

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU103122\  
 Data File : VU051610.D  
 Acq On : 31 Oct 2022 14:39  
 Operator : JC/MD  
 Sample : N5301-03  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBXC4

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: VU051610.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.385       | 7             | 14          | 30           | rVB      | 129766         | 149858        | 7.37%           | 0.833%        |
| 2         | 1.469       | 30            | 40          | 52           | rBV      | 147358         | 267460        | 13.16%          | 1.487%        |
| 3         | 1.601       | 74            | 81          | 111          | rVB2     | 247598         | 411421        | 20.24%          | 2.287%        |
| 4         | 1.729       | 114           | 121         | 128          | rBV      | 71636          | 79373         | 3.90%           | 0.441%        |
| 5         | 1.925       | 168           | 182         | 203          | rVB2     | 295755         | 511736        | 25.17%          | 2.844%        |
| 6         | 2.575       | 369           | 384         | 392          | rBV3     | 630940         | 1220523       | 60.04%          | 6.784%        |
| 7         | 2.620       | 392           | 398         | 420          | rVB      | 380624         | 646285        | 31.79%          | 3.592%        |
| 8         | 2.945       | 488           | 499         | 517          | rBV      | 66246          | 124497        | 6.12%           | 0.692%        |
| 9         | 3.186       | 560           | 574         | 590          | rBV2     | 12602          | 29337         | 1.44%           | 0.163%        |
| 10        | 3.350       | 612           | 625         | 643          | rBV      | 113468         | 224747        | 11.06%          | 1.249%        |
| 11        | 3.867       | 755           | 786         | 811          | rBV3     | 68416          | 187254        | 9.21%           | 1.041%        |
| 12        | 4.616       | 1007          | 1019        | 1027         | rBV      | 191686         | 425232        | 20.92%          | 2.363%        |
| 13        | 4.970       | 1113          | 1129        | 1144         | rBV      | 146792         | 318187        | 15.65%          | 1.768%        |
| 14        | 5.083       | 1144          | 1164        | 1188         | rVB3     | 341150         | 976317        | 48.03%          | 5.426%        |
| 15        | 5.314       | 1215          | 1236        | 1251         | rBV2     | 77231          | 177700        | 8.74%           | 0.988%        |
| 16        | 5.523       | 1285          | 1301        | 1317         | rBV      | 102958         | 229453        | 11.29%          | 1.275%        |
| 17        | 5.723       | 1341          | 1363        | 1376         | rBV2     | 240978         | 665610        | 32.74%          | 3.699%        |
| 18        | 5.793       | 1377          | 1385        | 1403         | rVB2     | 54868          | 111498        | 5.48%           | 0.620%        |
| 19        | 6.247       | 1510          | 1526        | 1544         | rBV      | 196282         | 376239        | 18.51%          | 2.091%        |
| 20        | 6.539       | 1604          | 1617        | 1636         | rBV      | 116592         | 221241        | 10.88%          | 1.230%        |
| 21        | 6.690       | 1650          | 1664        | 1683         | rBV      | 173343         | 340897        | 16.77%          | 1.895%        |
| 22        | 7.565       | 1922          | 1936        | 1941         | rBV      | 68061          | 114071        | 5.61%           | 0.634%        |
| 23        | 7.607       | 1941          | 1949        | 1969         | rVB      | 186282         | 331336        | 16.30%          | 1.842%        |
| 24        | 7.790       | 1992          | 2006        | 2027         | rBV      | 1169858        | 2032826       | 100.00%         | 11.298%       |
| 25        | 7.896       | 2028          | 2039        | 2054         | rVV      | 277646         | 490264        | 24.12%          | 2.725%        |
| 26        | 7.970       | 2054          | 2062        | 2075         | rVB2     | 19302          | 35216         | 1.73%           | 0.196%        |
| 27        | 8.182       | 2115          | 2128        | 2130         | rBV      | 50494          | 74566         | 3.67%           | 0.414%        |
| 28        | 8.208       | 2131          | 2136        | 2157         | rVB      | 89221          | 149944        | 7.38%           | 0.833%        |
| 29        | 8.398       | 2183          | 2195        | 2209         | rBV2     | 98912          | 166743        | 8.20%           | 0.927%        |
| 30        | 8.552       | 2231          | 2243        | 2256         | rBV      | 195947         | 329970        | 16.23%          | 1.834%        |
| 31        | 8.629       | 2256          | 2267        | 2299         | rBV      | 608862         | 1113861       | 54.79%          | 6.191%        |
| 32        | 8.922       | 2345          | 2358        | 2374         | rBV      | 108047         | 184774        | 9.09%           | 1.027%        |
| 33        | 9.417       | 2498          | 2512        | 2514         | rBV      | 321954         | 423884        | 20.85%          | 2.356%        |
| 34        | 9.446       | 2515          | 2521        | 2549         | rVB      | 533488         | 896840        | 44.12%          | 4.985%        |
| 35        | 10.288      | 2771          | 2783        | 2799         | rBV      | 65853          | 109125        | 5.37%           | 0.607%        |
| 36        | 10.754      | 2913          | 2928        | 2949         | rBV2     | 188642         | 399849        | 19.67%          | 2.222%        |

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR102822WMA.M  
 Title : TRACE VOA SFAM1.0

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 11.465 | 3137 | 3149 | 3170 | rBV  | 369397 | 574755 | 28.27% | 3.194% |
| 38 | 11.745 | 3224 | 3236 | 3246 | rBV  | 243368 | 388287 | 19.10% | 2.158% |
| 39 | 11.812 | 3246 | 3257 | 3279 | rVB2 | 308358 | 737314 | 36.27% | 4.098% |
| 40 | 12.192 | 3362 | 3375 | 3394 | rBV  | 245559 | 408110 | 20.08% | 2.268% |
| 41 | 13.217 | 3682 | 3694 | 3714 | rBV  | 354928 | 560095 | 27.55% | 3.113% |
| 42 | 13.838 | 3875 | 3887 | 3908 | rBV2 | 256997 | 415883 | 20.46% | 2.311% |
| 43 | 14.327 | 4028 | 4039 | 4061 | rBV  | 151347 | 251654 | 12.38% | 1.399% |
| 44 | 16.677 | 4760 | 4770 | 4780 | rBV4 | 23168  | 35475  | 1.75%  | 0.197% |
| 45 | 16.886 | 4823 | 4835 | 4844 | rBV2 | 47502  | 72800  | 3.58%  | 0.405% |

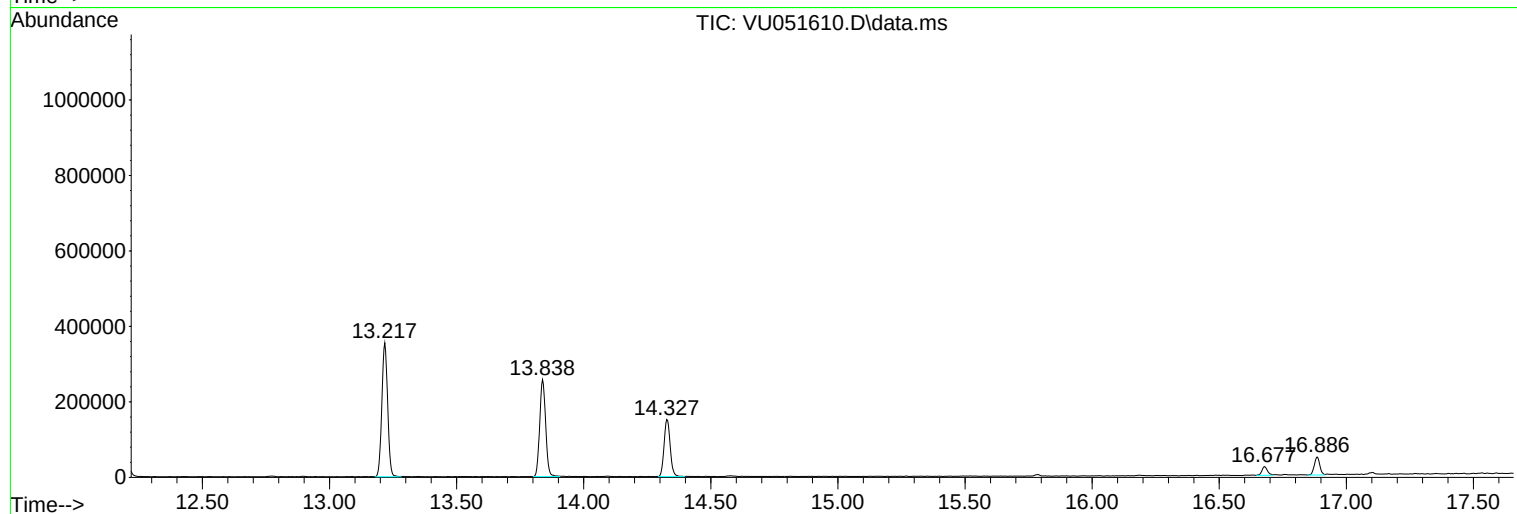
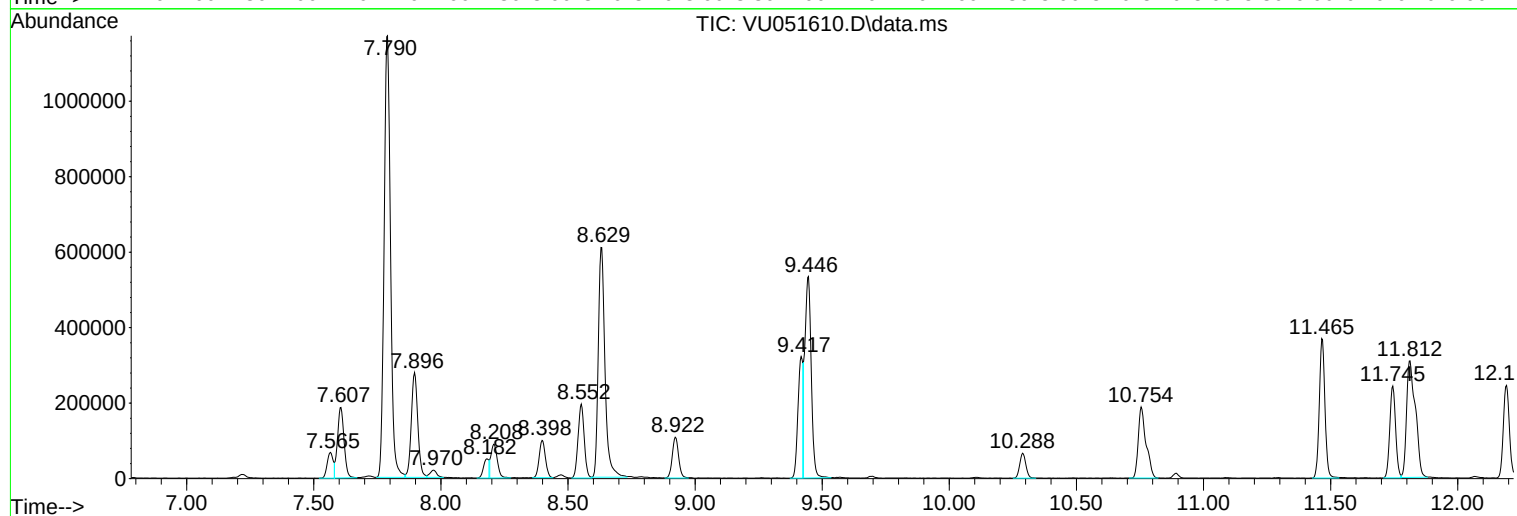
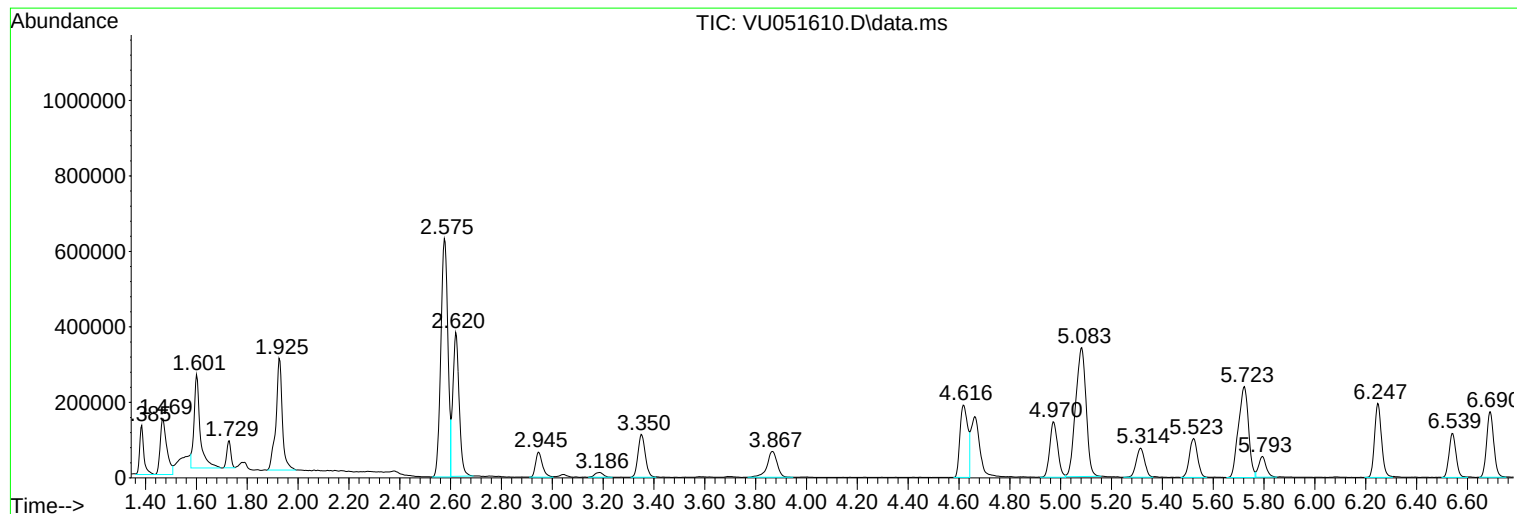
Sum of corrected areas: 17992507

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ALS Vial : 8 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DBXC4

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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ALS Vial : 8 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DBXC4

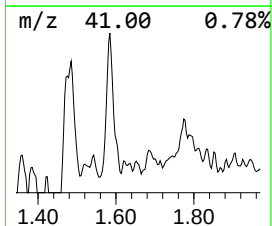
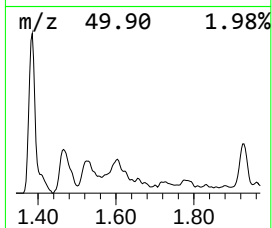
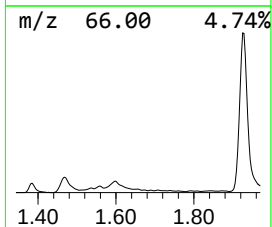
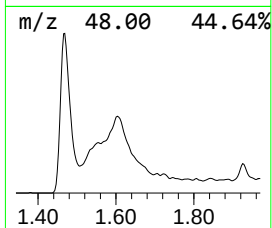
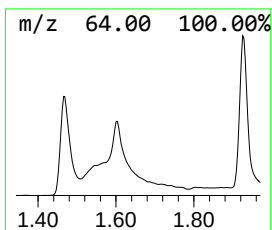
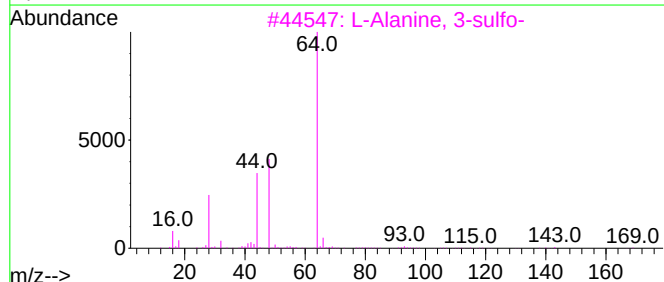
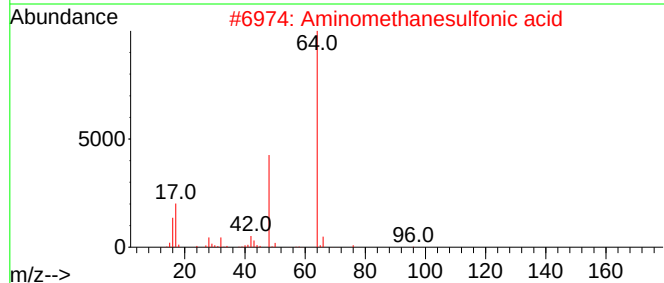
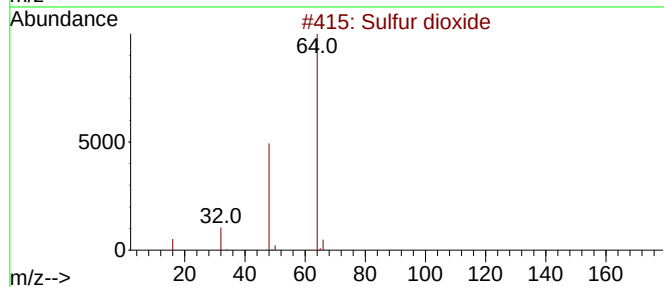
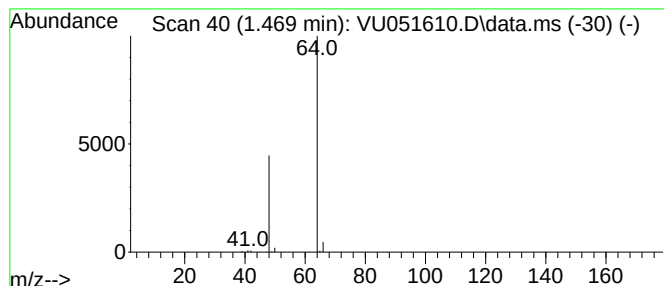
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR102822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.469 | 3.55 ug/L | 267460 | 1,4-Difluorobenzene | 6.247 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 83   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 4    |
| 5    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |



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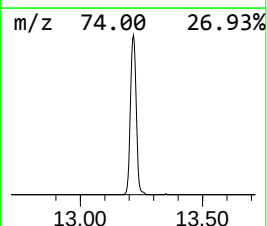
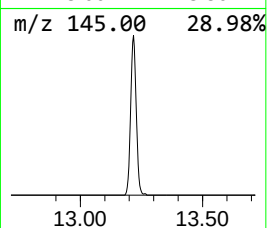
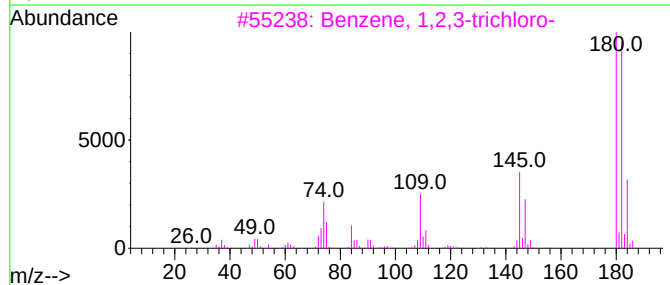
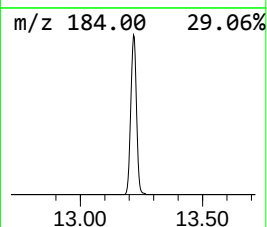
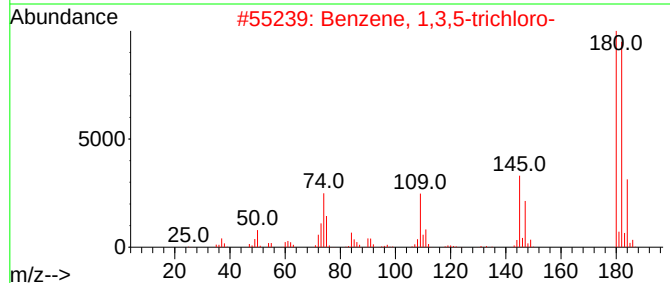
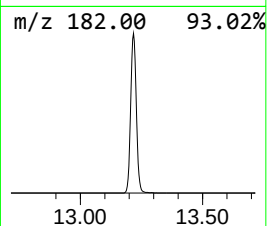
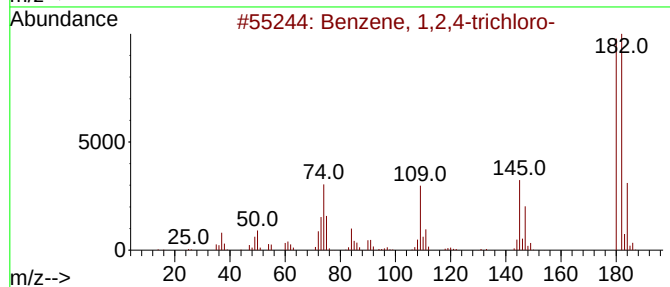
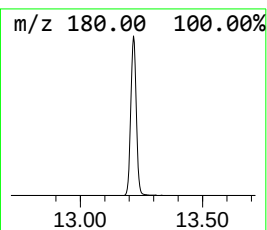
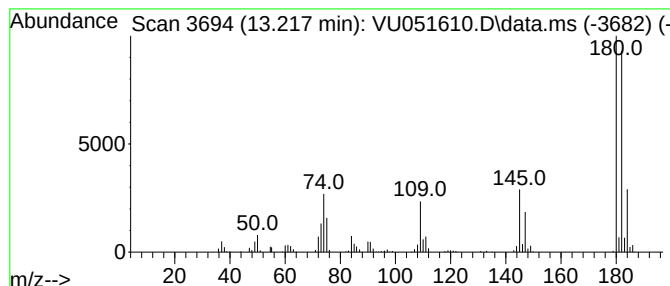
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR102822WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 Benzene, 1,3,5-trichloro- Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.217 | 3.80 ug/L | 560095 | 1,4-Dichlorobenzene-d4 | 11.809 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzene, 1,2,4-trichloro- | 180 | C6H3Cl3 | 000120-82-1 | 98   |
| 2    |    |   | Benzene, 1,3,5-trichloro- | 180 | C6H3Cl3 | 000108-70-3 | 98   |
| 3    |    |   | Benzene, 1,2,3-trichloro- | 180 | C6H3Cl3 | 000087-61-6 | 98   |
| 4    |    |   | Benzene, 1,3,5-trichloro- | 180 | C6H3Cl3 | 000108-70-3 | 98   |
| 5    |    |   | Benzene, 1,2,3-trichloro- | 180 | C6H3Cl3 | 000087-61-6 | 98   |



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Quant Title : TRACE VOA SFAM1.0

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Sulfur dioxide     | 1.469  | 3.5     | ug/L  | 267460   | 1                     | 6.247  | 376239 | 5.0  |
| Benzene, 1,3,5-... | 13.217 | 3.8     | ug/L  | 560095   | 3                     | 11.809 | 737314 | 5.0  |