LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
Data File : VU051597.D
Acq On : 29 Oct 2022 04:00
Operator : JC/MD
Sample : N5276-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
EW4X7

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU051597.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.359 | 3 | 6 | 21 | rVB2 | 21798 | 26276 | 2.42% | 0.357% |
| 2 | 1.488 | 36 | 46 | 61 | rBV | 140090 | 433237 | 39.82% | 5.892% |
| 3 | 1.594 | 72 | 79 | 86 | rBV2 | 92446 | 123329 | 11.34% | 1.677% |
| 4 | 1.912 | 172 | 178 | 189 | rVB | 94397 | 120796 | 11.10% | 1.643% |
| 5 | 2.565 | 369 | 381 | 397 | rVB | 130899 | 213667 | 19.64% | 2.906% |
| 6 | 2.658 | 399 | 410 | 416 | rBV4 | 5054 | 11350 | 1.04% | 0.154% |
| 7 | 2.790 | 440 | 451 | 464 | rBV | 30153 | 50065 | 4.60% | 0.681% |
| 8 | 3.880 | 761 | 790 | 792 | rBV | 15486 | 55510 | 5.10% | 0.755% |
| 9 | 4.642 | 1013 | 1027 | 1072 | rBV | 115289 | 461784 | 42.44% | 6.280% |
| 10 | 5.060 | 1142 | 1157 | 1191 | rBV | 174153 | 413415 | 38.00% | 5.622% |
| 11 | 5.722 | 1342 | 1363 | 1393 | rBV2 | 312469 | 841354 | 77.33% | 11.442% |
| 12 | 6.247 | 1512 | 1526 | 1552 | rBV | 220681 | 429196 | 39.45% | 5.837% |
| 13 | 6.690 | 1650 | 1664 | 1684 | rBV | 219078 | 432440 | 39.75% | 5.881% |
| 14 | 7.169 | 1802 | 1813 | 1830 | rBV6 | 4759 | 11164 | 1.03% | 0.152% |
| 15 | 7.565 | 1925 | 1936 | 1958 | rBV | 70007 | 126245 | 11.60% | 1.717% |
| 16 | 7.896 | 2026 | 2039 | 2054 | rVV | 285696 | 498278 | 45.80% | 6.776% |
| 17 | 7.970 | 2055 | 2062 | 2077 | rVB2 | 18101 | 31967 | 2.94% | 0.435% |
| 18 | 8.179 | 2116 | 2127 | 2145 | rBV | 41640 | 72214 | 6.64% | 0.982% |
| 19 | 8.636 | 2256 | 2269 | 2300 | rBV | 547189 | 1088002 | 100.00% | 14.796% |
| 20 | 9.417 | 2499 | 2512 | 2539 | rBV | 336910 | 569947 | 52.38% | 7.751% |
| 21 | 10.754 | 2913 | 2928 | 2945 | rBV | 195626 | 319557 | 29.37% | 4.346% |
| 22 | 10.889 | 2959 | 2970 | 2981 | rVB3 | 9035 | 15099 | 1.39% | 0.205% |
| 23 | 11.809 | 3243 | 3256 | 3273 | rBV | 281926 | 463485 | 42.60% | 6.303% |
| 24 | 12.192 | 3360 | 3375 | 3397 | rBV | 285397 | 475784 | 43.73% | 6.470% |
| 25 | 15.481 | 4386 | 4398 | 4413 | rBV | 41351 | 69353 | 6.37% | 0.943% |

Sum of corrected areas: 7353514

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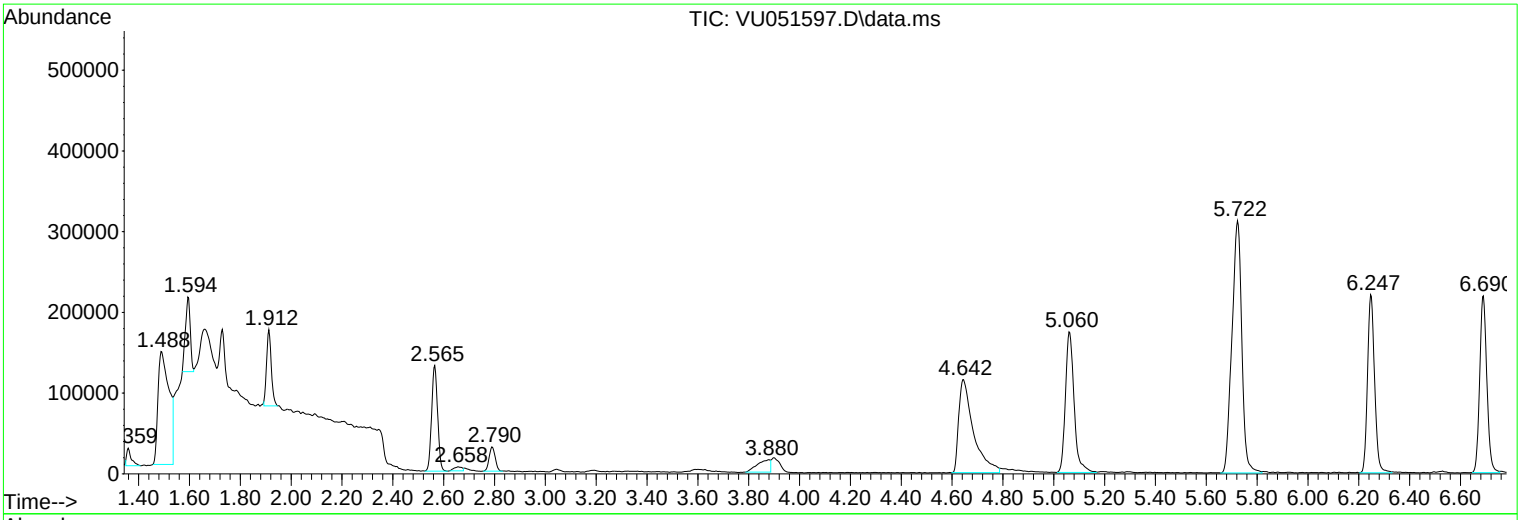
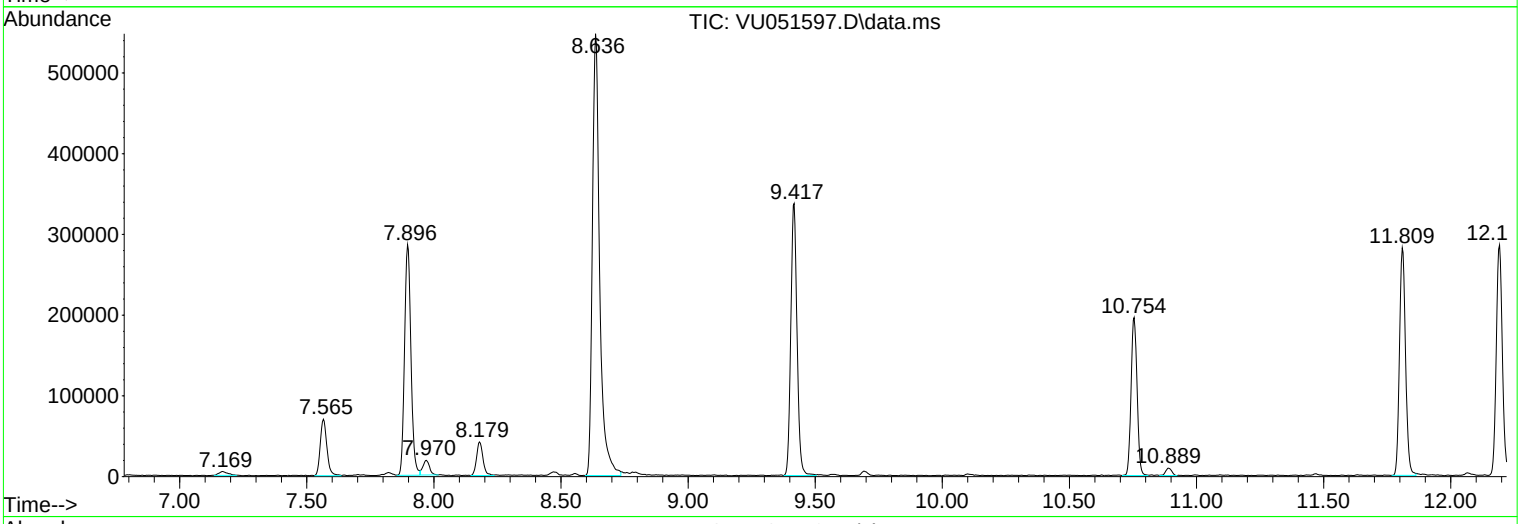
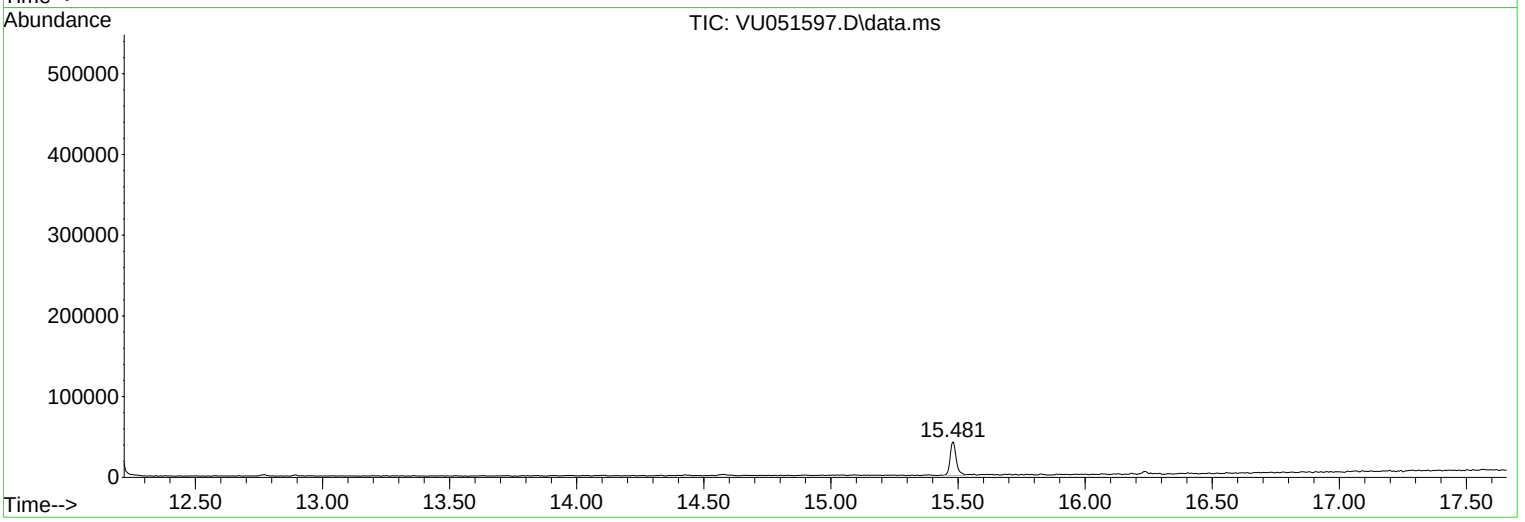
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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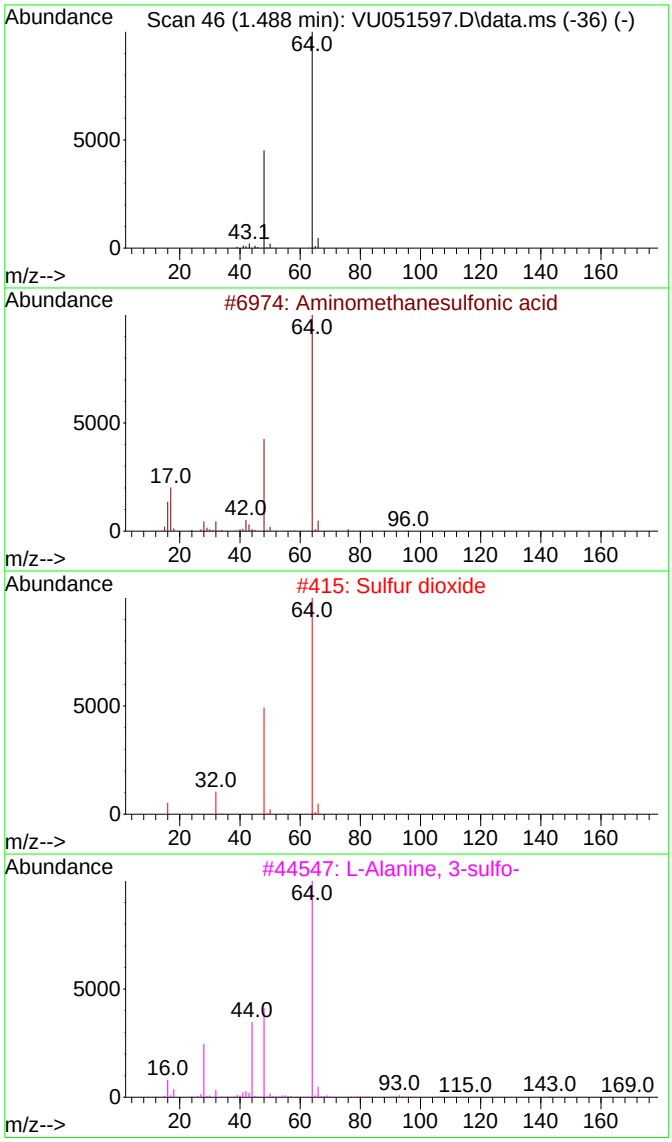
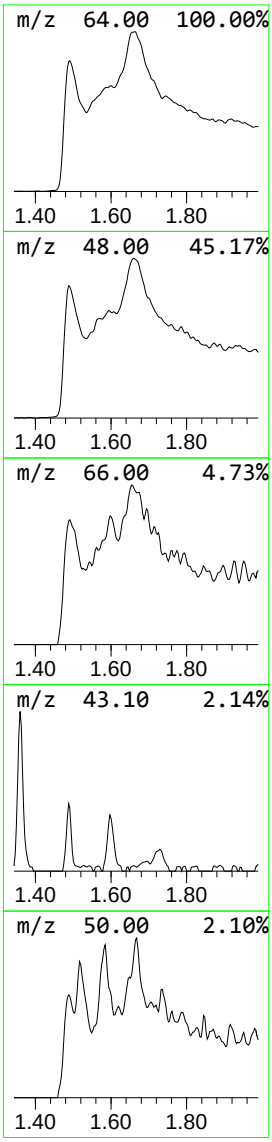
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.488 | 5.05 ug/L | 433237 | 1,4-Difluorobenzene | 6.247 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 83 |
| 2 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 83 |
| 3 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 9 |
| 4 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 5 |
| 5 | Ethene, 1,1-difluoro- | 64 | C2H2F2 | 000075-38-7 | 5 |



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Quant Title : TRACE VOA SFAM1.0

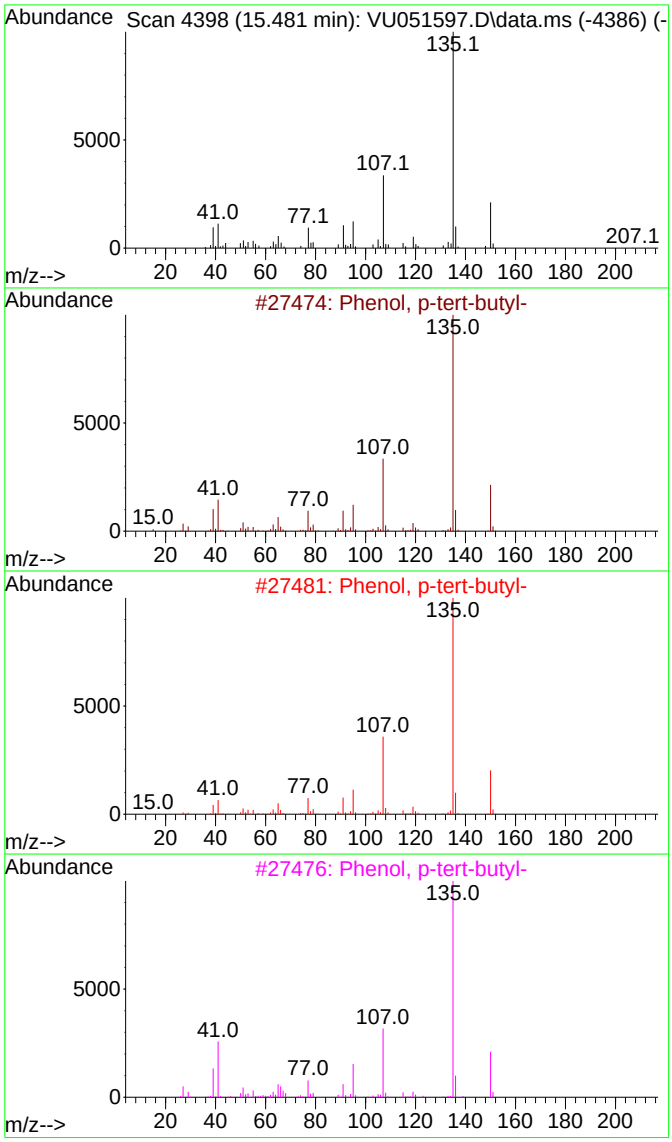
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

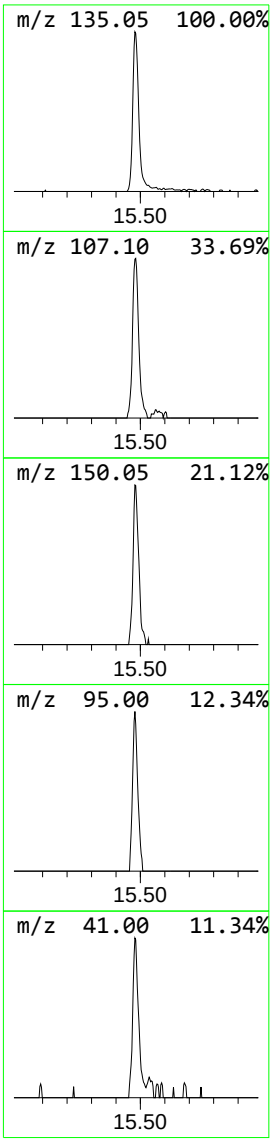
**********

Peak Number 4 Phenol, p-tert-butyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.481 | 0.75 ug/L | 69353 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, p-tert-butyl- | 150 | C10H14O | 000098-54-4 | 97 |
| 2 | Phenol, p-tert-butyl- | 150 | C10H14O | 000098-54-4 | 97 |
| 3 | Phenol, p-tert-butyl- | 150 | C10H14O | 000098-54-4 | 94 |
| 4 | Phenol, m-tert-butyl- | 150 | C10H14O | 000585-34-2 | 93 |
| 5 | Phenol, p-tert-butyl- | 150 | C10H14O | 000098-54-4 | 80 |



Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Aminomethanesul... | 1.488 | 5.0 | ug/L | 433237 | 1 | 6.247 | 429196 | 5.0 |
| Phenol, p-tert-... | 15.481 | 0.8 | ug/L | 69353 | 3 | 11.809 | 463485 | 5.0 |