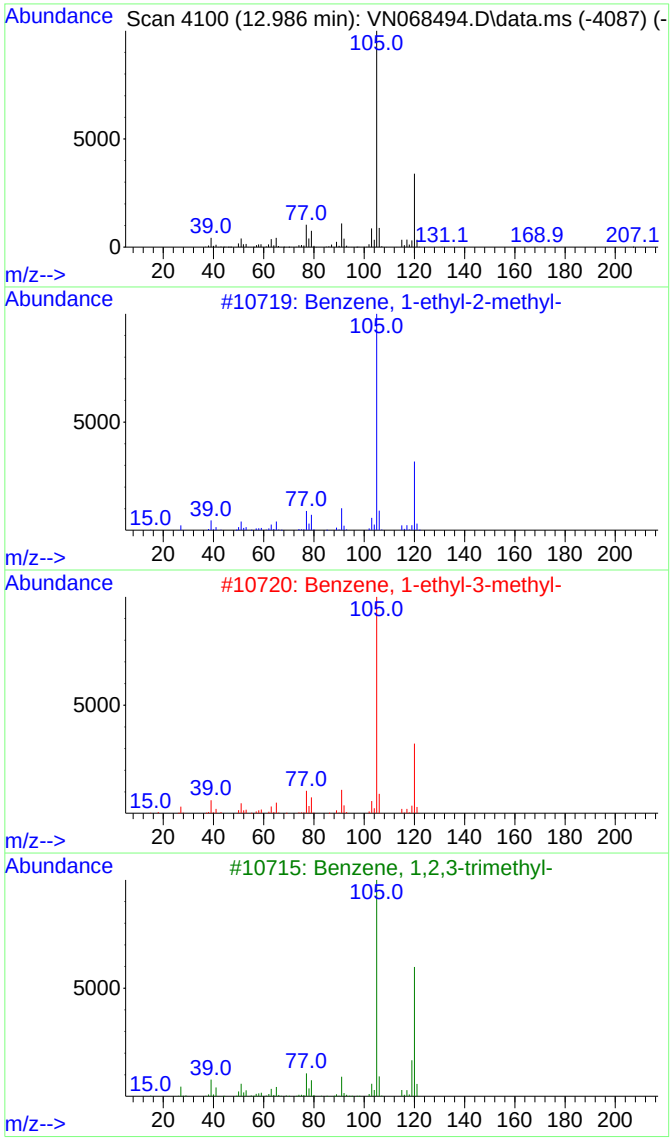
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

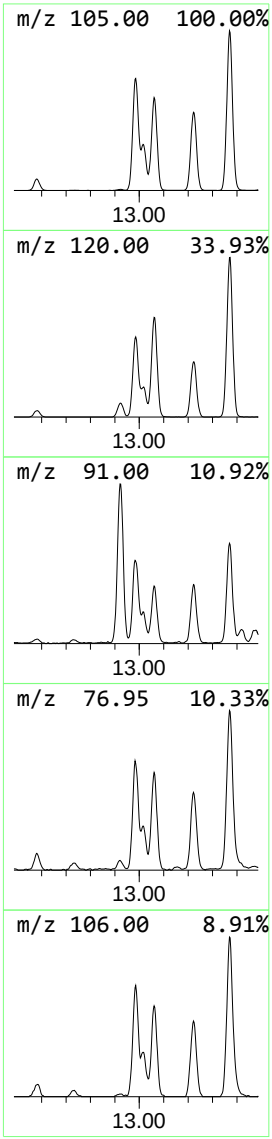
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.986 | 17.17 ug/l | 1038160 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-ethyl-2-methyl- | 120 | C9H12 | 000611-14-3 | 95 |
| 2 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 95 |
| 3 | Benzene, 1,2,3-trimethyl- | 120 | C9H12 | 000526-73-8 | 91 |
| 4 | Benzene, 1,2,4-trimethyl- | 120 | C9H12 | 000095-63-6 | 91 |
| 5 | Mesitylene | 120 | C9H12 | 000108-67-8 | 91 |



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** 31209

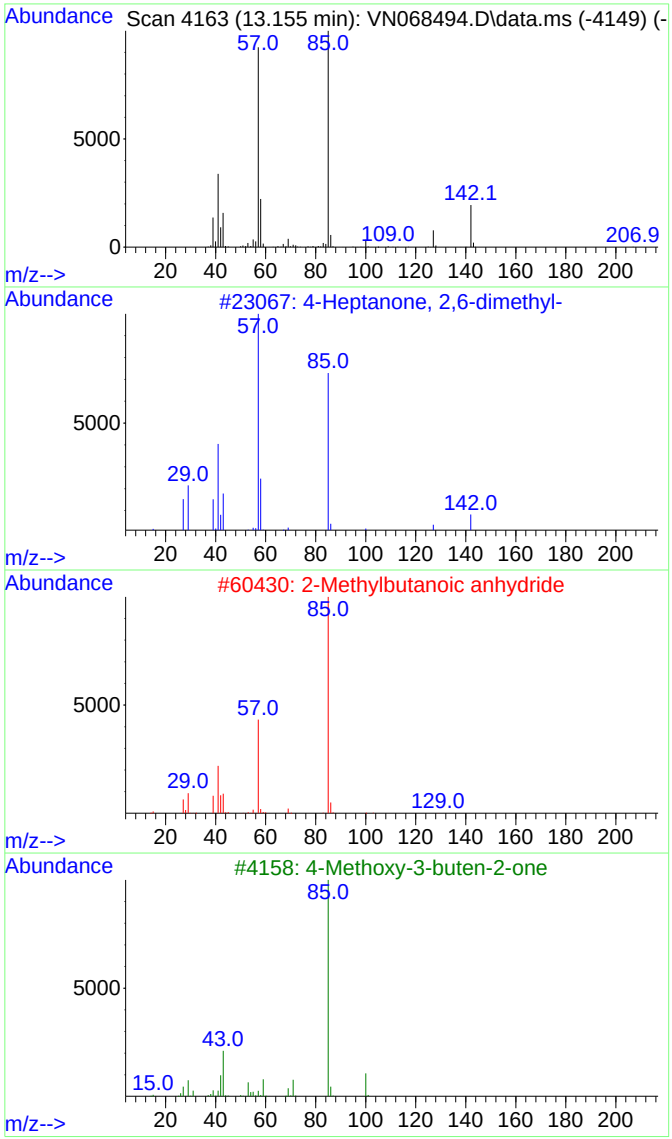
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

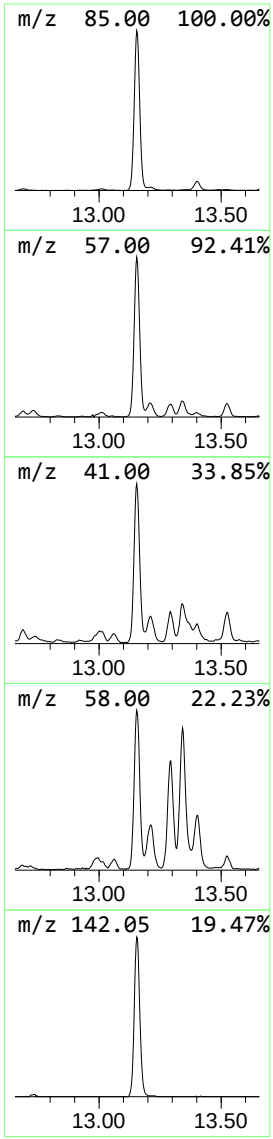
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 4-Heptanone, 2,6-dimethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.155 | 19.84 ug/l | 1199700 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Heptanone, 2,6-dimethyl- | 142 | C9H18O | 000108-83-8 | 91 |
| 2 | 2-Methylbutanoic anhydride | 186 | C10H18O3 | 001468-39-9 | 53 |
| 3 | 4-Methoxy-3-buten-2-one | 100 | C5H8O2 | 004652-27-1 | 49 |
| 4 | Acetaldehyde, bis(1-methylethyl)... | 142 | C8H18N2 | 067660-50-8 | 45 |
| 5 | t-Butyl isobutyl ketone | 142 | C9H18O | 014705-50-1 | 42 |



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Operator : JC/MD
Sample : M3759-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

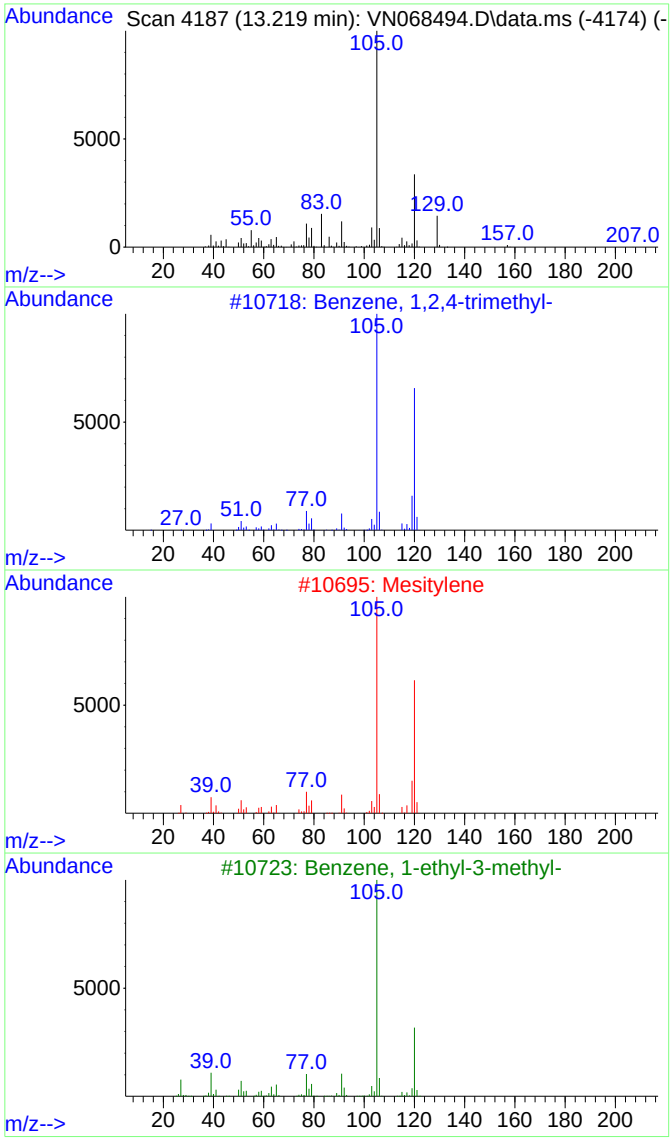
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

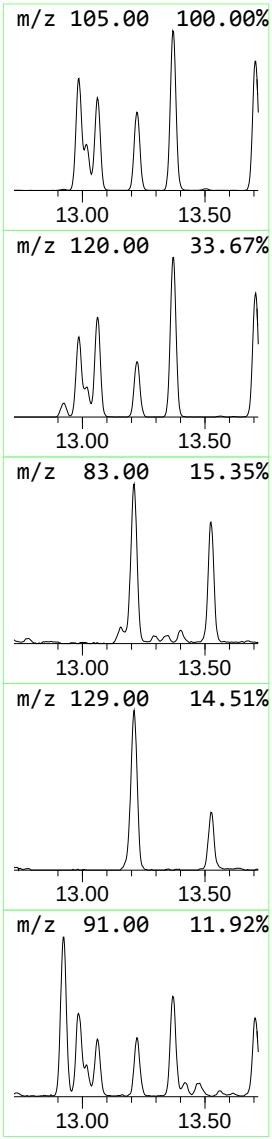
**********

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.219 | 18.24 ug/l | 1102530 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1,2,4-trimethyl- | 120 | C9H12 | 000095-63-6 | 70 |
| 2 | Mesitylene | 120 | C9H12 | 000108-67-8 | 70 |
| 3 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 70 |
| 4 | Benzene, 1,2,3-trimethyl- | 120 | C9H12 | 000526-73-8 | 70 |
| 5 | Benzene, 1-ethyl-4-methyl- | 120 | C9H12 | 000622-96-8 | 70 |



Tentatively Identified Compound (LSC) summary

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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 |
| unknown2.563 | 2.563 | 1656.3 | ug/l | 89945800 | 1 | 8.086 | 2715240 | 50.0 |
| unknown4.090 | 4.090 | 1259.8 | ug/l | 68411000 | 1 | 8.086 | 2715240 | 50.0 |
| 1-Propanol | 6.616 | 487.7 | ug/l | 26486200 | 1 | 8.086 | 2715240 | 50.0 |
| Butanal | 7.064 | 48.5 | ug/l | 2631330 | 1 | 8.086 | 2715240 | 50.0 |
| Benzene, 1-ethy... | 12.986 | 17.2 | ug/l | 1038160 | 4 | 13.675 | 3023080 | 50.0 |
| 4-Heptanone, 2,... | 13.155 | 19.8 | ug/l | 1199700 | 4 | 13.675 | 3023080 | 50.0 |
| Benzene, 1,2,3-... | 13.219 | 18.2 | ug/l | 1102530 | 4 | 13.675 | 3023080 | 50.0 |