

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100124\  
 Data File : VU061058.D  
 Acq On : 01 Oct 2024 21:04  
 Operator : MD/SY  
 Sample : P4227-14 10X  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 30 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 PMW-7S(20240927)

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\SFAMUTR100124WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU061058.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         | 1.596       | 88            | 95          | 113          | rVB      | 85182          | 107473        | 3.30%           | 1.123%        |
| 2         | 1.911       | 184           | 193         | 205          | rBV      | 55559          | 87685         | 2.69%           | 0.916%        |
| 3         | 2.554       | 382           | 393         | 413          | rVB      | 134333         | 224694        | 6.90%           | 2.348%        |
| 4         | 3.174       | 571           | 586         | 604          | rBV2     | 21666          | 51853         | 1.59%           | 0.542%        |
| 5         | 3.348       | 627           | 640         | 656          | rBV      | 23993          | 53299         | 1.64%           | 0.557%        |
| 6         | 3.686       | 730           | 745         | 765          | rBV2     | 38286          | 86136         | 2.64%           | 0.900%        |
| 7         | 3.859       | 784           | 799         | 819          | rVB2     | 25731          | 62627         | 1.92%           | 0.654%        |
| 8         | 4.650       | 1024          | 1045        | 1089         | rBV2     | 220118         | 661699        | 20.32%          | 6.915%        |
| 9         | 5.052       | 1155          | 1170        | 1201         | rBV      | 112910         | 255386        | 7.84%           | 2.669%        |
| 10        | 5.714       | 1357          | 1376        | 1406         | rBV2     | 232986         | 630013        | 19.34%          | 6.584%        |
| 11        | 6.242       | 1527          | 1540        | 1567         | rBV      | 231867         | 455558        | 13.99%          | 4.761%        |
| 12        | 6.682       | 1663          | 1677        | 1697         | rBV      | 145825         | 292363        | 8.98%           | 3.055%        |
| 13        | 7.560       | 1935          | 1950        | 1975         | rBV      | 80098          | 152595        | 4.68%           | 1.595%        |
| 14        | 7.891       | 2040          | 2053        | 2073         | rBV      | 293124         | 527326        | 16.19%          | 5.511%        |
| 15        | 8.174       | 2130          | 2141        | 2160         | rBV      | 47199          | 88984         | 2.73%           | 0.930%        |
| 16        | 8.640       | 2273          | 2286        | 2316         | rBV      | 308440         | 703844        | 21.61%          | 7.356%        |
| 17        | 9.412       | 2514          | 2526        | 2532         | rBV      | 326998         | 601615        | 18.47%          | 6.287%        |
| 18        | 10.753      | 2931          | 2943        | 2966         | rBV      | 104232         | 175061        | 5.37%           | 1.829%        |
| 19        | 11.740      | 3238          | 3250        | 3261         | rBV      | 345907         | 563523        | 17.30%          | 5.889%        |
| 20        | 11.827      | 3261          | 3277        | 3303         | rVB2     | 1698316        | 3257171       | 100.00%         | 34.039%       |
| 21        | 12.187      | 3377          | 3389        | 3410         | rBV      | 262966         | 477110        | 14.65%          | 4.986%        |
| 22        | 13.839      | 3889          | 3903        | 3917         | rBV3     | 26700          | 52860         | 1.62%           | 0.552%        |

Sum of corrected areas: 9568875

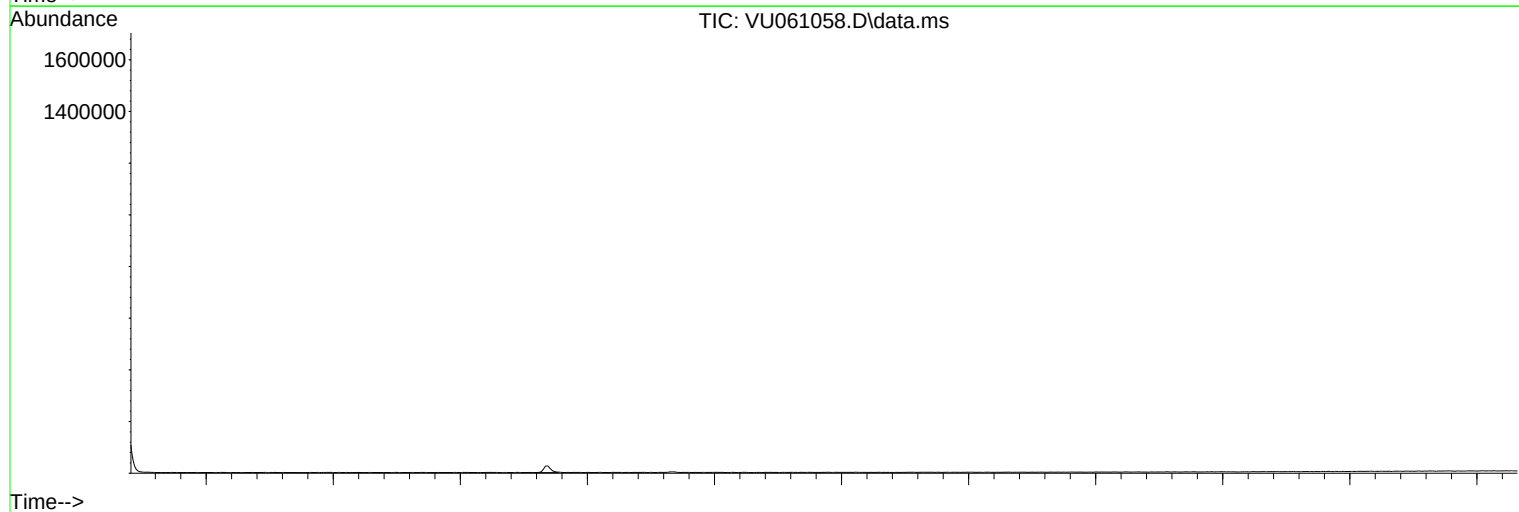
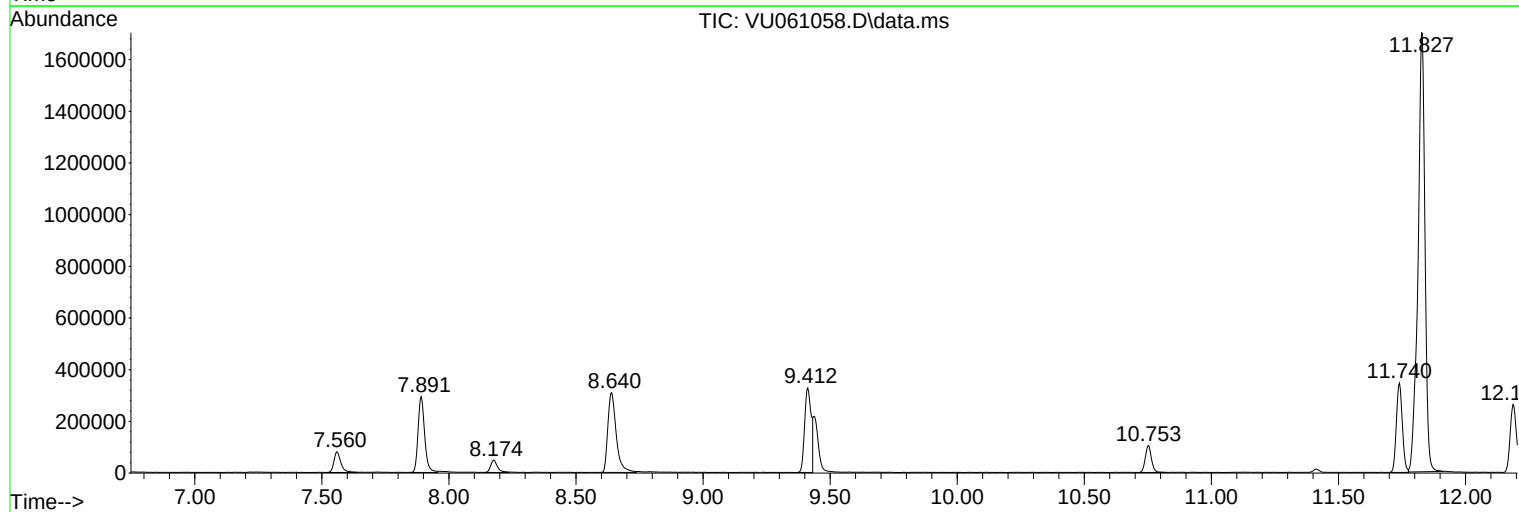
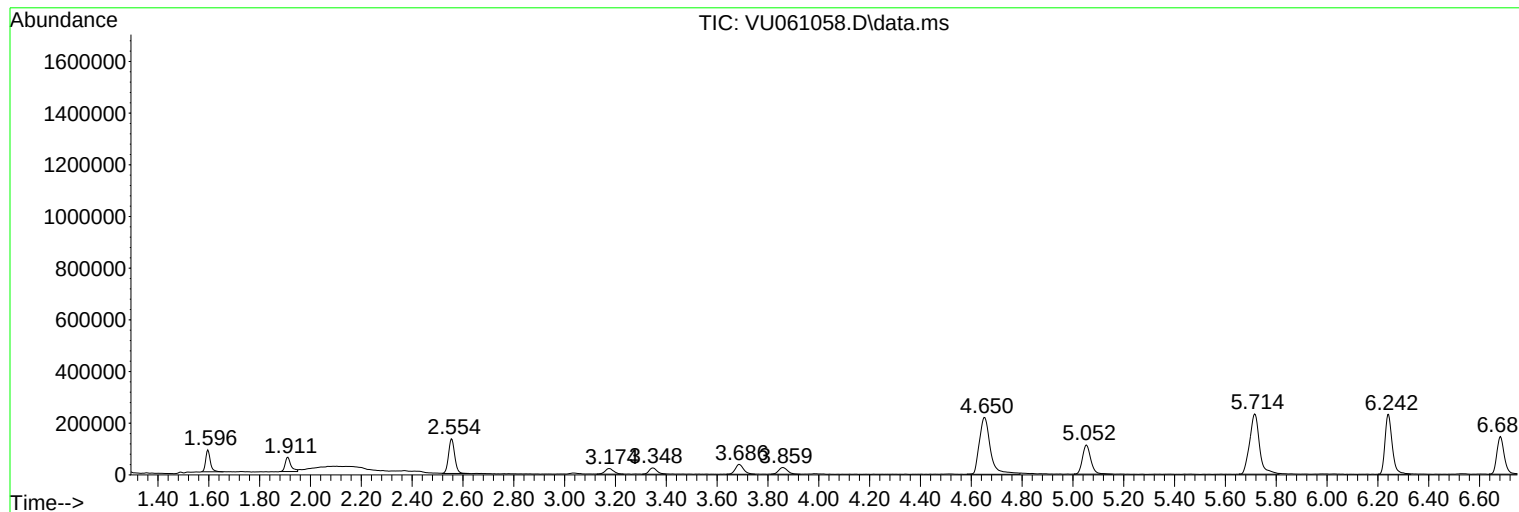
Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100124\  
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ALS Vial : 30 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
PMW-7S(20240927)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR100124WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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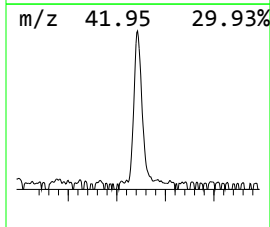
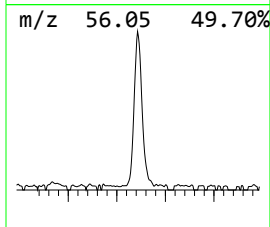
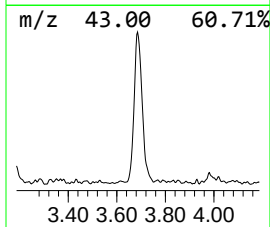
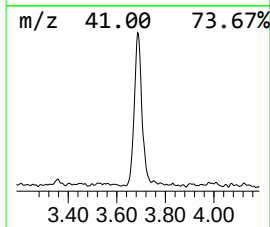
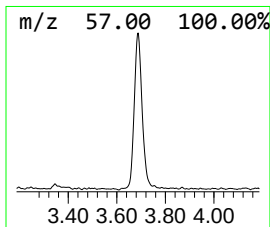
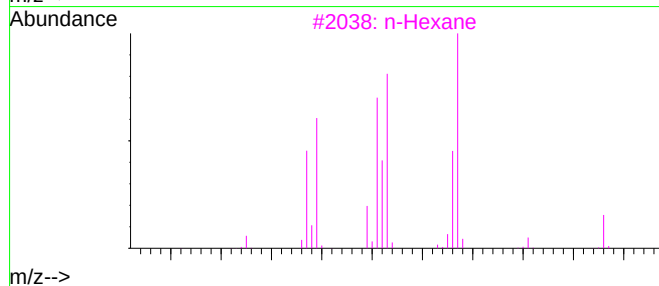
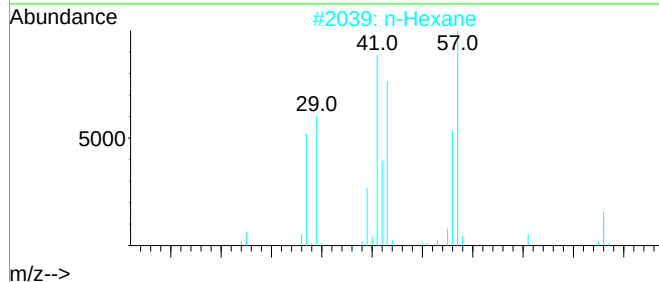
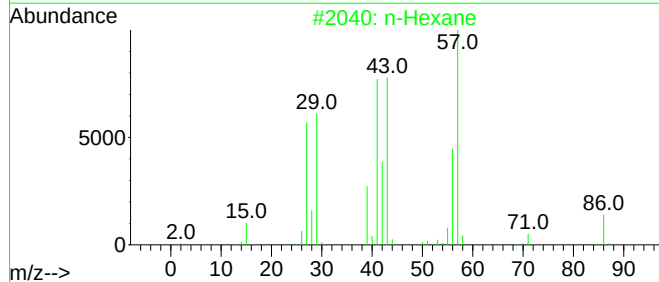
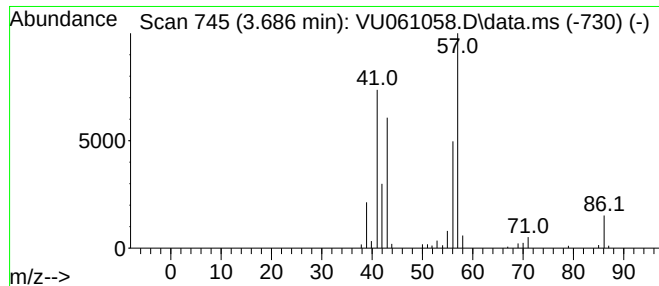
Instrument :  
MSVOA\_U  
ClientSampleId :  
PMW-7S(20240927)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR100124WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

| R.T.      | EstConc         | Area  | Relative to ISTD    | R.T.         |      |
|-----------|-----------------|-------|---------------------|--------------|------|
| 3.686     | 0.95 ug/L       | 86136 | 1,4-Difluorobenzene | 6.242        |      |
| Hit# of 5 | Tentative ID    | MW    | MolForm             | CAS#         | Qual |
| 1         | n-Hexane        | 86    | C6H14               | 000110-54-3  | 91   |
| 2         | n-Hexane        | 86    | C6H14               | 000110-54-3  | 91   |
| 3         | n-Hexane        | 86    | C6H14               | 000110-54-3  | 91   |
| 4         | 2-Ethyl-oxetane | 86    | C5H10O              | 1010386-40-2 | 86   |
| 5         | n-Hexane        | 86    | C6H14               | 000110-54-3  | 59   |



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Instrument :  
MSVOA\_U  
ClientSampleId :  
PMW-7S(20240927)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR100124WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

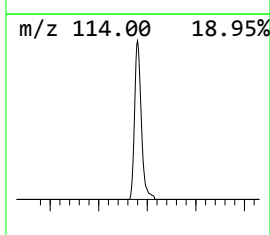
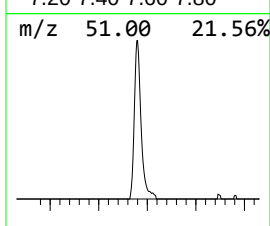
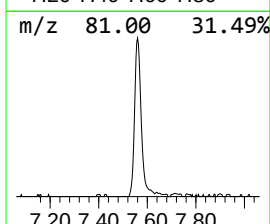
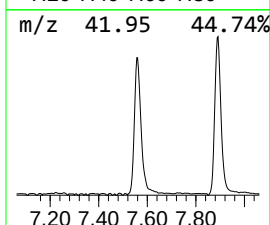
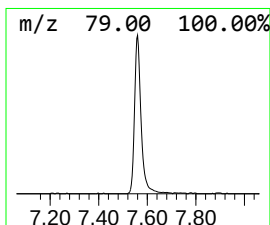
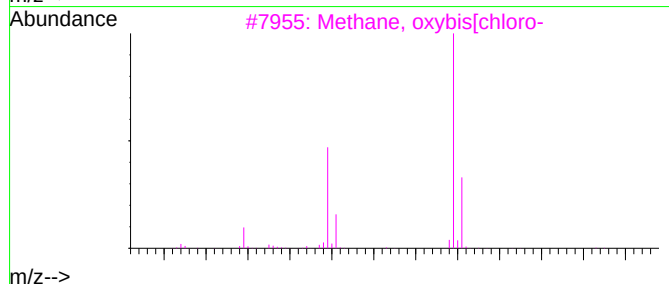
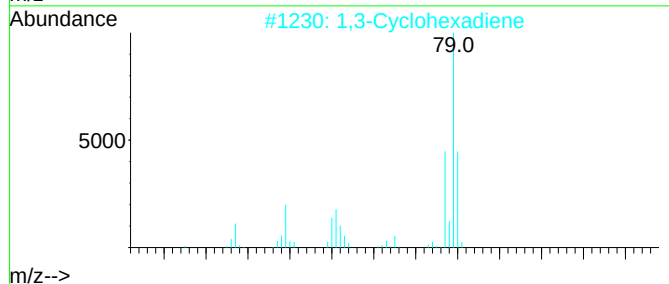
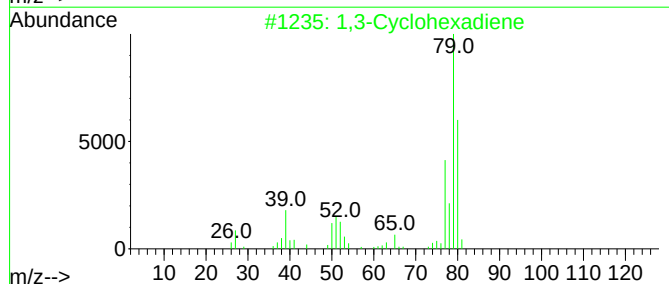
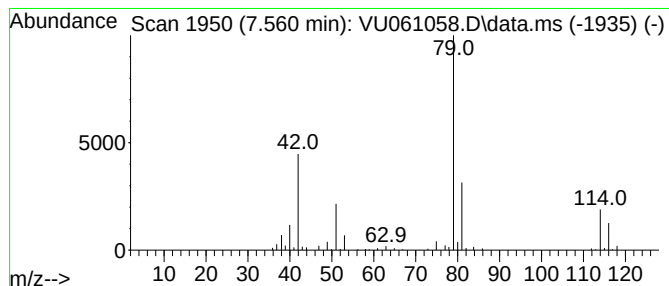
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Peak Number 3 unknown-01 Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 7.560 | 1.67 ug/L | 152595 | 1,4-Difluorobenzene | 6.242 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|-----------|-------------------------------------|-----|----------|--------------|------|
| 1         | 1,3-Cyclohexadiene                  | 80  | C6H8     | 000592-57-4  | 28   |
| 2         | 1,3-Cyclohexadiene                  | 80  | C6H8     | 000592-57-4  | 28   |
| 3         | Methane, oxybis[chloro-             | 114 | C2H4Cl2O | 000542-88-1  | 25   |
| 4         | Thiophosgene                        | 114 | CCl2S    | 000463-71-8  | 16   |
| 5         | 3-Thiatricyclo[3.1.1.0(2,4)]heptane | 112 | C6H8S    | 1000221-37-0 | 9    |



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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 |
| (DEL) Alkane: S... | 3.686 | 0.9     | ug/L  | 86136    | 1                     | 6.242 | 455558 | 5.0  |
| unknown-01         | 7.560 | 1.7     | ug/L  | 152595   | 1                     | 6.242 | 455558 | 5.0  |