LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

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\82N072418W.M
Title : SW846 8260

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.661 | 3 | 22 | 39 | rBV | 1323890 | 2053758 | 51.28% | 5.373% |
| 2 | 1.815 | 60 | 70 | 89 | rBV | 444390 | 593578 | 14.82% | 1.553% |
| 3 | 2.018 | 117 | 133 | 141 | rBV2 | 30431 | 57768 | 1.44% | 0.151% |
| 4 | 2.149 | 166 | 174 | 177 | rBV | 71496 | 94561 | 2.36% | 0.247% |
| 5 | 2.310 | 217 | 224 | 237 | rVB | 47222 | 73919 | 1.85% | 0.193% |
| 6 | 3.825 | 676 | 695 | 709 | rBV | 1086356 | 2798154 | 69.87% | 7.321% |
| 7 | 4.082 | 757 | 775 | 808 | rBV | 167886 | 477906 | 11.93% | 1.250% |
| 8 | 4.805 | 978 | 1000 | 1032 | rVB3 | 147808 | 523031 | 13.06% | 1.368% |
| 9 | 6.551 | 1528 | 1543 | 1559 | rBV7 | 14513 | 45825 | 1.14% | 0.120% |
| 10 | 6.654 | 1559 | 1575 | 1596 | rVB10 | 15433 | 49724 | 1.24% | 0.130% |
| 11 | 6.847 | 1613 | 1635 | 1669 | rBV | 443766 | 1295032 | 32.34% | 3.388% |
| 12 | 7.204 | 1730 | 1746 | 1773 | rBV2 | 57822 | 162434 | 4.06% | 0.425% |
| 13 | 7.593 | 1845 | 1867 | 1879 | rBV | 554498 | 1386689 | 34.63% | 3.628% |
| 14 | 7.670 | 1879 | 1891 | 1922 | rVB | 837625 | 2004815 | 50.06% | 5.245% |
| 15 | 8.030 | 1984 | 2003 | 2025 | rBV | 564975 | 1322458 | 33.02% | 3.460% |
| 16 | 8.233 | 2042 | 2066 | 2067 | rBV | 140563 | 392995 | 9.81% | 1.028% |
| 17 | 8.451 | 2124 | 2134 | 2160 | rVB | 113865 | 275477 | 6.88% | 0.721% |
| 18 | 8.590 | 2161 | 2177 | 2209 | rVB | 1215505 | 2507812 | 62.62% | 6.561% |
| 19 | 8.979 | 2285 | 2298 | 2306 | rBV6 | 27097 | 66298 | 1.66% | 0.173% |
| 20 | 9.046 | 2306 | 2319 | 2339 | rVV | 617506 | 1241607 | 31.00% | 3.249% |
| 21 | 9.194 | 2355 | 2365 | 2385 | rVB | 82926 | 177824 | 4.44% | 0.465% |
| 22 | 9.368 | 2406 | 2419 | 2427 | rBV3 | 77079 | 148933 | 3.72% | 0.390% |
| 23 | 9.432 | 2428 | 2439 | 2460 | rVB | 303273 | 633718 | 15.82% | 1.658% |
| 24 | 9.895 | 2572 | 2583 | 2600 | rVB2 | 48929 | 95767 | 2.39% | 0.251% |
| 25 | 9.988 | 2600 | 2612 | 2621 | rBV | 169430 | 320365 | 8.00% | 0.838% |
| 26 | 10.094 | 2631 | 2645 | 2658 | rBV | 2174926 | 4004653 | 100.00% | 10.478% |
| 27 | 10.159 | 2658 | 2665 | 2673 | rVV | 150273 | 270922 | 6.77% | 0.709% |
| 28 | 10.201 | 2674 | 2678 | 2692 | rVB | 70585 | 110580 | 2.76% | 0.289% |
| 29 | 10.612 | 2793 | 2806 | 2811 | rBV | 157245 | 285187 | 7.12% | 0.746% |
| 30 | 10.757 | 2837 | 2851 | 2872 | rBV | 390516 | 717857 | 17.93% | 1.878% |
| 31 | 10.853 | 2874 | 2881 | 2890 | rVB4 | 30448 | 48711 | 1.22% | 0.127% |
| 32 | 10.914 | 2892 | 2900 | 2908 | rBV | 48085 | 85403 | 2.13% | 0.223% |
| 33 | 11.410 | 3041 | 3054 | 3074 | rVB | 1655167 | 2951251 | 73.70% | 7.722% |
| 34 | 11.525 | 3076 | 3090 | 3100 | rVB2 | 86875 | 181785 | 4.54% | 0.476% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

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\82N072418W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 11.586 | 3100 | 3109 | 3117 | rBV3 | 30851 | 53660 | 1.34% | 0.140% |
| 36 | 11.660 | 3123 | 3132 | 3142 | rVB | 143055 | 231102 | 5.77% | 0.605% |
| 37 | 11.728 | 3142 | 3153 | 3163 | rBV5 | 81645 | 183320 | 4.58% | 0.480% |
| 38 | 11.950 | 3214 | 3222 | 3236 | rVV | 334827 | 579302 | 14.47% | 1.516% |
| 39 | 12.030 | 3239 | 3247 | 3267 | rVB2 | 443780 | 933343 | 23.31% | 2.442% |
| 40 | 12.117 | 3268 | 3274 | 3285 | rVB3 | 75336 | 129065 | 3.22% | 0.338% |
| 41 | 12.249 | 3307 | 3315 | 3325 | rVB6 | 33024 | 64093 | 1.60% | 0.168% |
| 42 | 12.358 | 3337 | 3349 | 3352 | rBV7 | 46067 | 84695 | 2.11% | 0.222% |
| 43 | 12.403 | 3353 | 3363 | 3375 | rVV | 1455455 | 2404657 | 60.05% | 6.292% |
| 44 | 12.731 | 3457 | 3465 | 3477 | rVB | 672075 | 1122415 | 28.03% | 2.937% |
| 45 | 12.792 | 3479 | 3484 | 3496 | rVB2 | 241120 | 389979 | 9.74% | 1.020% |
| 46 | 12.856 | 3496 | 3504 | 3520 | rBV4 | 64005 | 148364 | 3.70% | 0.388% |
| 47 | 13.091 | 3569 | 3577 | 3585 | rVV | 114340 | 166064 | 4.15% | 0.434% |
| 48 | 13.136 | 3586 | 3591 | 3598 | rVB | 39540 | 50188 | 1.25% | 0.131% |
| 49 | 13.345 | 3643 | 3656 | 3680 | rVV | 1697011 | 3114912 | 77.78% | 8.150% |
| 50 | 13.451 | 3682 | 3689 | 3701 | rVB2 | 74313 | 125193 | 3.13% | 0.328% |
| 51 | 13.683 | 3750 | 3761 | 3768 | rBV3 | 96347 | 203952 | 5.09% | 0.534% |
| 52 | 14.033 | 3854 | 3870 | 3884 | rBV7 | 45346 | 139575 | 3.49% | 0.365% |
| 53 | 14.252 | 3932 | 3938 | 3946 | rVB | 35448 | 47399 | 1.18% | 0.124% |
| 54 | 14.422 | 3984 | 3991 | 4001 | rVB3 | 41329 | 66876 | 1.67% | 0.175% |
| 55 | 14.589 | 4036 | 4043 | 4053 | rBV3 | 32795 | 64274 | 1.60% | 0.168% |
| 56 | 15.795 | 4412 | 4418 | 4429 | rVB | 95916 | 166129 | 4.15% | 0.435% |
| 57 | 16.358 | 4583 | 4593 | 4608 | rVB2 | 142105 | 294887 | 7.36% | 0.772% |

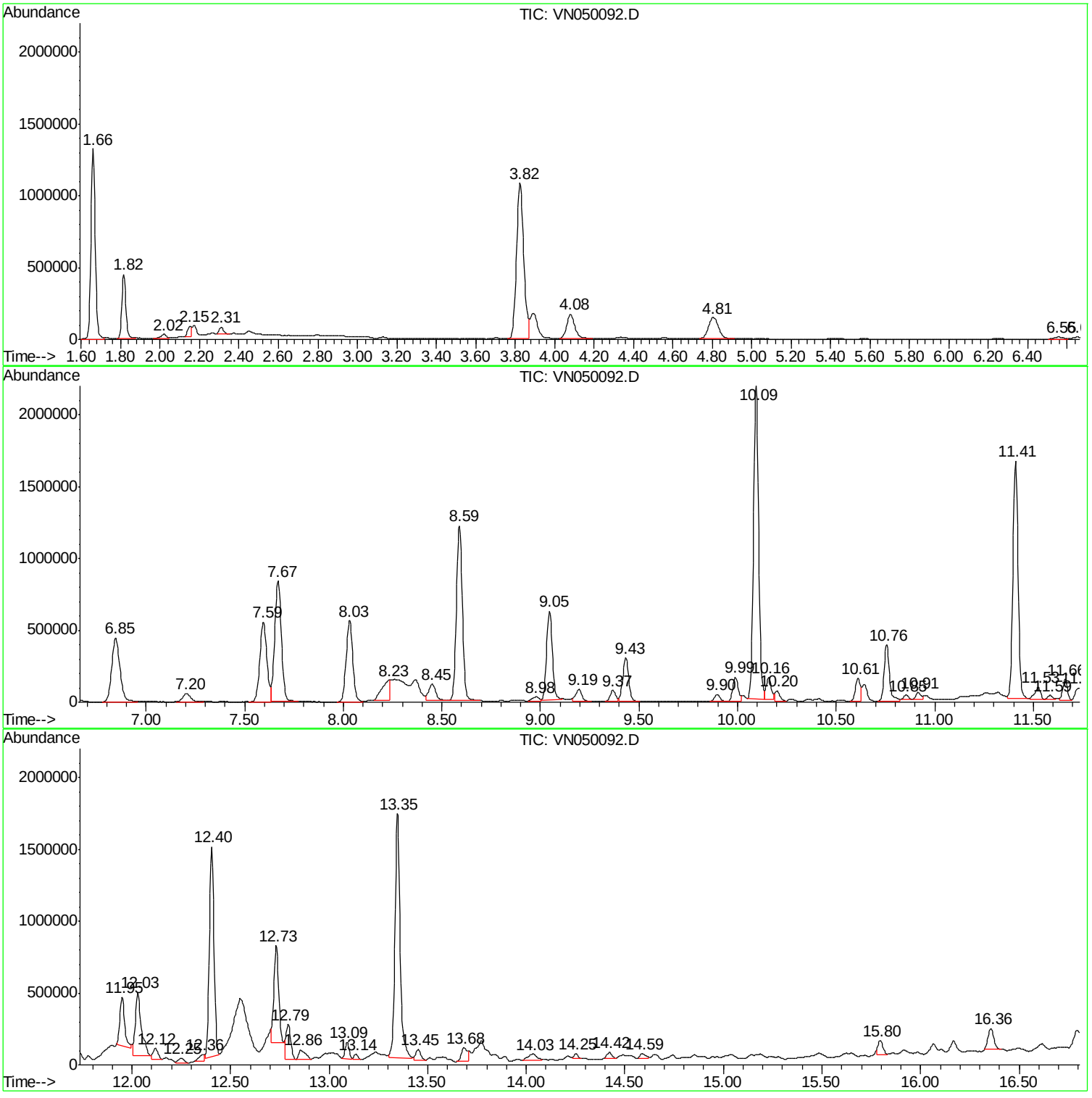
Sum of corrected areas: 38220241

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

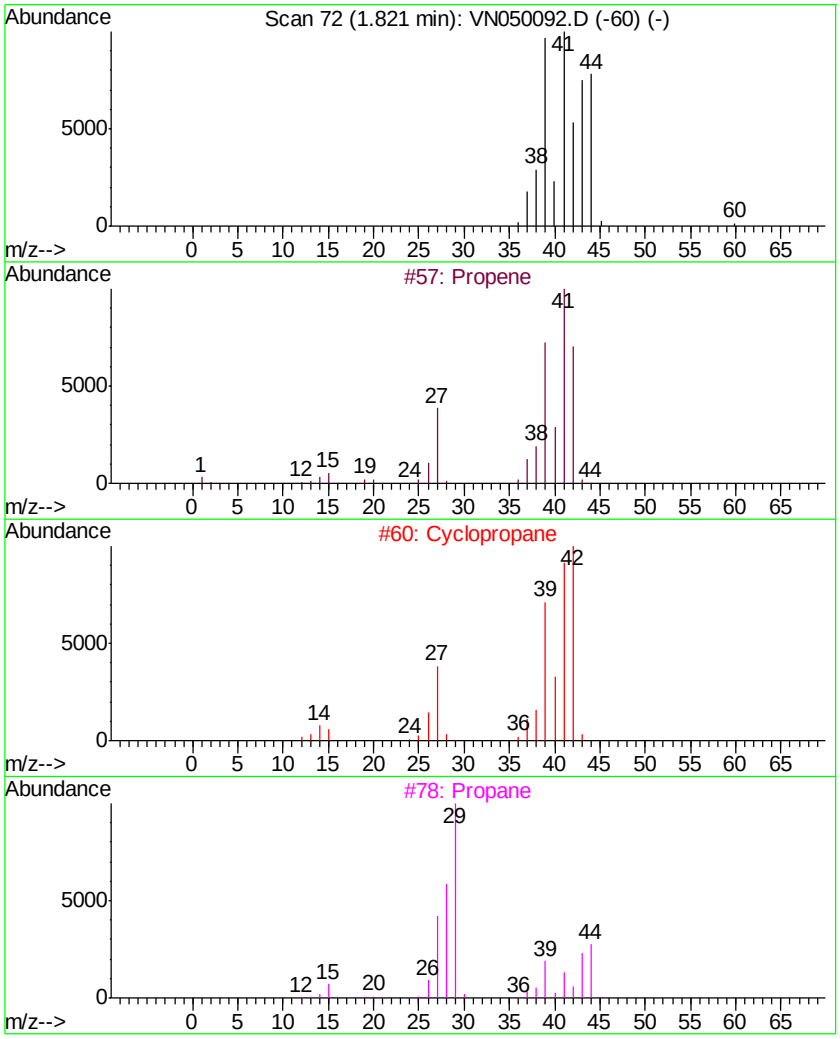
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

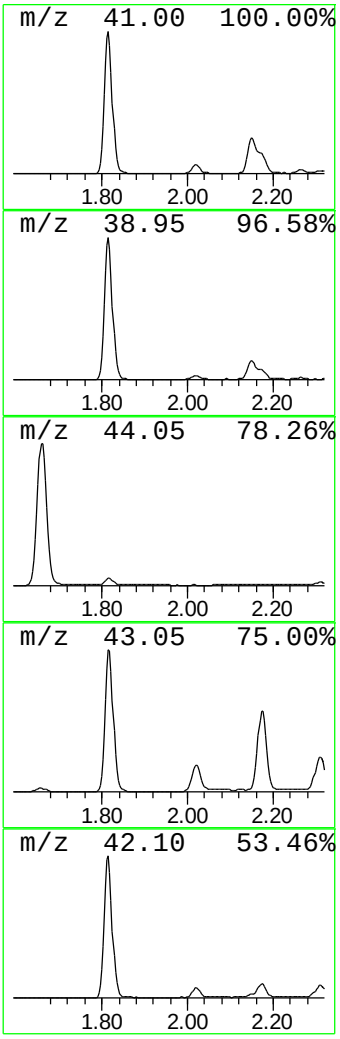
**********

Peak Number 2 Propene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.82 | 14.80 ug/l | 593578 | Pentafluorobenzene | 7.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propene | 42 | C3H6 | 000115-07-1 | 59 |
| 2 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 4 |
| 3 | Propane | 44 | C3H8 | 000074-98-6 | 4 |
| 4 | Cyclobutylamine | 71 | C4H9N | 002516-34-9 | 2 |
| 5 | 4-Amino-1-butanol | 89 | C4H11NO | 013325-10-5 | 2 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

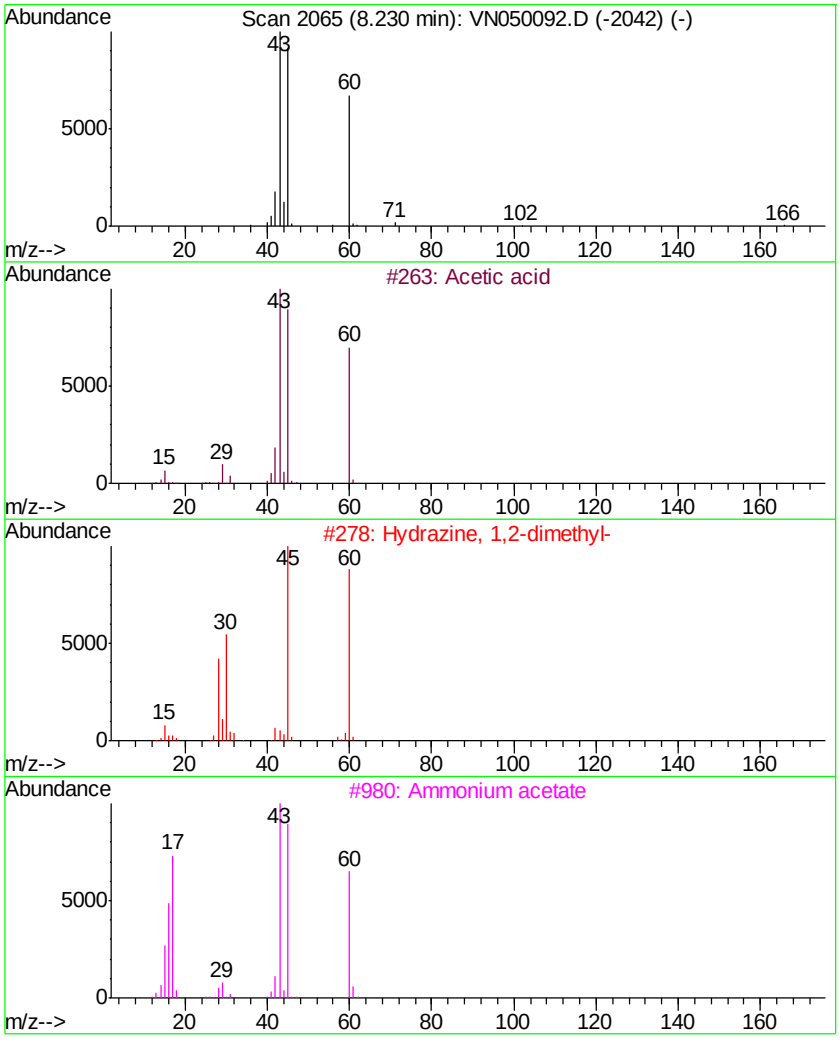
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

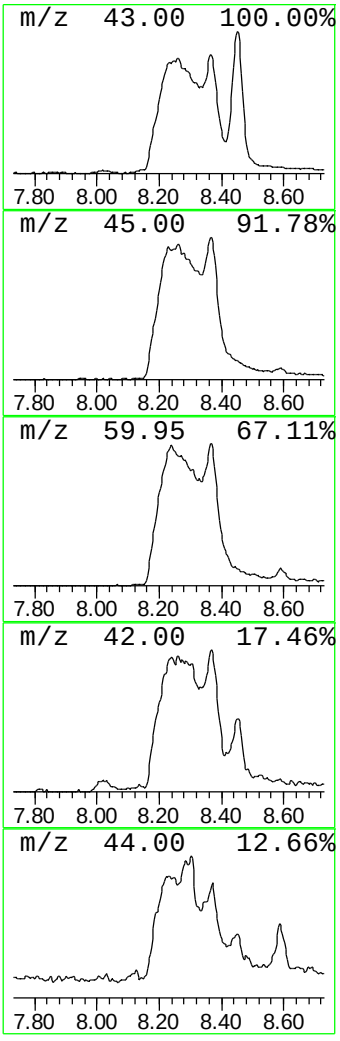
**********

Peak Number 3 Acetic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.23 | 7.84 ug/l | 392995 | 1,4-Difluorobenzene | 8.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid | 60 | C2H4O2 | 000064-19-7 | 90 |
| 2 | Hydrazine, 1,2-dimethyl- | 60 | C2H8N2 | 000540-73-8 | 50 |
| 3 | Ammonium acetate | 77 | C2H7NO2 | 000631-61-8 | 43 |
| 4 | Formic acid hydrazide | 60 | CH4N2O | 000624-84-0 | 9 |
| 5 | Hydrazine, 1,1-dimethyl- | 60 | C2H8N2 | 000057-14-7 | 9 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

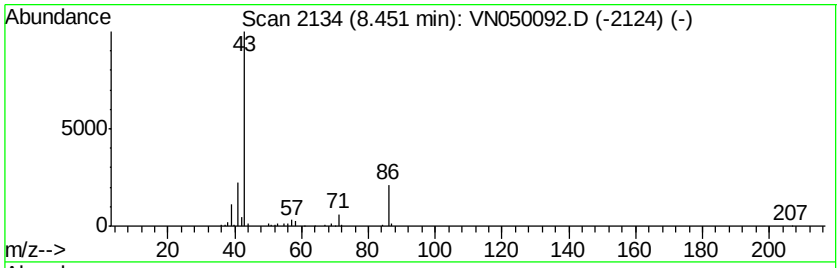
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

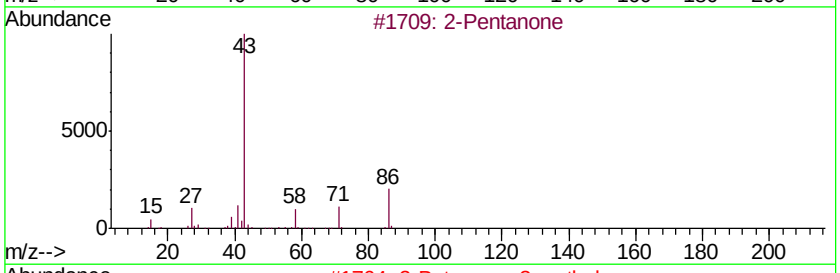
**********

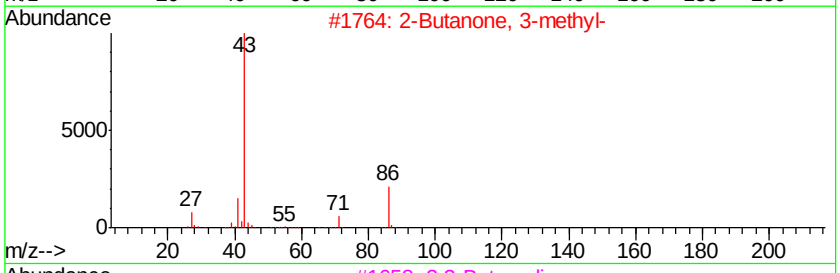
Peak Number 4 2-Pentanone Concentration Rank 8

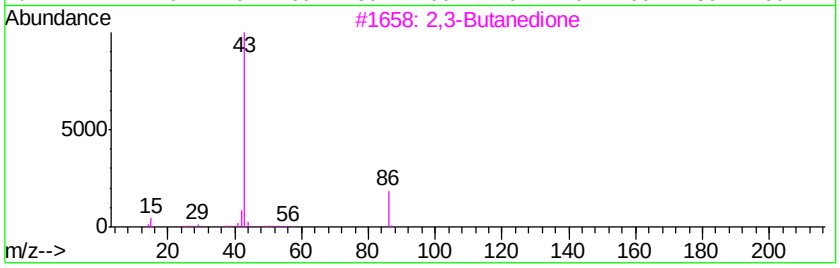
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.45 | 5.49 ug/l | 275477 | 1,4-Difluorobenzene | 8.59 |

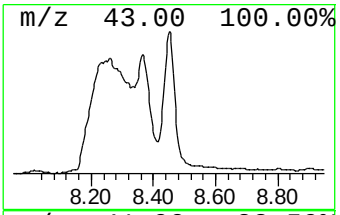
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone | 86 | C5H10O | 000107-87-9 | 59 |
| 2 | 2-Butanone, 3-methyl- | 86 | C5H10O | 000563-80-4 | 50 |
| 3 | 2,3-Butanedione | 86 | C4H6O2 | 000431-03-8 | 40 |
| 4 | 2-Propanone, methylhydrazone | 86 | C4H10N2 | 005771-02-8 | 32 |
| 5 | 2-Imidazolidinone | 86 | C3H6N2O | 000120-93-4 | 9 |

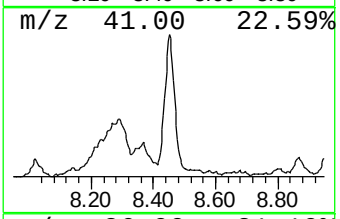


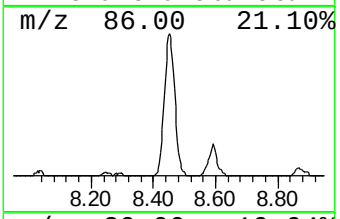



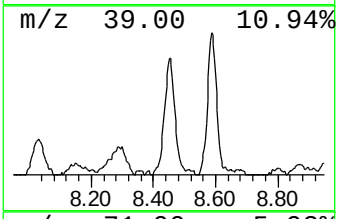



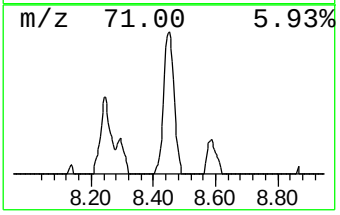



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

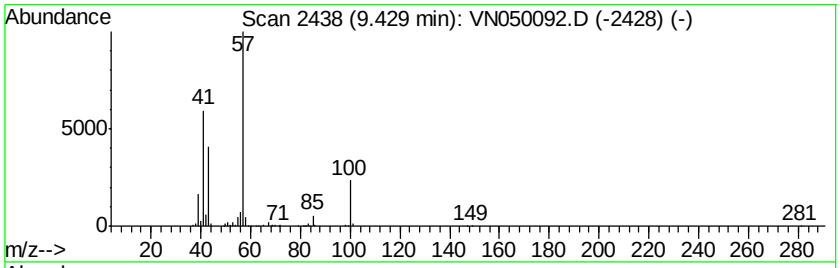
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

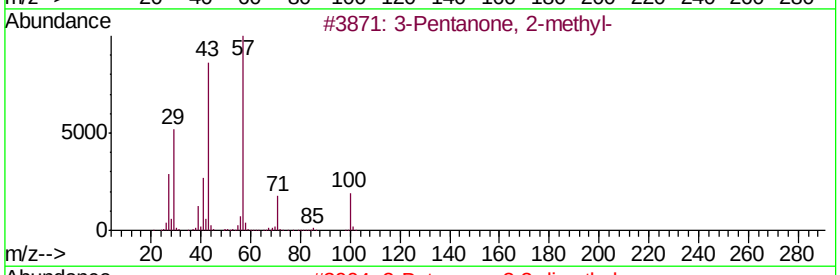
**********

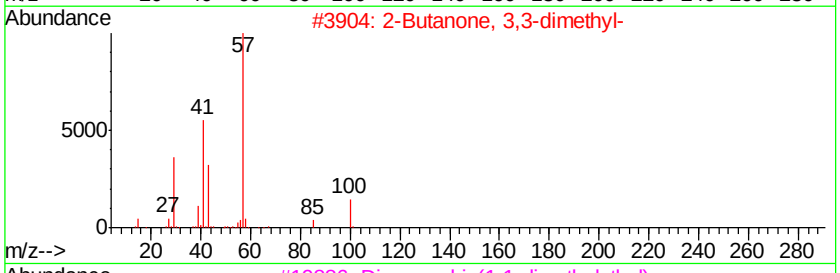
Peak Number 5 3-Pentanone, 2-methyl- Concentration Rank 5

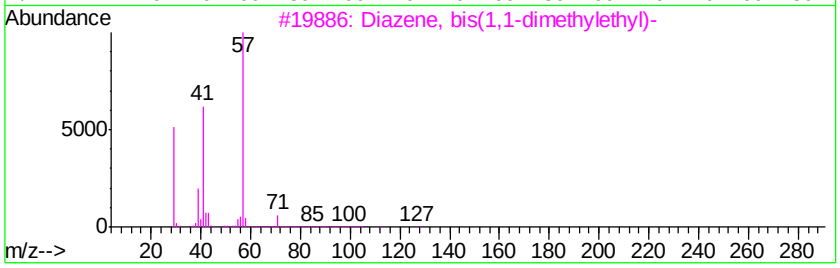
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.43 | 12.63 ug/l | 633718 | 1,4-Difluorobenzene | 8.59 |

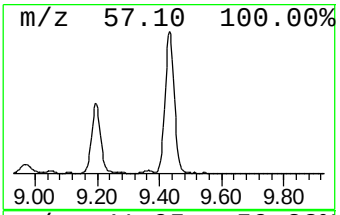
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 80 |
| 2 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 72 |
| 3 | Diazene, bis(1,1-dimethylethyl)- | 142 | C8H18N2 | 000927-83-3 | 43 |
| 4 | 3-Hexanone | 100 | C6H12O | 000589-38-8 | 42 |
| 5 | Propane, 1-(ethenyloxy)-2-methyl- | 100 | C6H12O | 000109-53-5 | 40 |

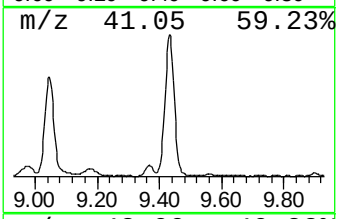


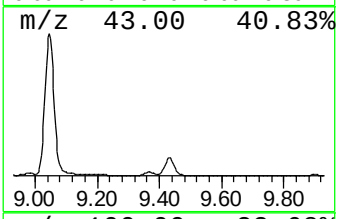



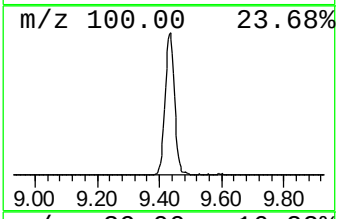



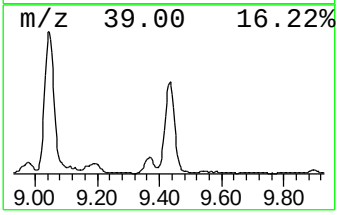



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

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

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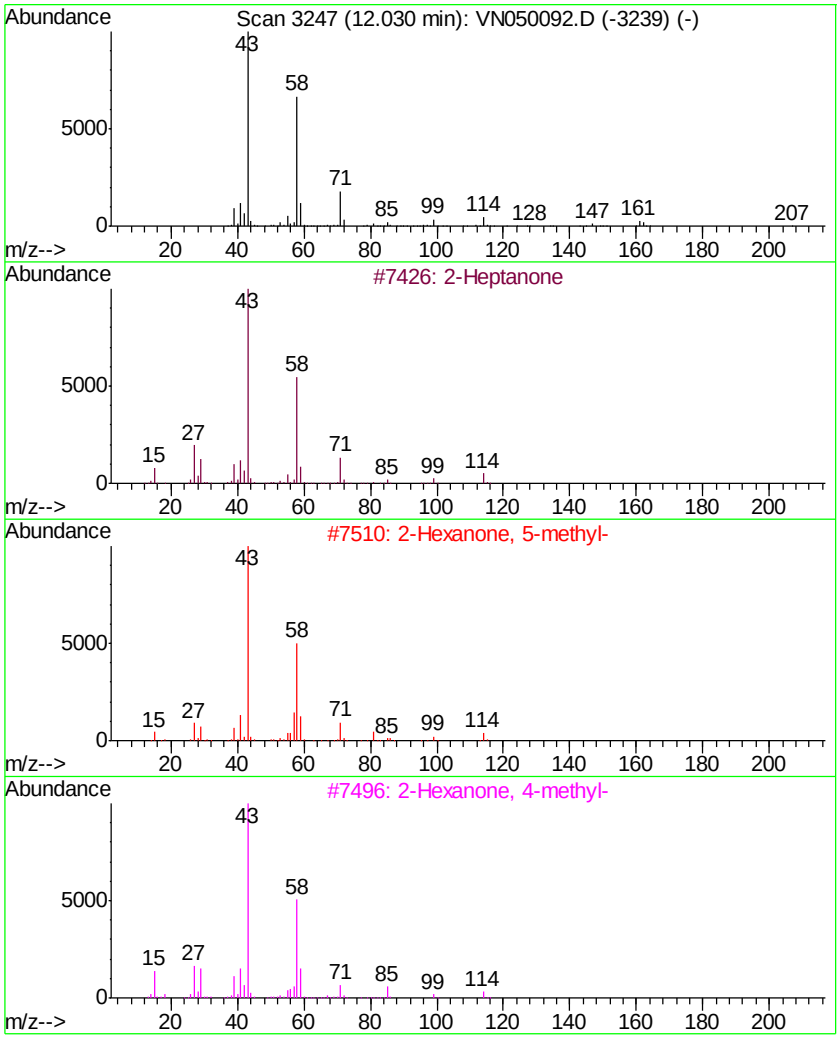
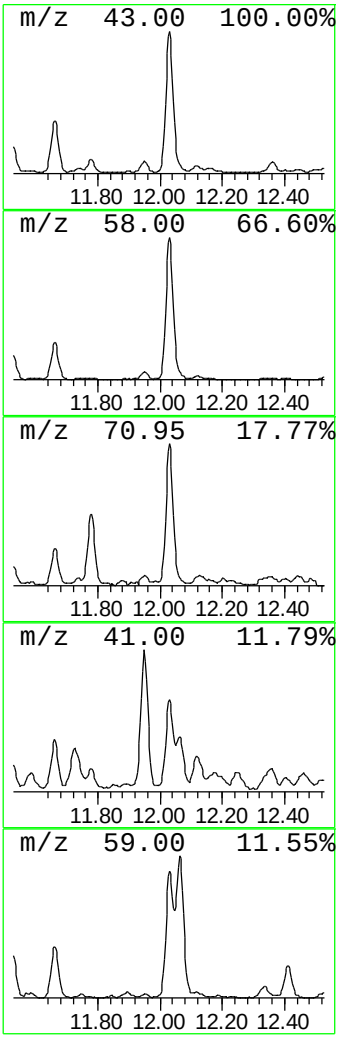
Peak Number 6 2-Heptanone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.03 | 15.81 ug/l | 933343 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptanone | 114 | C7H14O | 000110-43-0 | 90 |
| 2 | 2-Hexanone, 5-methyl- | 114 | C7H14O | 000110-12-3 | 86 |
| 3 | 2-Hexanone, 4-methyl- | 114 | C7H14O | 000105-42-0 | 59 |
| 4 | 2-Octanone | 128 | C8H16O | 000111-13-7 | 50 |
| 5 | 2-Pentanone, 4,4-dimethyl- | 114 | C7H14O | 000590-50-1 | 47 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

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

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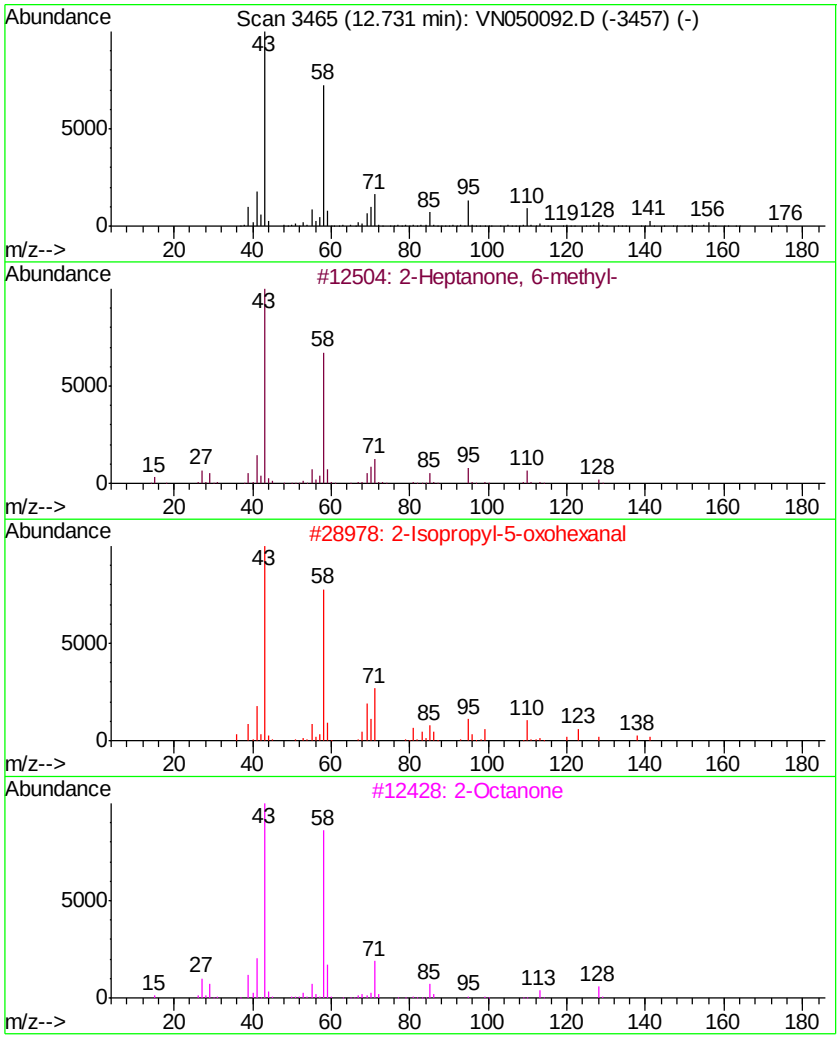
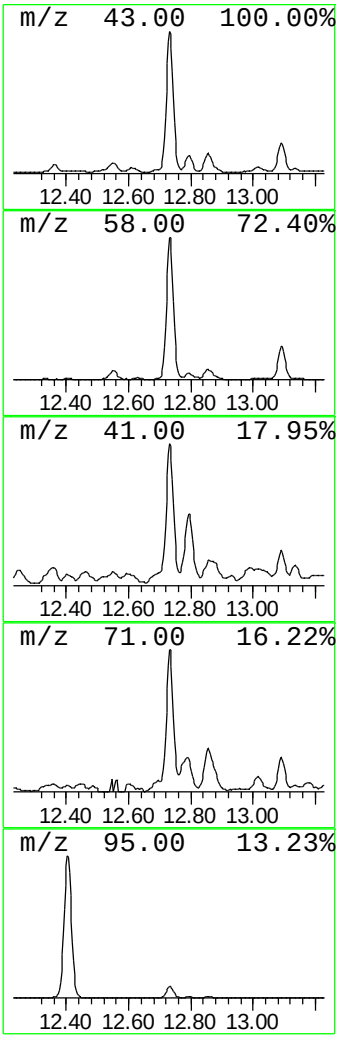
Peak Number 7 2-Heptanone, 6-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.73 | 18.02 ug/l | 1122420 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptanone, 6-methyl- | 128 | C8H16O | 000928-68-7 | 94 |
| 2 | 2-Isopropyl-5-oxohexanal | 156 | C9H16O2 | 015303-46-5 | 56 |
| 3 | 2-Octanone | 128 | C8H16O | 000111-13-7 | 53 |
| 4 | 2-Heptanone | 114 | C7H14O | 000110-43-0 | 53 |
| 5 | 2-Nonanone | 142 | C9H18O | 000821-55-6 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

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

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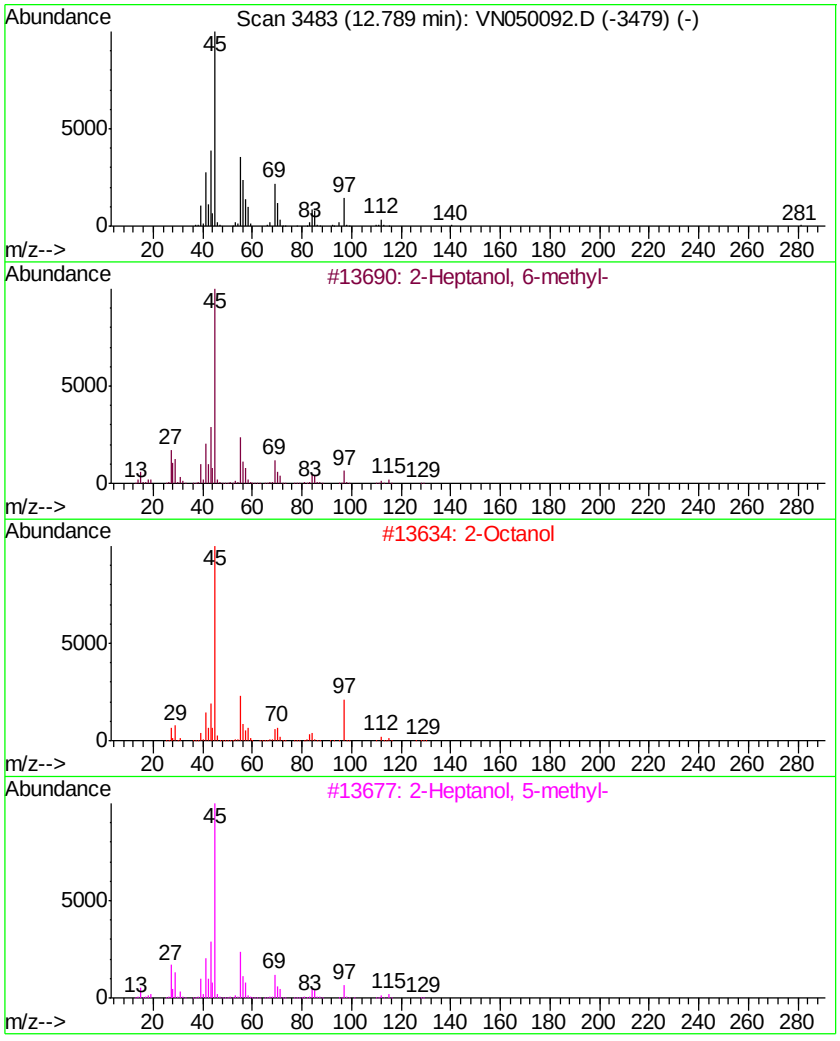
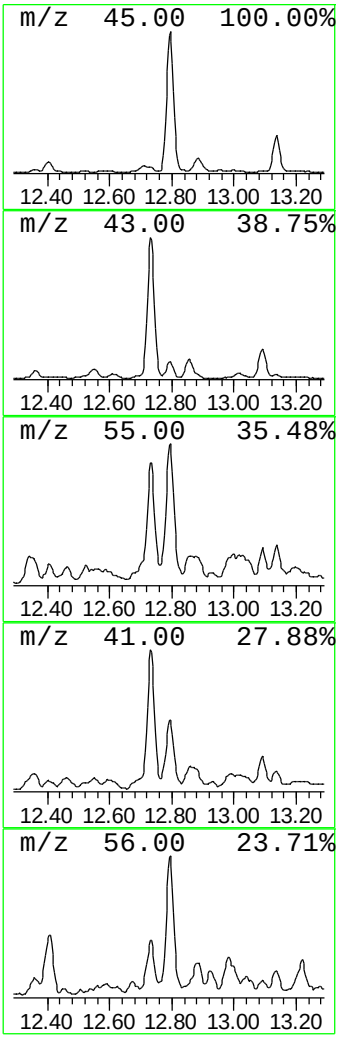
Peak Number 8 2-Heptanol, 6-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.79 | 6.26 ug/l | 389979 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptanol, 6-methyl- | 130 | C8H18O | 004730-22-7 | 72 |
| 2 | 2-Octanol | 130 | C8H18O | 000123-96-6 | 72 |
| 3 | 2-Heptanol, 5-methyl- | 130 | C8H18O | 054630-50-1 | 72 |
| 4 | 2-Octanol, (S)- | 130 | C8H18O | 006169-06-8 | 64 |
| 5 | 2-Octanol, (R)- | 130 | C8H18O | 005978-70-1 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN072618\
Data File : VN050092.D
Acq On : 26 Jul 2018 19:21
Operator : MD\SY
Sample : J4158-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** OILY-WATER-TOTES

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N072418W.M
Quant Title : SW846 8260

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Propene | 1.82 | 14.8 | ug/l | 593578 | 1 | 7.67 | 2004820 | 50.0 |
| Acetic acid | 8.23 | 7.8 | ug/l | 392995 | 2 | 8.59 | 2507810 | 50.0 |
| 2-Pentanone | 8.45 | 5.5 | ug/l | 275477 | 2 | 8.59 | 2507810 | 50.0 |
| 3-Pentanone, 2-me... | 9.43 | 12.6 | ug/l | 633718 | 2 | 8.59 | 2507810 | 50.0 |
| 2-Heptanone | 12.03 | 15.8 | ug/l | 933343 | 3 | 11.41 | 2951250 | 50.0 |
| 2-Heptanone, 6-me... | 12.73 | 18.0 | ug/l | 1122420 | 4 | 13.35 | 3114910 | 50.0 |
| 2-Heptanol, 6-met... | 12.79 | 6.3 | ug/l | 389979 | 4 | 13.35 | 3114910 | 50.0 |