LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

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\82N052319W.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 | 2.699 | 272 | 288 | 323 | rVB | 5393994 | 11781865 | 6.21% | 0.783% |
| 2 | 3.066 | 386 | 402 | 433 | rVB3 | 4497636 | 11828092 | 6.23% | 0.786% |
| 3 | 3.259 | 445 | 462 | 484 | rBV | 1423566 | 3095879 | 1.63% | 0.206% |
| 4 | 3.507 | 524 | 539 | 573 | rVB | 2852751 | 6828635 | 3.60% | 0.454% |
| 5 | 3.744 | 586 | 613 | 641 | rBV | 655230 | 2042792 | 1.08% | 0.136% |
| 6 | 4.381 | 775 | 811 | 826 | rBV8 | 602393 | 2338429 | 1.23% | 0.155% |
| 7 | 4.551 | 826 | 864 | 890 | rBV | 9773813 | 40336171 | 21.26% | 2.680% |
| 8 | 5.021 | 978 | 1010 | 1057 | rVB | 6373197 | 22950814 | 12.10% | 1.525% |
| 9 | 5.349 | 1083 | 1112 | 1144 | rBV | 1323266 | 4615447 | 2.43% | 0.307% |
| 10 | 5.542 | 1144 | 1172 | 1203 | rBV | 7399084 | 23086568 | 12.17% | 1.534% |
| 11 | 5.719 | 1204 | 1227 | 1243 | rBV | 1609100 | 4962154 | 2.62% | 0.330% |
| 12 | 5.838 | 1244 | 1264 | 1274 | rVV | 2196812 | 7446918 | 3.93% | 0.495% |
| 13 | 5.905 | 1276 | 1285 | 1308 | rVB | 2906654 | 8217792 | 4.33% | 0.546% |
| 14 | 6.050 | 1308 | 1330 | 1346 | rBV | 1644214 | 5323945 | 2.81% | 0.354% |
| 15 | 6.185 | 1348 | 1372 | 1402 | rVV2 | 1378455 | 5881645 | 3.10% | 0.391% |
| 16 | 6.355 | 1403 | 1425 | 1452 | rVV3 | 3315769 | 10873780 | 5.73% | 0.722% |
| 17 | 6.503 | 1453 | 1471 | 1487 | rVV | 2142890 | 6825942 | 3.60% | 0.453% |
| 18 | 6.609 | 1487 | 1504 | 1521 | rVV | 4249714 | 13294324 | 7.01% | 0.883% |
| 19 | 6.696 | 1523 | 1531 | 1551 | rVB | 795469 | 2081005 | 1.10% | 0.138% |
| 20 | 7.313 | 1704 | 1723 | 1731 | rBV4 | 1295366 | 3576977 | 1.89% | 0.238% |
| 21 | 7.378 | 1732 | 1743 | 1760 | rVB | 3617308 | 9171205 | 4.83% | 0.609% |
| 22 | 7.629 | 1804 | 1821 | 1841 | rBV2 | 12634650 | 34762052 | 18.32% | 2.309% |
| 23 | 7.738 | 1842 | 1855 | 1876 | rVB3 | 6125147 | 17792942 | 9.38% | 1.182% |
| 24 | 7.870 | 1876 | 1896 | 1929 | rVB | 14314594 | 34603040 | 18.24% | 2.299% |
| 25 | 8.037 | 1929 | 1948 | 1969 | rBV | 3107885 | 8554161 | 4.51% | 0.568% |
| 26 | 8.153 | 1970 | 1984 | 1988 | rBV4 | 3514189 | 7288544 | 3.84% | 0.484% |
| 27 | 8.204 | 1990 | 2000 | 2023 | rVB | 9553196 | 28531433 | 15.04% | 1.896% |
| 28 | 8.432 | 2051 | 2071 | 2097 | rVB2 | 10536236 | 30410187 | 16.03% | 2.020% |
| 29 | 8.574 | 2097 | 2115 | 2127 | rBV3 | 10247829 | 25339178 | 13.36% | 1.683% |
| 30 | 8.741 | 2156 | 2167 | 2179 | rVB | 2866412 | 5398145 | 2.85% | 0.359% |
| 31 | 8.821 | 2179 | 2192 | 2194 | rBV3 | 2900819 | 4708445 | 2.48% | 0.313% |
| 32 | 9.082 | 2243 | 2273 | 2283 | rBV5 | 8464317 | 24370826 | 12.85% | 1.619% |
| 33 | 9.140 | 2283 | 2291 | 2305 | rVB | 4482457 | 8723412 | 4.60% | 0.580% |
| 34 | 9.268 | 2322 | 2331 | 2343 | rVB | 2074083 | 4004893 | 2.11% | 0.266% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
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Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

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\82N052319W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.362 | 2343 | 2360 | 2374 | rBV4 | 1526488 | 4631916 | 2.44% | 0.308% |
| 36 | 9.519 | 2397 | 2409 | 2418 | rBV | 6732939 | 13636891 | 7.19% | 0.906% |
| 37 | 9.616 | 2429 | 2439 | 2443 | rBV2 | 4288283 | 7122773 | 3.75% | 0.473% |
| 38 | 9.657 | 2444 | 2452 | 2464 | rVB4 | 8564221 | 18219613 | 9.60% | 1.210% |
| 39 | 9.728 | 2464 | 2474 | 2481 | rBV | 9209542 | 16748780 | 8.83% | 1.113% |
| 40 | 9.870 | 2499 | 2518 | 2538 | rBV | 10474634 | 25117855 | 13.24% | 1.669% |
| 41 | 9.966 | 2538 | 2548 | 2556 | rBV3 | 2342259 | 4199475 | 2.21% | 0.279% |
| 42 | 10.021 | 2556 | 2565 | 2575 | rVB3 | 2816760 | 5082885 | 2.68% | 0.338% |
| 43 | 10.085 | 2575 | 2585 | 2594 | rBV4 | 2817371 | 6225334 | 3.28% | 0.414% |
| 44 | 10.156 | 2596 | 2607 | 2619 | rVV | 17390279 | 31370938 | 16.54% | 2.084% |
| 45 | 10.288 | 2631 | 2648 | 2659 | rVB3 | 10862727 | 23345152 | 12.30% | 1.551% |
| 46 | 10.349 | 2659 | 2667 | 2675 | rBV3 | 2788375 | 4564780 | 2.41% | 0.303% |
| 47 | 10.519 | 2711 | 2720 | 2742 | rVB7 | 4108878 | 11167887 | 5.89% | 0.742% |
| 48 | 10.625 | 2744 | 2753 | 2763 | rVB4 | 1788413 | 3456714 | 1.82% | 0.230% |
| 49 | 10.718 | 2763 | 2782 | 2791 | rBV3 | 1876250 | 4282986 | 2.26% | 0.285% |
| 50 | 10.821 | 2791 | 2814 | 2826 | rBV4 | 3217127 | 8992698 | 4.74% | 0.597% |
| 51 | 10.918 | 2837 | 2844 | 2852 | rBV3 | 1374693 | 2121484 | 1.12% | 0.141% |
| 52 | 11.059 | 2881 | 2888 | 2899 | rVB4 | 1703934 | 3413216 | 1.80% | 0.227% |
| 53 | 11.124 | 2901 | 2908 | 2915 | rBV2 | 1305232 | 2032589 | 1.07% | 0.135% |
| 54 | 11.198 | 2922 | 2931 | 2952 | rVB3 | 8836634 | 19559079 | 10.31% | 1.299% |
| 55 | 11.300 | 2953 | 2963 | 2981 | rBV | 6939394 | 12183539 | 6.42% | 0.809% |
| 56 | 11.416 | 2989 | 2999 | 3015 | rBV7 | 2633697 | 5511468 | 2.90% | 0.366% |
| 57 | 11.513 | 3017 | 3029 | 3045 | rVV2 | 31129502 | 54912942 | 28.94% | 3.648% |
| 58 | 11.625 | 3048 | 3064 | 3085 | rVB3 | 79339030 | 189724197 | 100.00% | 12.605% |
| 59 | 11.853 | 3128 | 3135 | 3145 | rVV4 | 1329362 | 2527732 | 1.33% | 0.168% |
| 60 | 11.950 | 3148 | 3165 | 3180 | rVB2 | 37765232 | 66860920 | 35.24% | 4.442% |
| 61 | 12.249 | 3249 | 3258 | 3267 | rBV | 7495388 | 11848413 | 6.25% | 0.787% |
| 62 | 12.445 | 3313 | 3319 | 3328 | rVB | 2519796 | 3548415 | 1.87% | 0.236% |
| 63 | 12.593 | 3355 | 3365 | 3374 | rBV | 11187811 | 17465157 | 9.21% | 1.160% |
| 64 | 12.657 | 3374 | 3385 | 3392 | rBV2 | 42173593 | 73962373 | 38.98% | 4.914% |
| 65 | 12.734 | 3402 | 3409 | 3422 | rVB | 26239332 | 41692535 | 21.98% | 2.770% |
| 66 | 12.892 | 3446 | 3458 | 3474 | rBV | 14952971 | 25840992 | 13.62% | 1.717% |
| 67 | 13.043 | 3492 | 3505 | 3517 | rBV3 | 59881439 | 105227450 | 55.46% | 6.991% |
| 68 | 13.165 | 3531 | 3543 | 3551 | rBV3 | 1486707 | 3852952 | 2.03% | 0.256% |
| 69 | 13.233 | 3558 | 3564 | 3573 | rVB | 2272831 | 3422587 | 1.80% | 0.227% |
| 70 | 13.374 | 3595 | 3608 | 3619 | rVB | 14905436 | 24747683 | 13.04% | 1.644% |
| 71 | 13.541 | 3641 | 3660 | 3667 | rBV2 | 17984748 | 36182402 | 19.07% | 2.404% |

LSC Area Percent Report

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Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

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\82N052319W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 13.583 | 3667 | 3673 | 3692 | rVV4 | 15571994 | 30136747 | 15.88% | 2.002% |
| 73 | 13.670 | 3694 | 3700 | 3709 | rVV3 | 1498830 | 2229963 | 1.18% | 0.148% |
| 74 | 13.738 | 3711 | 3721 | 3731 | rVB | 3356615 | 5551870 | 2.93% | 0.369% |
| 75 | 13.802 | 3731 | 3741 | 3746 | rBV | 7234845 | 11723095 | 6.18% | 0.779% |
| 76 | 13.831 | 3746 | 3750 | 3759 | rVV | 6709272 | 9396371 | 4.95% | 0.624% |
| 77 | 13.889 | 3759 | 3768 | 3778 | rVB | 12129111 | 18188358 | 9.59% | 1.208% |
| 78 | 13.995 | 3791 | 3801 | 3811 | rVB2 | 4022373 | 6633174 | 3.50% | 0.441% |
| 79 | 14.127 | 3832 | 3842 | 3851 | rBV | 2362803 | 3731328 | 1.97% | 0.248% |
| 80 | 14.207 | 3857 | 3867 | 3873 | rBV | 6124157 | 9568373 | 5.04% | 0.636% |
| 81 | 14.246 | 3873 | 3879 | 3888 | rVV | 8460555 | 12481916 | 6.58% | 0.829% |
| 82 | 14.294 | 3888 | 3894 | 3901 | rVV2 | 2133824 | 2679776 | 1.41% | 0.178% |
| 83 | 14.474 | 3943 | 3950 | 3959 | rVV | 3766672 | 6305911 | 3.32% | 0.419% |
| 84 | 14.522 | 3960 | 3965 | 3973 | rVB2 | 1750086 | 2423846 | 1.28% | 0.161% |
| 85 | 14.586 | 3973 | 3985 | 3997 | rBV4 | 6336505 | 14390481 | 7.58% | 0.956% |
| 86 | 14.651 | 3997 | 4005 | 4017 | rVB2 | 1753914 | 3076115 | 1.62% | 0.204% |
| 87 | 14.853 | 4058 | 4068 | 4088 | rVB2 | 2359140 | 5681760 | 2.99% | 0.377% |
| 88 | 14.956 | 4089 | 4100 | 4113 | rVB2 | 1339137 | 2662297 | 1.40% | 0.177% |
| 89 | 15.130 | 4135 | 4154 | 4167 | rVB | 6448739 | 11434090 | 6.03% | 0.760% |
| 90 | 16.159 | 4460 | 4474 | 4508 | rVB | 3684245 | 7525681 | 3.97% | 0.500% |
| 91 | 16.348 | 4518 | 4533 | 4556 | rVB | 1620747 | 3536327 | 1.86% | 0.235% |

Sum of corrected areas: 1505209918

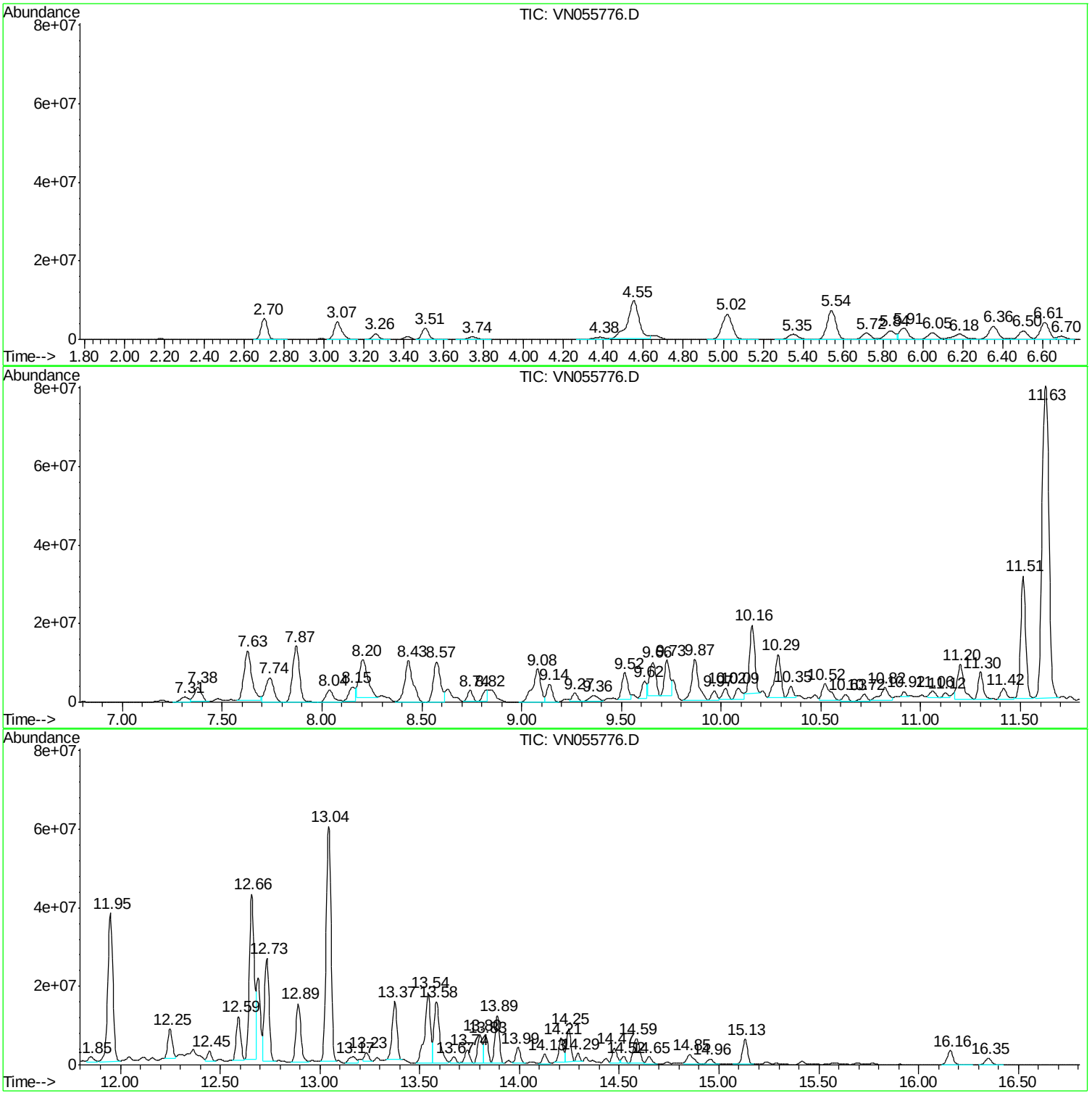
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

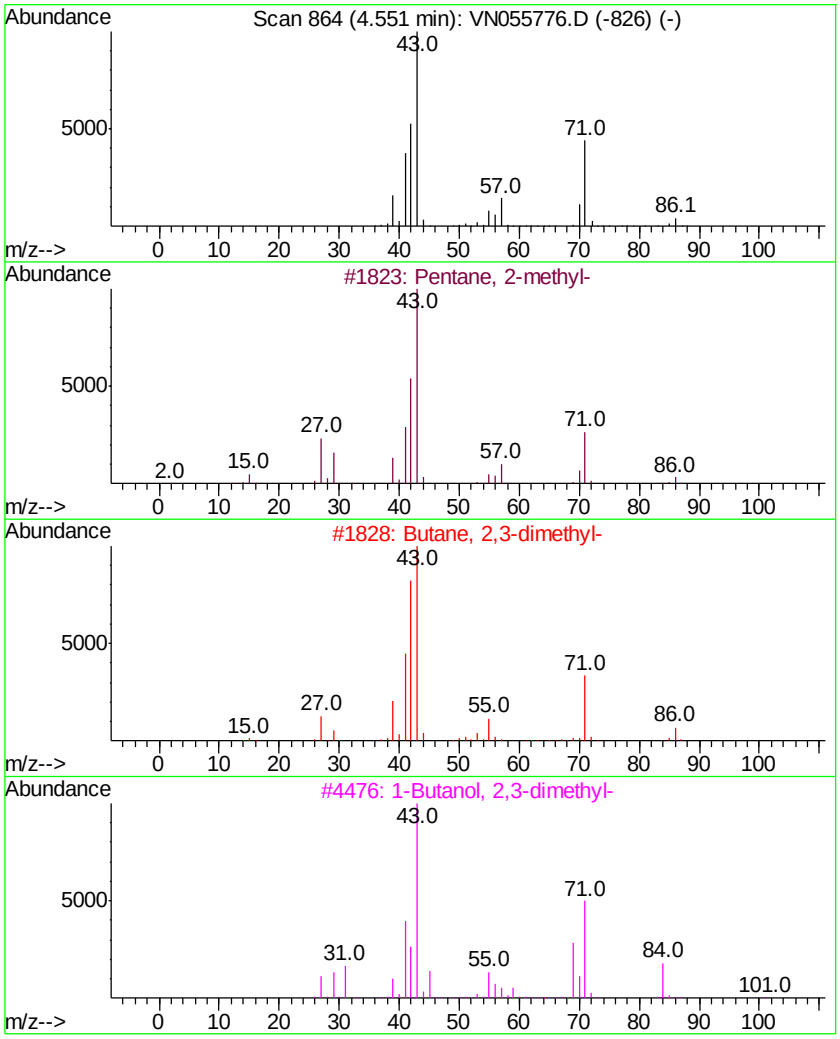
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

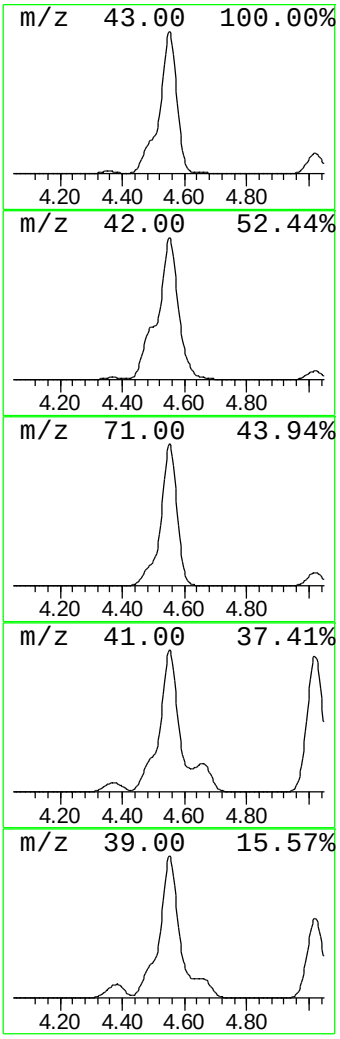
**********

Peak Number 1 Pentane, 2-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.55 | 58.02 ug/l | 40336200 | Pentafluorobenzene | 7.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentane, 2-methyl- | 86 | C6H14 | 000107-83-5 | 91 |
| 2 | Butane, 2,3-dimethyl- | 86 | C6H14 | 000079-29-8 | 72 |
| 3 | 1-Butanol, 2,3-dimethyl- | 102 | C6H14O | 019550-30-2 | 45 |
| 4 | Pentane | 72 | C5H12 | 000109-66-0 | 43 |
| 5 | Ether, hexyl pentyl | 172 | C11H24O | 032357-83-8 | 33 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

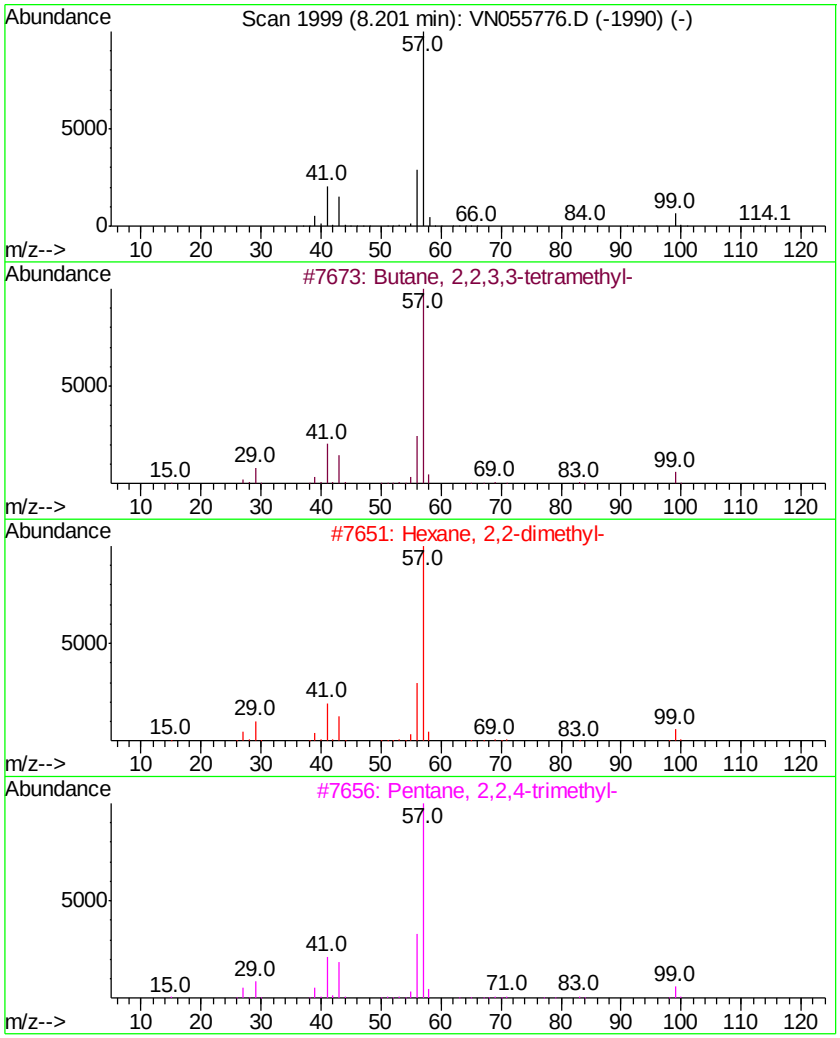
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

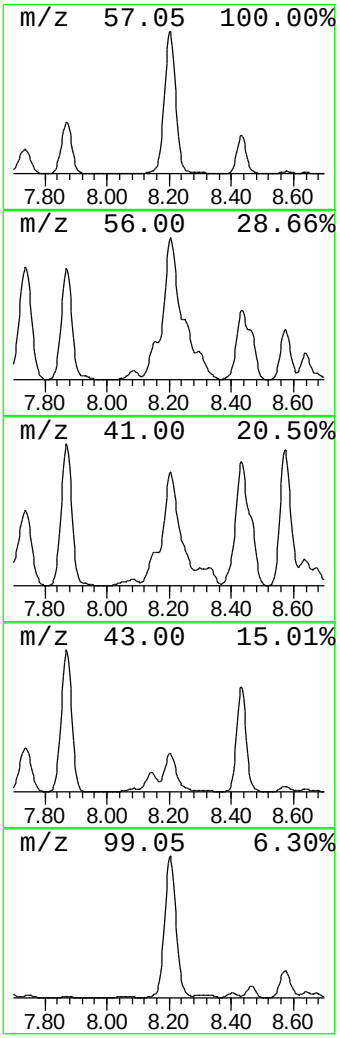
**********

Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.20 | 56.30 ug/l | 28531400 | 1,4-Difluorobenzene | 8.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2,2,3,3-tetramethyl- | 114 | C8H18 | 000594-82-1 | 78 |
| 2 | Hexane, 2,2-dimethyl- | 114 | C8H18 | 000590-73-8 | 78 |
| 3 | Pentane, 2,2,4-trimethyl- | 114 | C8H18 | 000540-84-1 | 78 |
| 4 | Pentane, 2,2,4,4-tetramethyl- | 128 | C9H20 | 001070-87-7 | 9 |
| 5 | Propanoic acid, 2-methylpropyl e... | 130 | C7H14O2 | 000540-42-1 | 9 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

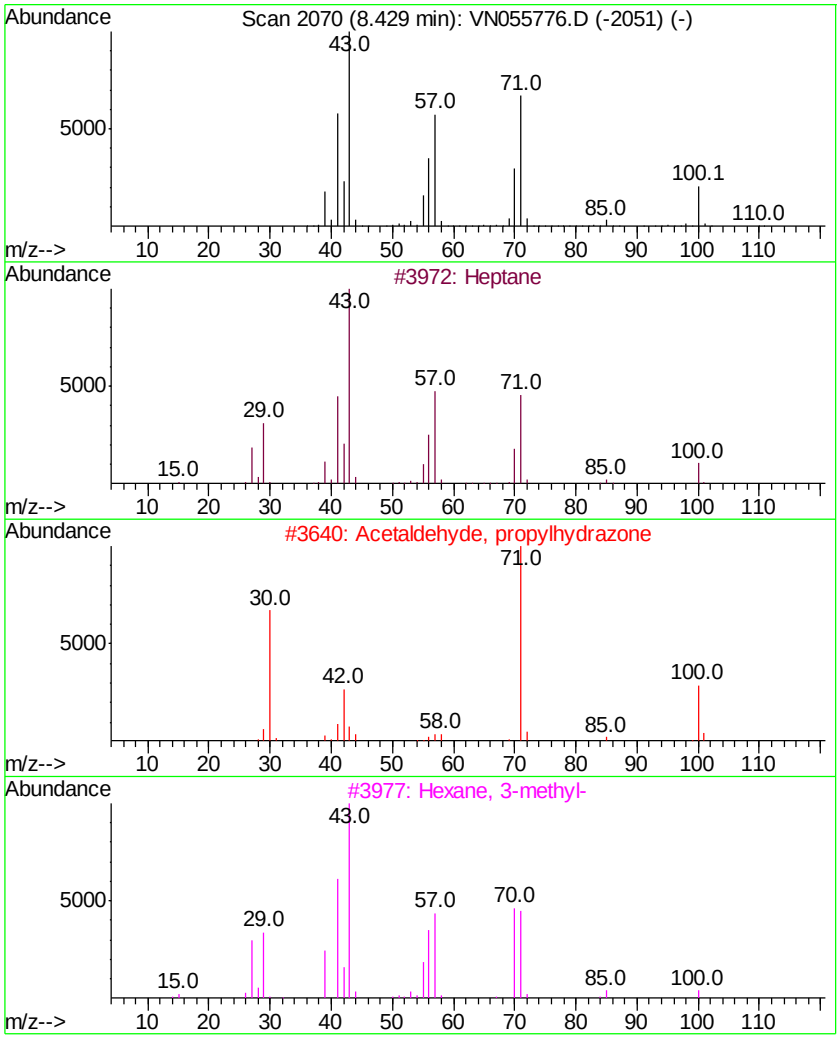
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

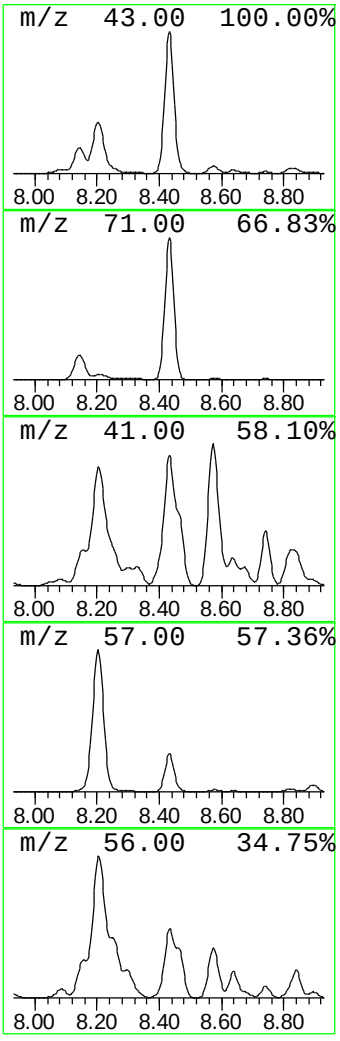
**********

Peak Number 3 Heptane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.43 | 60.01 ug/l | 30410200 | 1,4-Difluorobenzene | 8.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane | 100 | C7H16 | 000142-82-5 | 91 |
| 2 | Acetaldehyde, propylhydrazone | 100 | C5H12N2 | 007422-88-0 | 47 |
| 3 | Hexane, 3-methyl- | 100 | C7H16 | 000589-34-4 | 45 |
| 4 | Butane, 2,2-dimethyl- | 86 | C6H14 | 000075-83-2 | 40 |
| 5 | Pentane, 2,3,4-trimethyl- | 114 | C8H18 | 000565-75-3 | 40 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
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Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

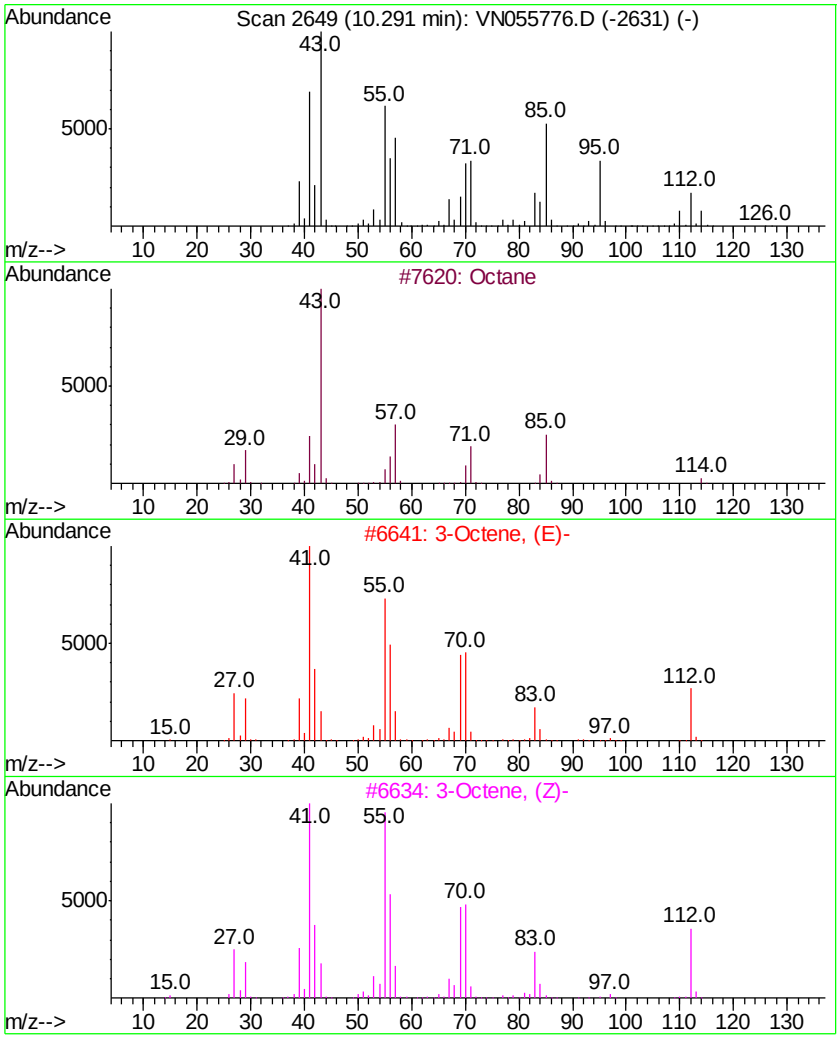
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

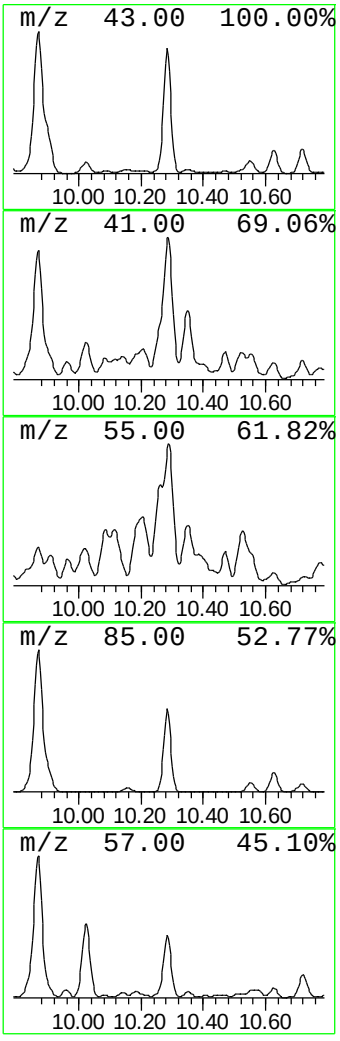
**********

Peak Number 4 Octane Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.29 | 211.79 ug/l | 23345200 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane | 114 | C8H18 | 000111-65-9 | 58 |
| 2 | 3-Octene, (E)- | 112 | C8H16 | 014919-01-8 | 46 |
| 3 | 3-Octene, (Z)- | 112 | C8H16 | 014850-22-7 | 46 |
| 4 | 2-Octene | 112 | C8H16 | 000111-67-1 | 41 |
| 5 | 2-Octene, (Z)- | 112 | C8H16 | 007642-04-8 | 41 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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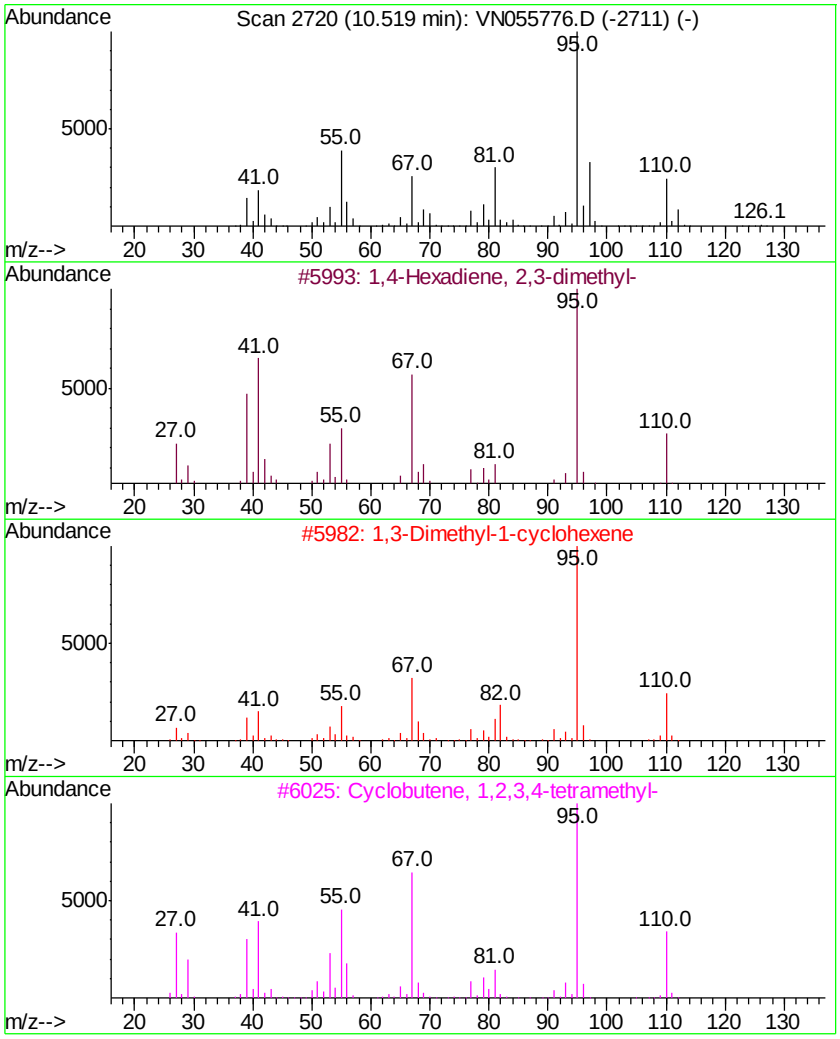
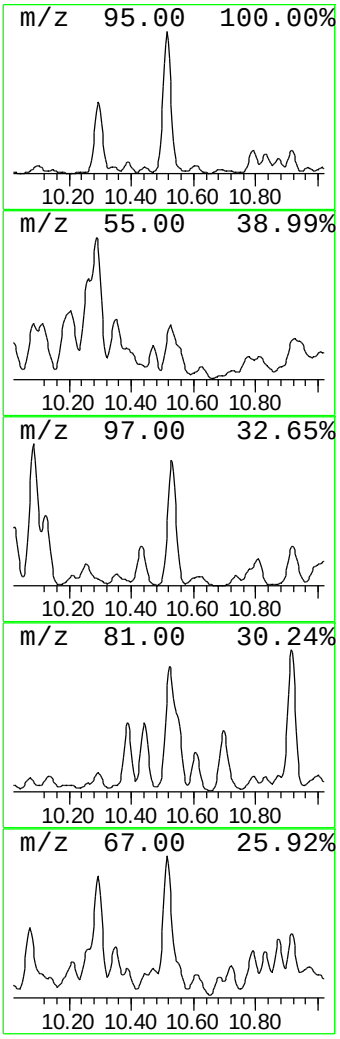
Peak Number 5 1,4-Hexadiene, 2,3-dimethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.52 | 101.32 ug/l | 11167900 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Hexadiene, 2,3-dimethyl- | 110 | C8H14 | 018669-52-8 | 76 |
| 2 | 1,3-Dimethyl-1-cyclohexene | 110 | C8H14 | 002808-76-6 | 62 |
| 3 | Cyclobutene, 1,2,3,4-tetramethyl- | 110 | C8H14 | 090346-45-5 | 62 |
| 4 | 1,4-Pentadiene, 2,3,3-trimethyl- | 110 | C8H14 | 000756-02-5 | 59 |
| 5 | 5,5-Dimethyl-1,3-hexadiene | 110 | C8H14 | 001515-79-3 | 59 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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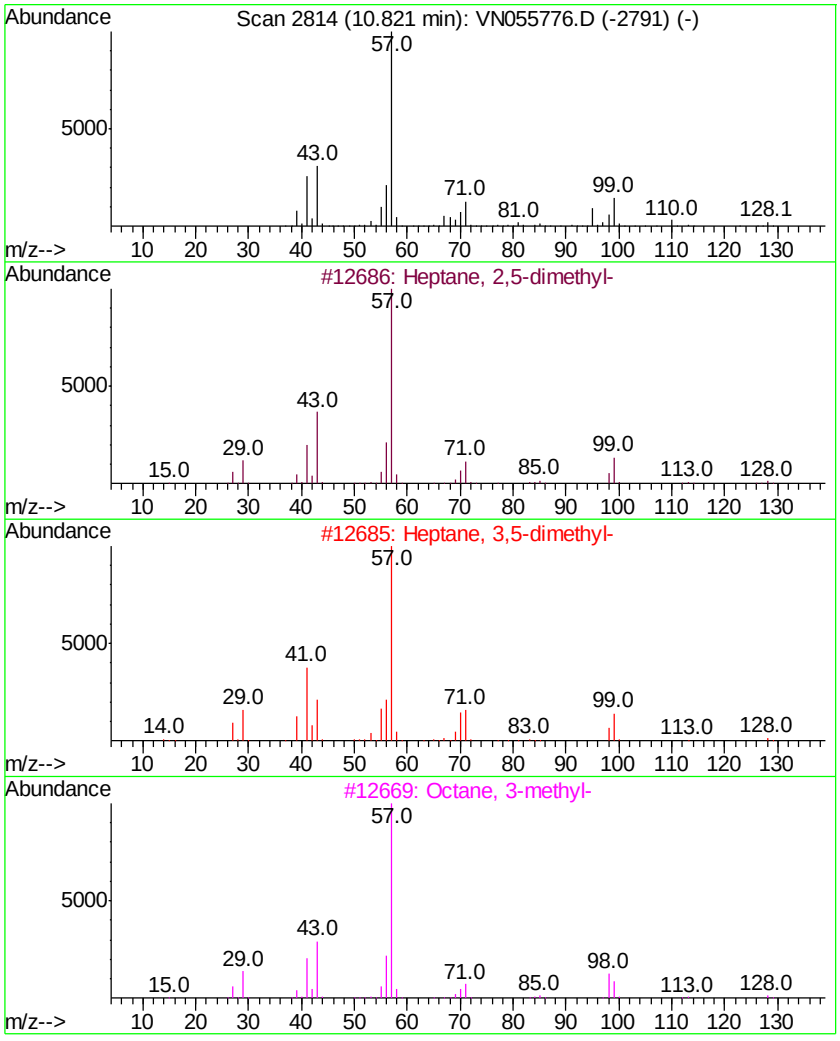
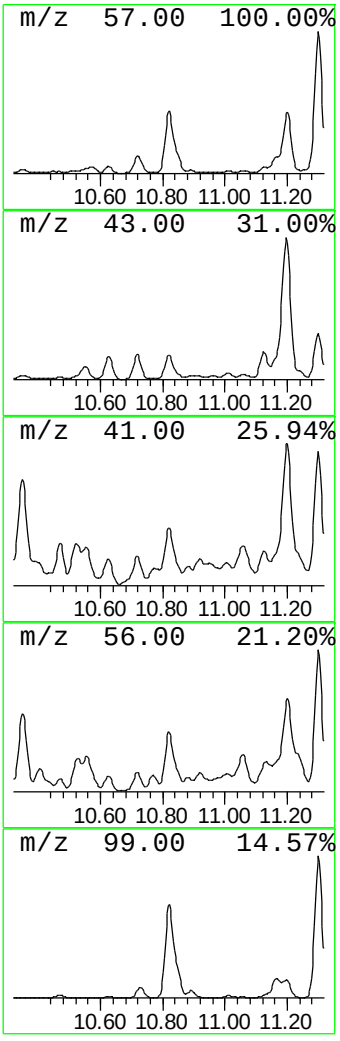
Peak Number 6 Heptane, 2,5-dimethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.82 | 81.58 ug/l | 8992700 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptane, 2,5-dimethyl- | 128 | C9H20 | 002216-30-0 | 81 |
| 2 | Heptane, 3,5-dimethyl- | 128 | C9H20 | 000926-82-9 | 74 |
| 3 | Octane, 3-methyl- | 128 | C9H20 | 002216-33-3 | 70 |
| 4 | Hexane, 3-ethyl-4-methyl- | 128 | C9H20 | 003074-77-9 | 47 |
| 5 | 2,2,4,4-Tetramethyloctane | 170 | C12H26 | 062183-79-3 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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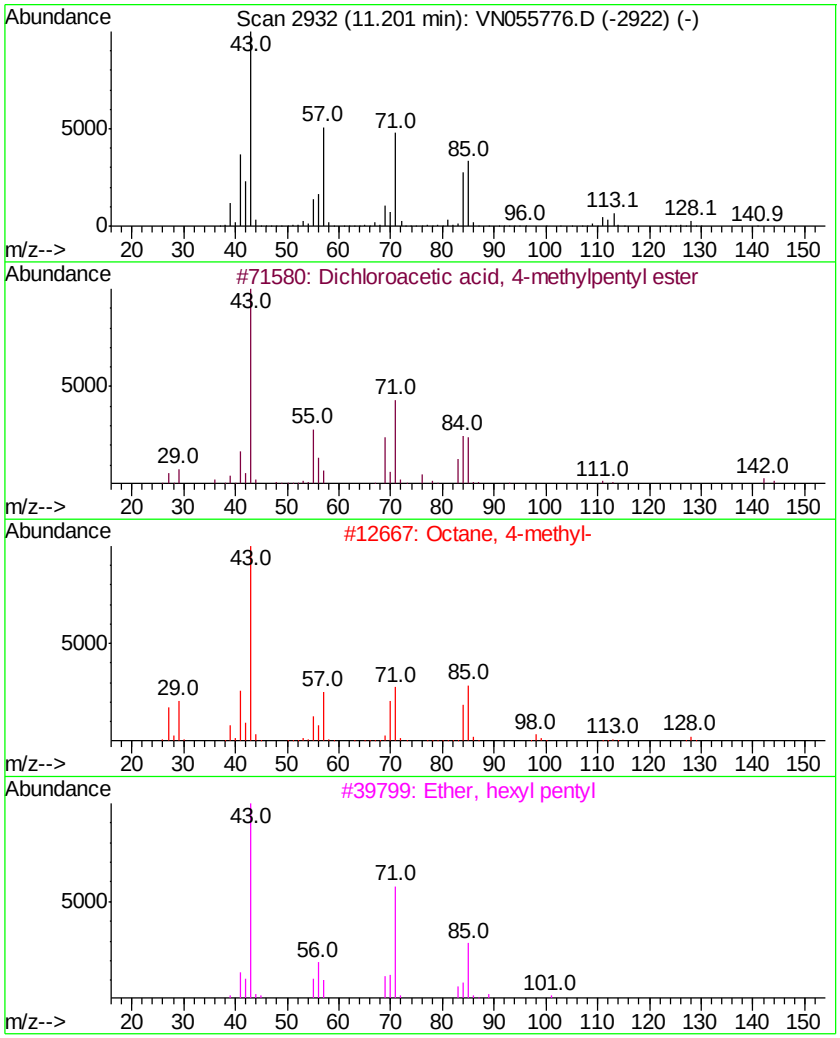
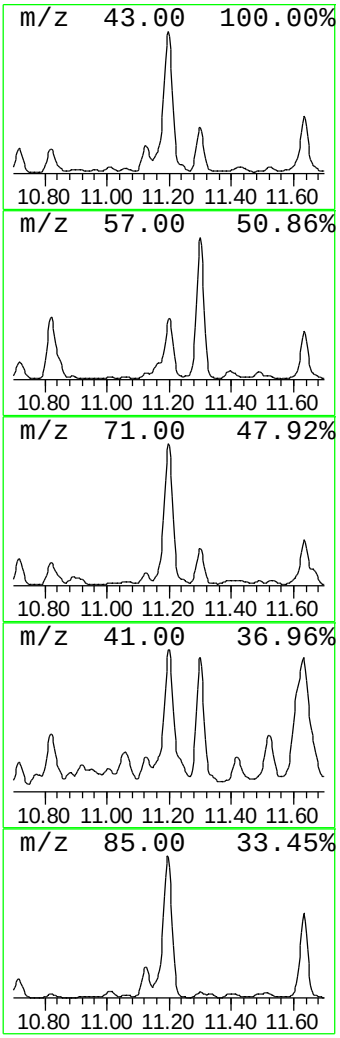
Peak Number 7 Dichloroacetic acid, 4-meth... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.20 | 177.44 ug/l | 19559100 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dichloroacetic acid, 4-methylpen... | 212 | C8H14Cl2O2 | 1000282-43-7 | 59 |
| 2 | Octane, 4-methyl- | 128 | C9H20 | 002216-34-4 | 53 |
| 3 | Ether, hexyl pentyl | 172 | C11H24O | 032357-83-8 | 53 |
| 4 | Hexane, 2,3,4-trimethyl- | 128 | C9H20 | 000921-47-1 | 53 |
| 5 | Pentane, 3-ethyl-2-methyl- | 114 | C8H18 | 000609-26-7 | 53 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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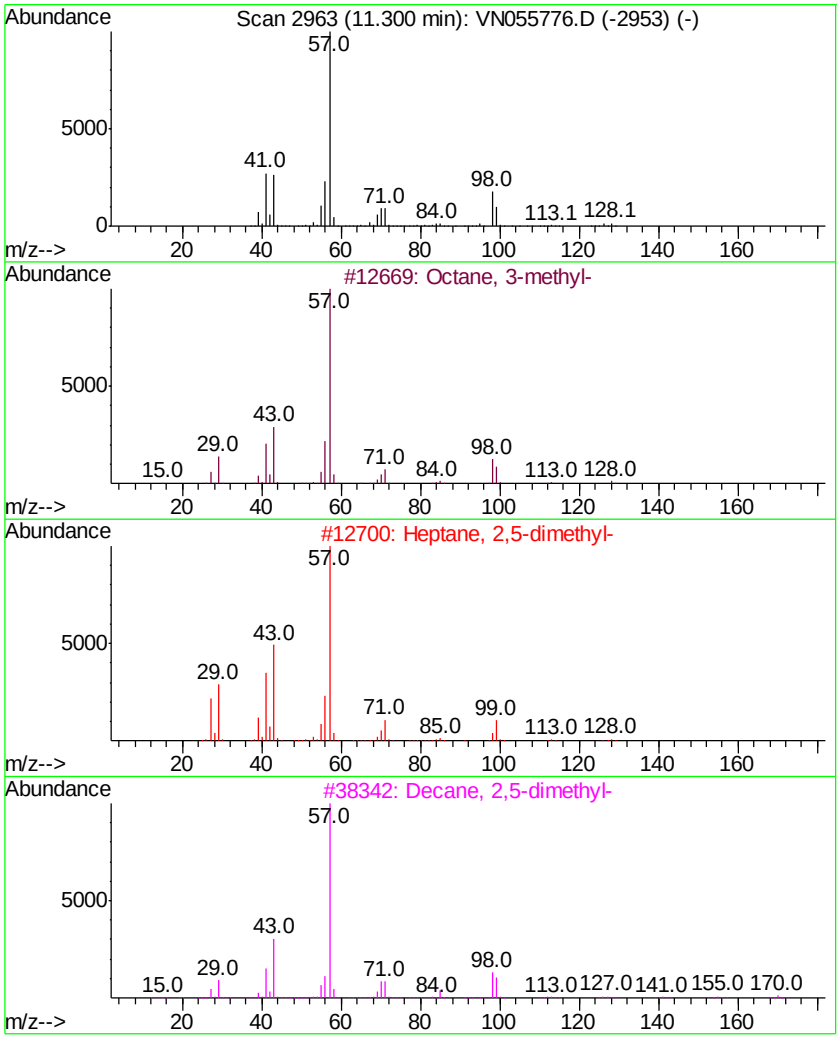
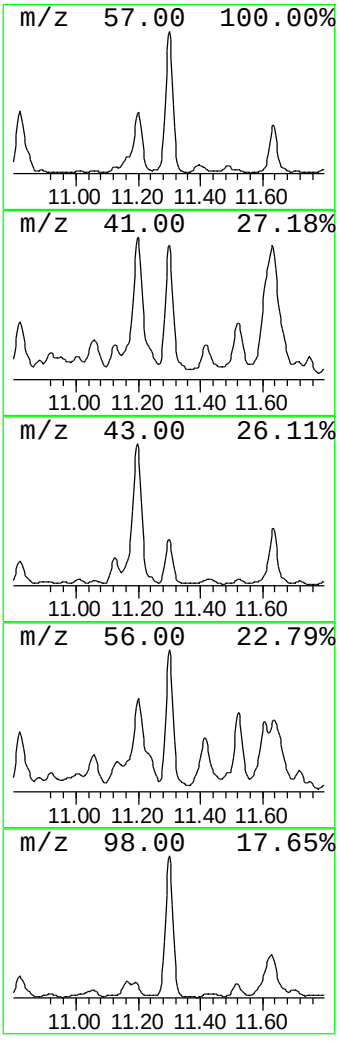
Peak Number 8 Octane, 3-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.30 | 110.53 ug/l | 12183500 | Chlorobenzene-d5 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane, 3-methyl- | 128 | C9H20 | 002216-33-3 | 91 |
| 2 | Heptane, 2,5-dimethyl- | 128 | C9H20 | 002216-30-0 | 83 |
| 3 | Decane, 2,5-dimethyl- | 170 | C12H26 | 017312-50-4 | 59 |
| 4 | Heptane, 4-propyl- | 142 | C10H22 | 003178-29-8 | 53 |
| 5 | Undecane, 6-methyl- | 170 | C12H26 | 017302-33-9 | 53 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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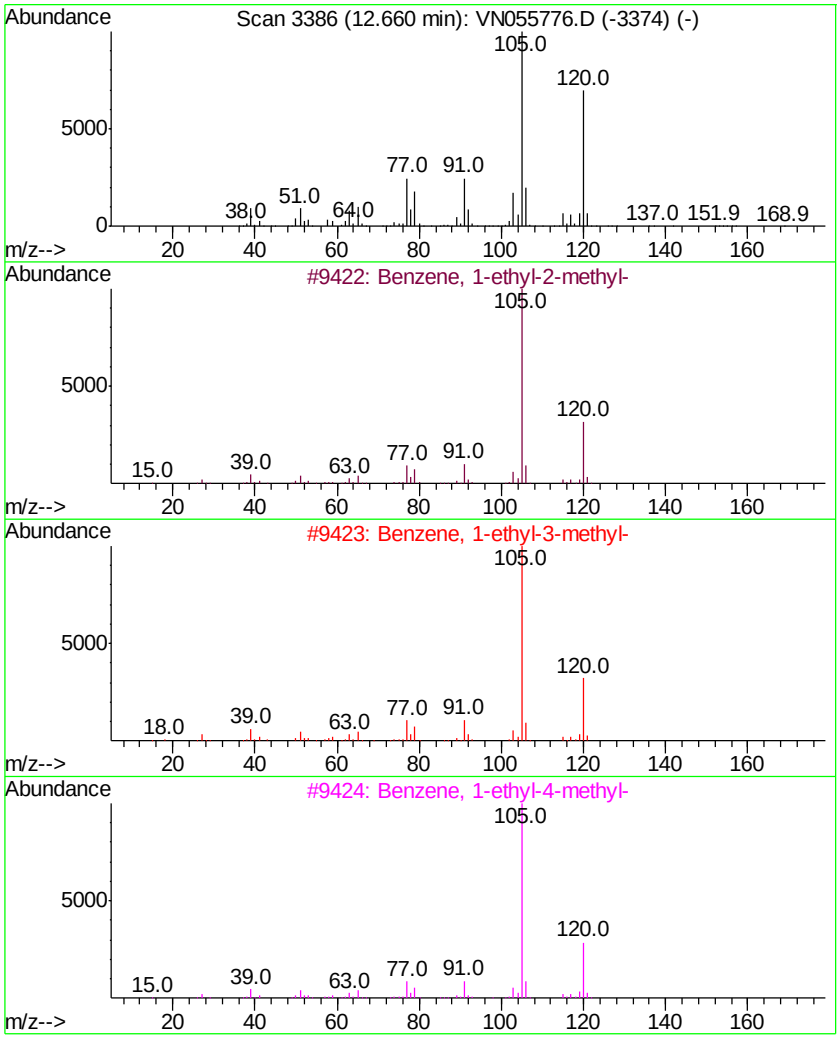
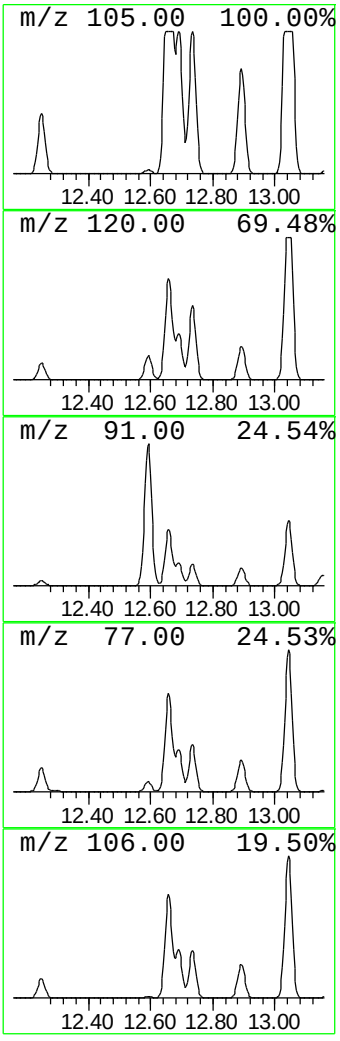
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.66 | 149.43 ug/l | 73962400 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-ethyl-2-methyl- | 120 | C9H12 | 000611-14-3 | 91 |
| 2 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 90 |
| 3 | Benzene, 1-ethyl-4-methyl- | 120 | C9H12 | 000622-96-8 | 81 |
| 4 | Benzene, 1,2,3-trimethyl- | 120 | C9H12 | 000526-73-8 | 76 |
| 5 | Benzene, (1-methylethyl)- | 120 | C9H12 | 000098-82-8 | 64 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.M
Quant Title : SW846 8260

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

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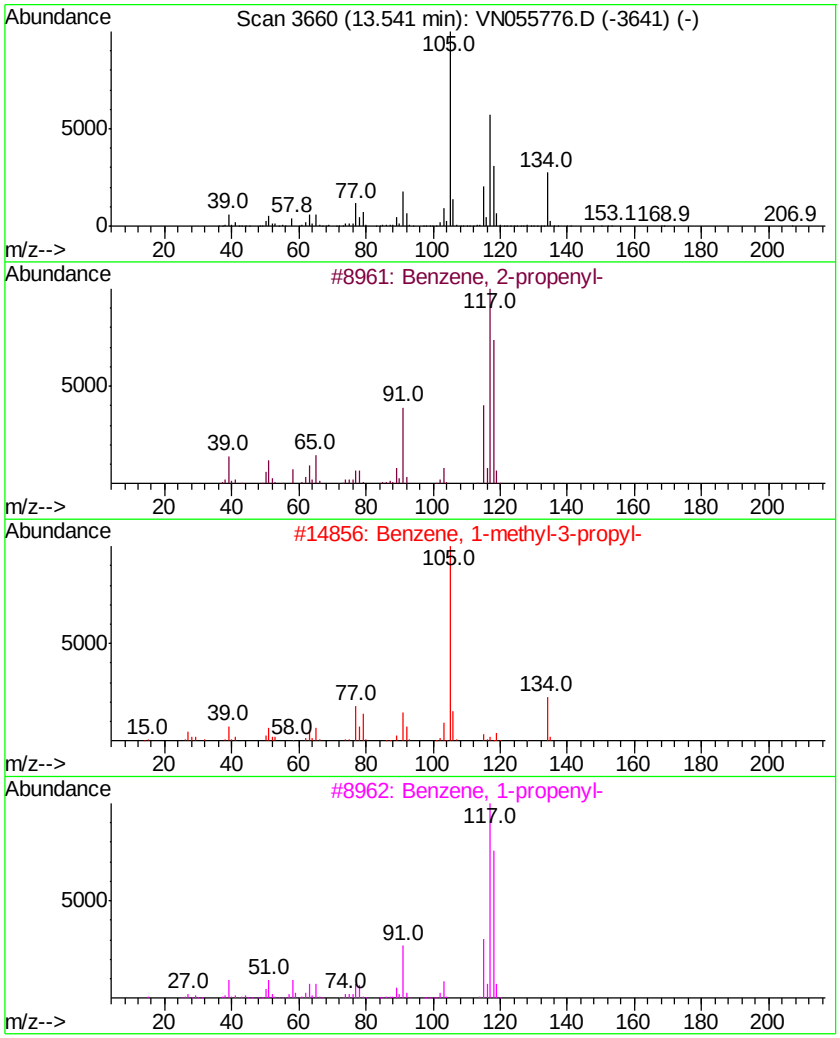
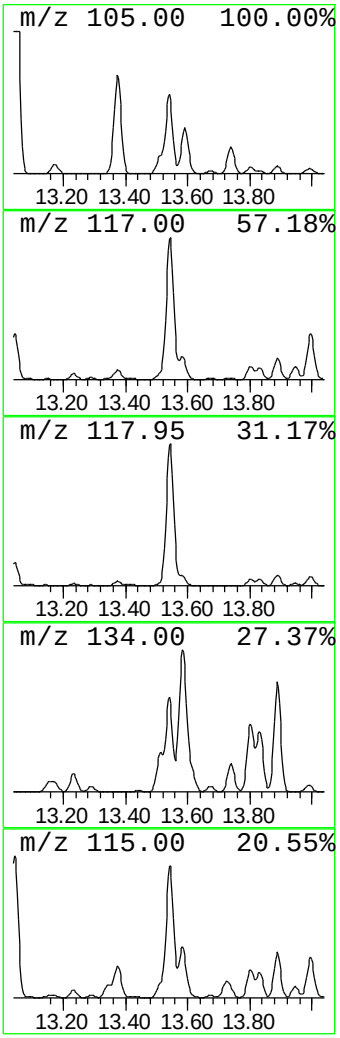
Peak Number 10 unknown13.54 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.54 | 73.10 ug/l | 36182400 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 2-propenyl- | 118 | C9H10 | 000300-57-2 | 46 |
| 2 | Benzene, 1-methyl-3-propyl- | 134 | C10H14 | 001074-43-7 | 46 |
| 3 | Benzene, 1-propenyl- | 118 | C9H10 | 000637-50-3 | 43 |
| 4 | Benzene, cyclopropyl- | 118 | C9H10 | 000873-49-4 | 43 |
| 5 | Indane | 118 | C9H10 | 000496-11-7 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN052319\
Data File : VN055776.D
Acq On : 24 May 2019 00:43
Operator : JC/SP
Sample : K2996-05
Misc : 5.27g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** MSVOA_N
**ClientSampleId :** P-3(4.5-5.0)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N052319W.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 |
| Pentane, 2-methyl- | 4.55 | 58.0 | ug/l | 40336200 | 1 | 7.66 | 34762100 | 50.0 |
| Butane, 2,2,3,3-t... | 8.20 | 56.3 | ug/l | 28531400 | 2 | 8.58 | 25339200 | 50.0 |
| Heptane | 8.43 | 60.0 | ug/l | 30410200 | 2 | 8.58 | 25339200 | 50.0 |
| Octane | 10.29 | 211.8 | ug/l | 23345200 | 3 | 11.41 | 5511470 | 50.0 |
| 1,4-Hexadiene, 2,... | 10.52 | 101.3 | ug/l | 11167900 | 3 | 11.41 | 5511470 | 50.0 |
| Heptane, 2,5-dime... | 10.82 | 81.6 | ug/l | 8992700 | 3 | 11.41 | 5511470 | 50.0 |
| Dichloroacetic ac... | 11.20 | 177.4 | ug/l | 19559100 | 3 | 11.41 | 5511470 | 50.0 |
| Octane, 3-methyl- | 11.30 | 110.5 | ug/l | 12183500 | 3 | 11.41 | 5511470 | 50.0 |
| Benzene, 1-ethyl-... | 12.66 | 149.4 | ug/l | 73962400 | 4 | 13.35 | 24747700 | 50.0 |
| unknown13.54 | 13.54 | 73.1 | ug/l | 36182400 | 4 | 13.35 | 24747700 | 50.0 |