LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052827.D
Acq On : 26 Jan 2023 19:36
Operator : JC/MD
Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
A44K9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMULM012623WMA.M
Title : VOC Analysis

Signal : TIC: VU052827.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.520 | 51 | 56 | 62 | rVB | 3266 | 2978 | 0.28% | 0.038% |
| 2 | 1.597 | 72 | 80 | 97 | rVB | 113042 | 135974 | 12.71% | 1.728% |
| 3 | 1.867 | 160 | 164 | 165 | rBV3 | 829 | 661 | 0.06% | 0.008% |
| 4 | 1.912 | 170 | 178 | 198 | rVV | 98909 | 137666 | 12.87% | 1.750% |
| 5 | 2.170 | 255 | 258 | 259 | rBV2 | 438 | 221 | 0.02% | 0.003% |
| 6 | 2.208 | 266 | 270 | 273 | rVB2 | 521 | 342 | 0.03% | 0.004% |
| 7 | 2.260 | 281 | 286 | 288 | rBV2 | 328 | 361 | 0.03% | 0.005% |
| 8 | 2.388 | 322 | 326 | 327 | rBV3 | 443 | 255 | 0.02% | 0.003% |
| 9 | 2.453 | 342 | 346 | 350 | rBV2 | 408 | 361 | 0.03% | 0.005% |
| 10 | 2.562 | 368 | 380 | 396 | rBV | 223600 | 365133 | 34.14% | 4.641% |
| 11 | 2.642 | 400 | 405 | 409 | rBV4 | 853 | 900 | 0.08% | 0.011% |
| 12 | 2.716 | 423 | 428 | 433 | rBV2 | 391 | 371 | 0.03% | 0.005% |
| 13 | 3.044 | 521 | 530 | 538 | rBV4 | 1237 | 2267 | 0.21% | 0.029% |
| 14 | 3.076 | 538 | 540 | 545 | rBV | 331 | 243 | 0.02% | 0.003% |
| 15 | 3.102 | 545 | 548 | 551 | rVB2 | 336 | 268 | 0.03% | 0.003% |
| 16 | 3.179 | 564 | 572 | 574 | rBV2 | 838 | 1109 | 0.10% | 0.014% |
| 17 | 3.192 | 574 | 576 | 578 | rVV | 927 | 467 | 0.04% | 0.006% |
| 18 | 3.205 | 578 | 580 | 586 | rVB2 | 345 | 290 | 0.03% | 0.004% |
| 19 | 3.427 | 646 | 649 | 654 | rVB2 | 293 | 307 | 0.03% | 0.004% |
| 20 | 3.559 | 684 | 690 | 693 | rBV2 | 203 | 278 | 0.03% | 0.004% |
| 21 | 3.674 | 722 | 726 | 733 | rBV2 | 256 | 291 | 0.03% | 0.004% |
| 22 | 3.751 | 746 | 750 | 753 | rBV2 | 341 | 407 | 0.04% | 0.005% |
| 23 | 3.877 | 786 | 789 | 795 | rBV2 | 242 | 264 | 0.02% | 0.003% |
| 24 | 4.211 | 890 | 893 | 899 | rBV2 | 256 | 260 | 0.02% | 0.003% |
| 25 | 4.411 | 951 | 955 | 962 | rVB2 | 298 | 449 | 0.04% | 0.006% |
| 26 | 4.530 | 986 | 992 | 997 | rVB2 | 254 | 277 | 0.03% | 0.004% |
| 27 | 4.555 | 997 | 1000 | 1003 | rBV | 363 | 273 | 0.03% | 0.003% |
| 28 | 4.623 | 1009 | 1021 | 1050 | rBV | 70640 | 191645 | 17.92% | 2.436% |
| 29 | 5.057 | 1139 | 1156 | 1178 | rBV | 199207 | 438533 | 41.01% | 5.574% |
| 30 | 5.211 | 1200 | 1204 | 1207 | rBV | 257 | 229 | 0.02% | 0.003% |
| 31 | 5.292 | 1220 | 1229 | 1238 | rVB5 | 737 | 1555 | 0.15% | 0.020% |
| 32 | 5.333 | 1238 | 1242 | 1245 | rVB2 | 289 | 268 | 0.03% | 0.003% |
| 33 | 5.523 | 1298 | 1301 | 1304 | rVV2 | 407 | 307 | 0.03% | 0.004% |
| 34 | 5.626 | 1330 | 1333 | 1336 | rBV | 258 | 217 | 0.02% | 0.003% |
| 35 | 5.719 | 1341 | 1362 | 1386 | rBV2 | 396497 | 1069431 | 100.00% | 13.592% |
| 36 | 5.903 | 1416 | 1419 | 1424 | rVB2 | 242 | 224 | 0.02% | 0.003% |

LSC Area Percent Report

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Data File : VU052827.D
Acq On : 26 Jan 2023 19:36
Operator : JC/MD
Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
A44K9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMULM012623WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 5.999 | 1445 | 1449 | 1452 | rVB2 | 447 | 361 | 0.03% | 0.005% |
| 38 | 6.243 | 1511 | 1525 | 1553 | rBV | 318122 | 603555 | 56.44% | 7.671% |
| 39 | 6.411 | 1574 | 1577 | 1582 | rVB3 | 315 | 301 | 0.03% | 0.004% |
| 40 | 6.491 | 1596 | 1602 | 1604 | rBV2 | 415 | 383 | 0.04% | 0.005% |
| 41 | 6.536 | 1604 | 1616 | 1632 | rBV7 | 9949 | 18759 | 1.75% | 0.238% |
| 42 | 6.594 | 1632 | 1634 | 1639 | rVB3 | 561 | 375 | 0.04% | 0.005% |
| 43 | 6.684 | 1644 | 1662 | 1686 | rBV | 244548 | 474058 | 44.33% | 6.025% |
| 44 | 6.806 | 1693 | 1700 | 1705 | rBV4 | 764 | 899 | 0.08% | 0.011% |
| 45 | 7.108 | 1789 | 1794 | 1797 | rBV2 | 322 | 302 | 0.03% | 0.004% |
| 46 | 7.189 | 1809 | 1819 | 1822 | rBV3 | 1816 | 2551 | 0.24% | 0.032% |
| 47 | 7.481 | 1908 | 1910 | 1912 | rVV | 417 | 252 | 0.02% | 0.003% |
| 48 | 7.562 | 1922 | 1935 | 1960 | rVV | 130757 | 228021 | 21.32% | 2.898% |
| 49 | 7.652 | 1960 | 1963 | 1969 | rVB3 | 457 | 465 | 0.04% | 0.006% |
| 50 | 7.693 | 1969 | 1976 | 1986 | rBV4 | 1091 | 2178 | 0.20% | 0.028% |
| 51 | 7.758 | 1993 | 1996 | 1999 | rVB | 572 | 386 | 0.04% | 0.005% |
| 52 | 7.803 | 2004 | 2010 | 2012 | rBV2 | 396 | 449 | 0.04% | 0.006% |
| 53 | 7.893 | 2025 | 2038 | 2059 | rBV | 488721 | 836822 | 78.25% | 10.636% |
| 54 | 8.086 | 2096 | 2098 | 2101 | rVB2 | 313 | 213 | 0.02% | 0.003% |
| 55 | 8.108 | 2101 | 2105 | 2107 | rBV2 | 469 | 288 | 0.03% | 0.004% |
| 56 | 8.176 | 2114 | 2126 | 2140 | rBV | 92644 | 154954 | 14.49% | 1.969% |
| 57 | 8.475 | 2209 | 2219 | 2228 | rVB3 | 2576 | 4472 | 0.42% | 0.057% |
| 58 | 8.636 | 2256 | 2269 | 2297 | rBV2 | 218014 | 443966 | 41.51% | 5.643% |
| 59 | 8.774 | 2310 | 2312 | 2316 | rVB3 | 409 | 242 | 0.02% | 0.003% |
| 60 | 8.857 | 2334 | 2338 | 2341 | rVB2 | 397 | 290 | 0.03% | 0.004% |
| 61 | 9.250 | 2458 | 2460 | 2464 | rBV | 256 | 219 | 0.02% | 0.003% |
| 62 | 9.414 | 2494 | 2511 | 2530 | rBV | 446526 | 729383 | 68.20% | 9.270% |
| 63 | 9.562 | 2553 | 2557 | 2560 | rBV3 | 422 | 379 | 0.04% | 0.005% |
| 64 | 9.639 | 2576 | 2581 | 2585 | rBV2 | 228 | 288 | 0.03% | 0.004% |
| 65 | 9.912 | 2660 | 2666 | 2670 | rBV2 | 236 | 253 | 0.02% | 0.003% |
| 66 | 9.935 | 2670 | 2673 | 2677 | rBV2 | 250 | 223 | 0.02% | 0.003% |
| 67 | 10.070 | 2709 | 2715 | 2718 | rBV2 | 248 | 322 | 0.03% | 0.004% |
| 68 | 10.099 | 2718 | 2724 | 2726 | rBV3 | 278 | 296 | 0.03% | 0.004% |
| 69 | 10.481 | 2839 | 2843 | 2851 | rVB3 | 713 | 918 | 0.09% | 0.012% |
| 70 | 10.529 | 2851 | 2858 | 2862 | rBV2 | 294 | 456 | 0.04% | 0.006% |
| 71 | 10.613 | 2878 | 2884 | 2889 | rBV | 292 | 416 | 0.04% | 0.005% |
| 72 | 10.700 | 2906 | 2911 | 2914 | rBV2 | 377 | 350 | 0.03% | 0.004% |
| 73 | 10.751 | 2914 | 2927 | 2941 | rBV | 332263 | 533308 | 49.87% | 6.778% |
| 74 | 10.832 | 2950 | 2952 | 2959 | rVB2 | 418 | 396 | 0.04% | 0.005% |
| 75 | 10.883 | 2960 | 2968 | 2976 | rBV5 | 2246 | 3549 | 0.33% | 0.045% |
| 76 | 11.131 | 3040 | 3045 | 3049 | rBV2 | 391 | 382 | 0.04% | 0.005% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
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Operator : JC/MD
Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** A44K9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMULM012623WMA.M
Title : VOC Analysis

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 11.471 | 3145 | 3151 | 3152 | rBV3 | 441 | 362 | 0.03% | 0.005% |
| 78 | 11.529 | 3166 | 3169 | 3176 | rVV2 | 294 | 265 | 0.02% | 0.003% |
| 79 | 11.745 | 3233 | 3236 | 3242 | rVB2 | 777 | 610 | 0.06% | 0.008% |
| 80 | 11.809 | 3243 | 3256 | 3273 | rBV | 428213 | 671566 | 62.80% | 8.535% |
| 81 | 11.899 | 3281 | 3284 | 3289 | rVB3 | 466 | 383 | 0.04% | 0.005% |
| 82 | 11.976 | 3304 | 3308 | 3312 | rBV2 | 476 | 297 | 0.03% | 0.004% |
| 83 | 12.053 | 3323 | 3332 | 3349 | rBV | 27856 | 47304 | 4.42% | 0.601% |
| 84 | 12.188 | 3362 | 3374 | 3391 | rBV | 457068 | 738714 | 69.08% | 9.389% |
| 85 | 12.301 | 3407 | 3409 | 3415 | rVB2 | 571 | 406 | 0.04% | 0.005% |
| 86 | 12.343 | 3420 | 3422 | 3425 | rBV | 335 | 233 | 0.02% | 0.003% |
| 87 | 12.401 | 3437 | 3440 | 3448 | rVB3 | 392 | 351 | 0.03% | 0.004% |
| 88 | 12.468 | 3458 | 3461 | 3468 | rVB2 | 303 | 272 | 0.03% | 0.003% |
| 89 | 12.497 | 3468 | 3470 | 3475 | rBV2 | 328 | 300 | 0.03% | 0.004% |
| 90 | 12.696 | 3527 | 3532 | 3536 | rBV2 | 384 | 535 | 0.05% | 0.007% |
| 91 | 12.764 | 3548 | 3553 | 3562 | rVB2 | 978 | 1516 | 0.14% | 0.019% |
| 92 | 12.941 | 3602 | 3608 | 3613 | rBV2 | 434 | 479 | 0.04% | 0.006% |
| 93 | 12.995 | 3622 | 3625 | 3627 | rBV | 407 | 275 | 0.03% | 0.003% |
| 94 | 13.217 | 3689 | 3694 | 3695 | rBV3 | 546 | 406 | 0.04% | 0.005% |
| 95 | 13.848 | 3887 | 3890 | 3895 | rVB4 | 749 | 656 | 0.06% | 0.008% |
| 96 | 14.095 | 3960 | 3967 | 3971 | rBV2 | 1032 | 1213 | 0.11% | 0.015% |
| 97 | 14.413 | 4064 | 4066 | 4072 | rBV2 | 325 | 283 | 0.03% | 0.004% |
| 98 | 14.831 | 4193 | 4196 | 4197 | rBV2 | 385 | 214 | 0.02% | 0.003% |
| 99 | 14.979 | 4239 | 4242 | 4244 | rBV2 | 376 | 255 | 0.02% | 0.003% |
| 100 | 15.973 | 4549 | 4551 | 4553 | rBV3 | 510 | 273 | 0.03% | 0.003% |

Sum of corrected areas: 7867930

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052827.D
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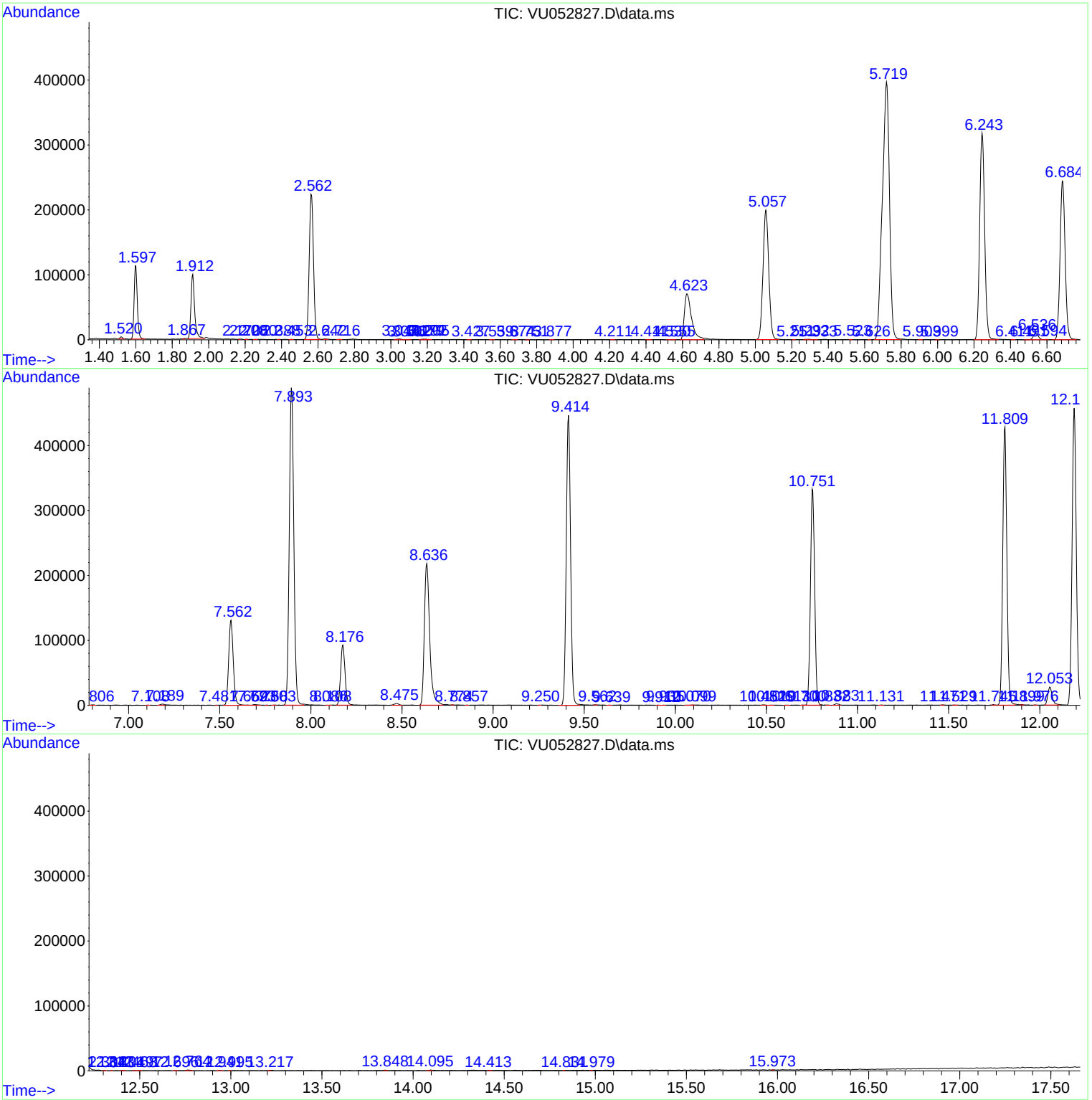
Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
A44K9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052827.D
Acq On : 26 Jan 2023 19:36
Operator : JC/MD
Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
A44K9

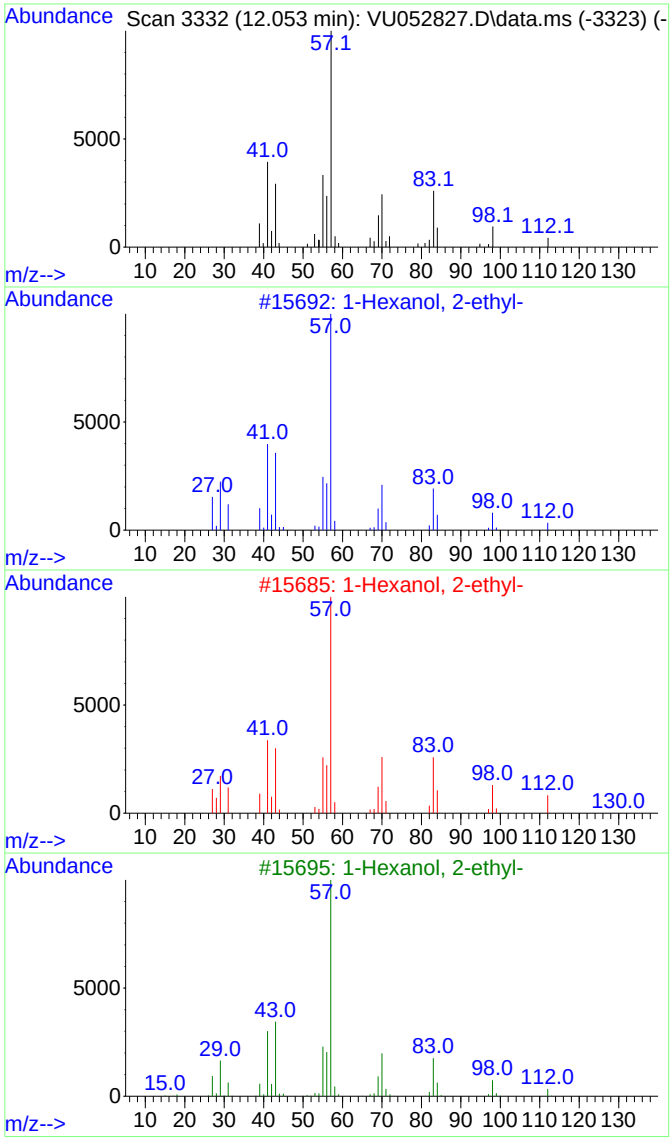
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

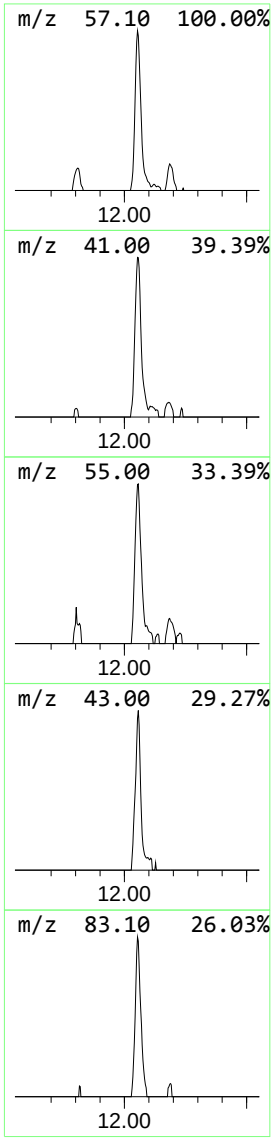
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.053 | 3.52 ug/L | 47304 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 3 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 4 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 72 |
| 5 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052827.D
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Sample : 01314-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
A44K9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

| | | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc | |
| 1-Hexanol, 2-et... | 12.053 | 3.5 | ug/L | 47304 | 3 | 11.809 | 671566 | 50.0 | |