

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV100923\  
 Data File : VV032351.D  
 Acq On : 10 Oct 2023 00:40  
 Operator : SY/MD  
 Sample : 04774-01  
 Misc : 25.0mL/MSVOA\_V/WATER  
 ALS Vial : 39 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 EX867

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\_V\Method\SFAMVTR092923WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV032351.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         | 1.085       | 8             | 14          | 40           | rVB      | 210251         | 266430        | 26.89%          | 5.082%        |
| 2         | 1.191       | 40            | 47          | 57           | rBV      | 81515          | 74214         | 7.49%           | 1.416%        |
| 3         | 1.278       | 65            | 74          | 86           | rBV3     | 158128         | 190941        | 19.27%          | 3.642%        |
| 4         | 1.384       | 102           | 107         | 115          | rVB2     | 8858           | 11892         | 1.20%           | 0.227%        |
| 5         | 1.532       | 146           | 153         | 164          | rVB      | 56067          | 66525         | 6.71%           | 1.269%        |
| 6         | 1.600       | 165           | 174         | 185          | rVB      | 45766          | 58573         | 5.91%           | 1.117%        |
| 7         | 1.767       | 219           | 226         | 238          | rVB2     | 31711          | 43874         | 4.43%           | 0.837%        |
| 8         | 2.059       | 308           | 317         | 331          | rBV2     | 94668          | 141948        | 14.33%          | 2.708%        |
| 9         | 2.159       | 332           | 348         | 362          | rVB6     | 21439          | 51123         | 5.16%           | 0.975%        |
| 10        | 2.696       | 502           | 515         | 533          | rBV      | 31049          | 58597         | 5.91%           | 1.118%        |
| 11        | 2.973       | 590           | 601         | 614          | rVB2     | 5525           | 11322         | 1.14%           | 0.216%        |
| 12        | 3.121       | 628           | 647         | 663          | rVB3     | 4354           | 11644         | 1.18%           | 0.222%        |
| 13        | 3.674       | 803           | 819         | 829          | rBV5     | 5270           | 13416         | 1.35%           | 0.256%        |
| 14        | 3.809       | 849           | 861         | 890          | rBV3     | 65293          | 216913        | 21.90%          | 4.137%        |
| 15        | 4.252       | 983           | 999         | 1020         | rBV3     | 61430          | 162086        | 16.36%          | 3.092%        |
| 16        | 4.587       | 1088          | 1103        | 1116         | rBV7     | 5574           | 15303         | 1.54%           | 0.292%        |
| 17        | 4.960       | 1204          | 1219        | 1236         | rBV3     | 143517         | 374290        | 37.78%          | 7.139%        |
| 18        | 5.538       | 1385          | 1399        | 1416         | rBV      | 110963         | 234511        | 23.67%          | 4.473%        |
| 19        | 5.834       | 1477          | 1491        | 1504         | rBV      | 498850         | 990696        | 100.00%         | 18.896%       |
| 20        | 5.992       | 1529          | 1540        | 1554         | rBV2     | 77988          | 166272        | 16.78%          | 3.171%        |
| 21        | 6.921       | 1815          | 1829        | 1850         | rBV      | 35995          | 78372         | 7.91%           | 1.495%        |
| 22        | 7.249       | 1919          | 1931        | 1947         | rBV      | 162644         | 301666        | 30.45%          | 5.754%        |
| 23        | 7.323       | 1947          | 1954        | 1981         | rVB      | 36711          | 75556         | 7.63%           | 1.441%        |
| 24        | 7.561       | 2020          | 2028        | 2053         | rBV      | 21416          | 45708         | 4.61%           | 0.872%        |
| 25        | 7.879       | 2112          | 2127        | 2143         | rBV2     | 24808          | 48124         | 4.86%           | 0.918%        |
| 26        | 8.030       | 2163          | 2174        | 2204         | rBV      | 228843         | 467598        | 47.20%          | 8.919%        |
| 27        | 8.789       | 2399          | 2410        | 2428         | rBV      | 176639         | 303271        | 30.61%          | 5.785%        |
| 28        | 8.953       | 2453          | 2461        | 2473         | rVB2     | 7519           | 12561         | 1.27%           | 0.240%        |
| 29        | 9.078       | 2492          | 2500        | 2517         | rBV3     | 16025          | 29671         | 2.99%           | 0.566%        |
| 30        | 9.487       | 2617          | 2627        | 2638         | rBV      | 8372           | 14752         | 1.49%           | 0.281%        |
| 31        | 10.156      | 2825          | 2835        | 2850         | rBV      | 69758          | 111327        | 11.24%          | 2.123%        |
| 32        | 10.329      | 2875          | 2889        | 2902         | rBV2     | 32715          | 54270         | 5.48%           | 1.035%        |
| 33        | 10.857      | 3046          | 3053        | 3069         | rBV      | 7451           | 11737         | 1.18%           | 0.224%        |
| 34        | 11.188      | 3144          | 3156        | 3177         | rBV      | 166154         | 269935        | 27.25%          | 5.149%        |
| 35        | 11.564      | 3262          | 3273        | 3291         | rVB      | 148829         | 239445        | 24.17%          | 4.567%        |
| 36        | 12.201      | 3459          | 3471        | 3480         | rBV2     | 11029          | 18199         | 1.84%           | 0.347%        |

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Misc : 25.0mL/MSVOA\_V/WATER  
ALS Vial : 39 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
EX867

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\_V\Method\SFAMVTR092923WMA.M  
Title : TRACE VOA SFAM1.0

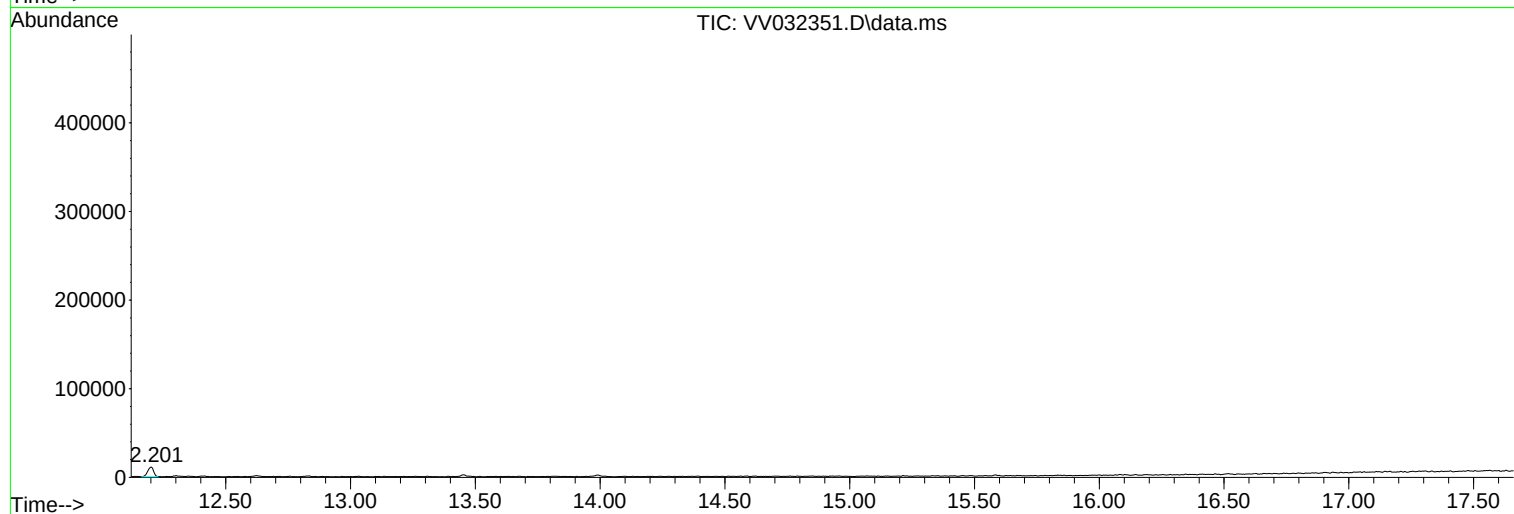
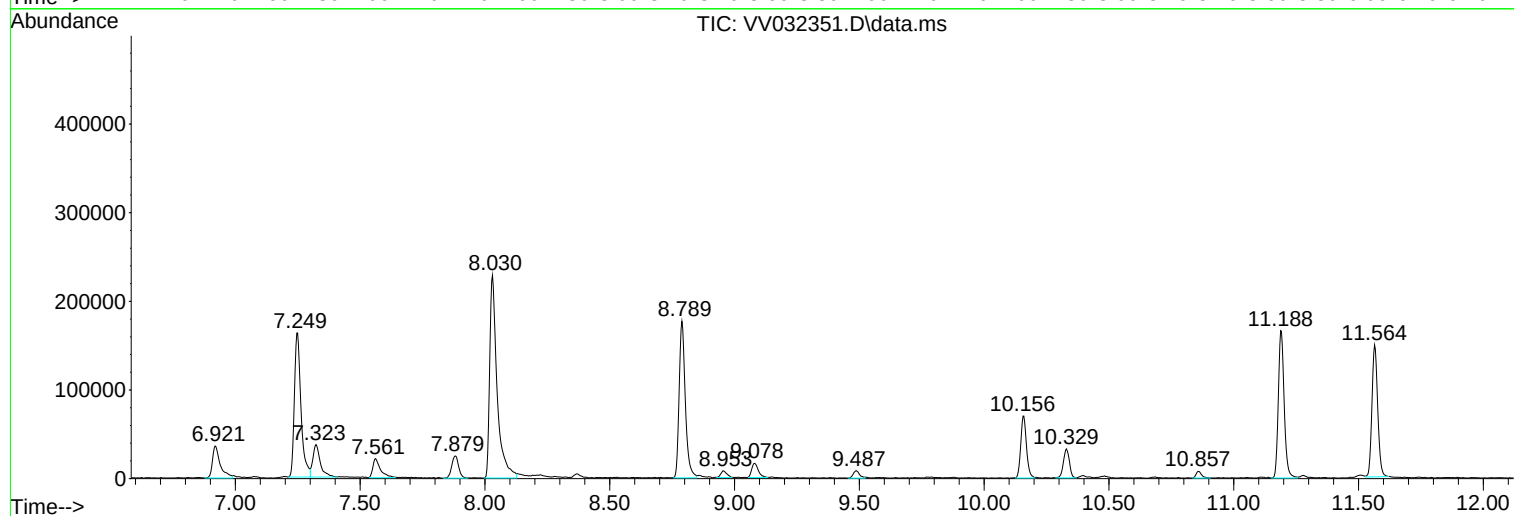
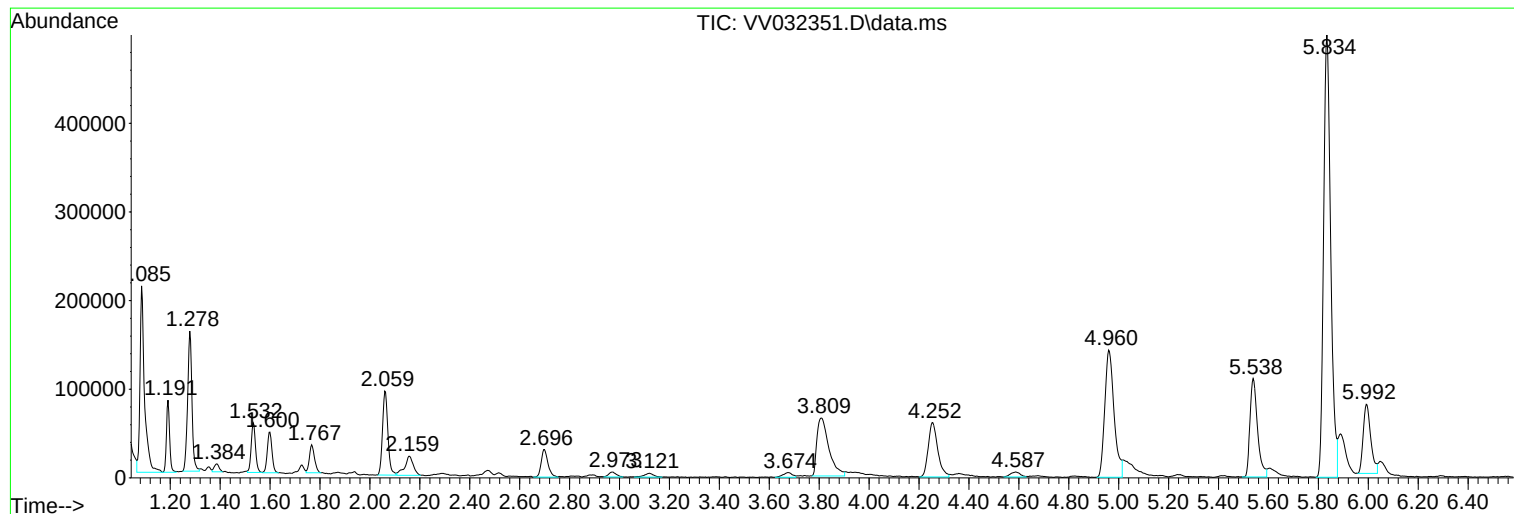
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR092923WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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MSVOA\_V  
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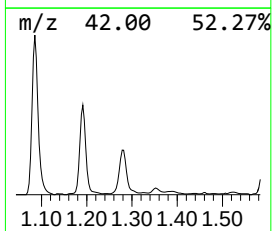
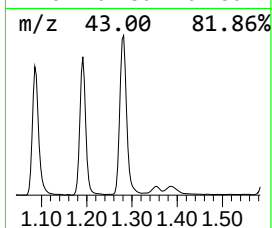
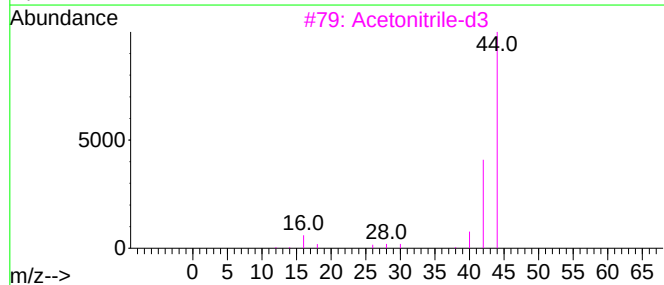
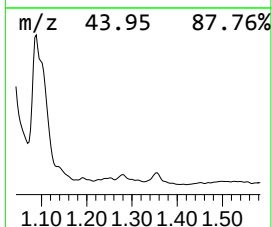
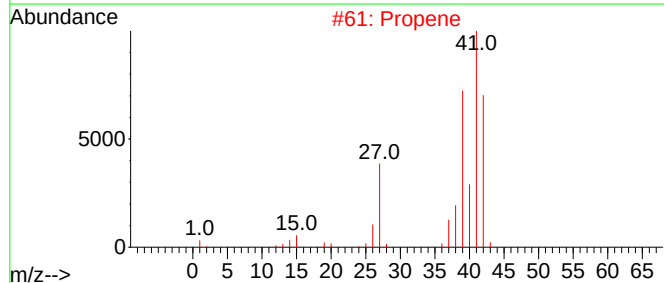
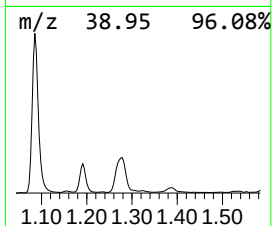
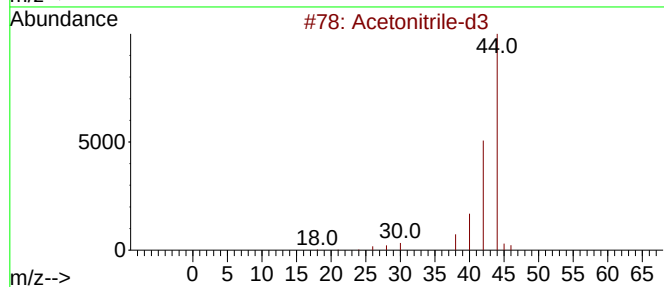
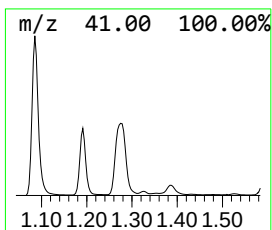
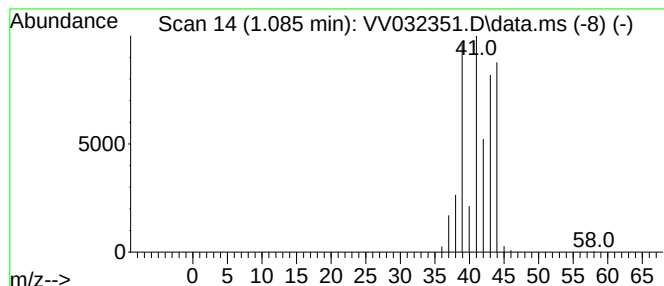
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR092923WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 1 unknown-01 Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.085 | 5.68 ug/L | 266430 | 1,4-Difluorobenzene | 5.538 |

| Hit# | of | 5 | Tentative ID    | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------|----|---------|-------------|------|
| 1    |    |   | Acetonitrile-d3 | 44 | C2D3N   | 002206-26-0 | 9    |
| 2    |    |   | Propene         | 42 | C3H6    | 000115-07-1 | 7    |
| 3    |    |   | Acetonitrile-d3 | 44 | C2D3N   | 002206-26-0 | 4    |
| 4    |    |   | Propane         | 44 | C3H8    | 000074-98-6 | 4    |
| 5    |    |   | Propane         | 44 | C3H8    | 000074-98-6 | 4    |



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ALS Vial : 39 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
EX867

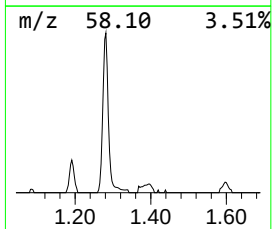
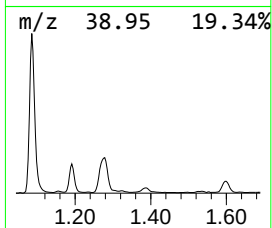
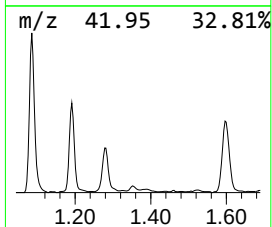
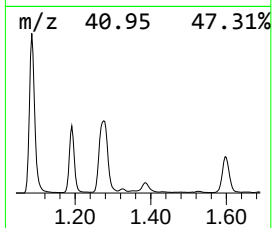
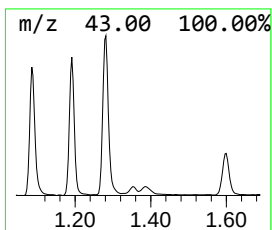
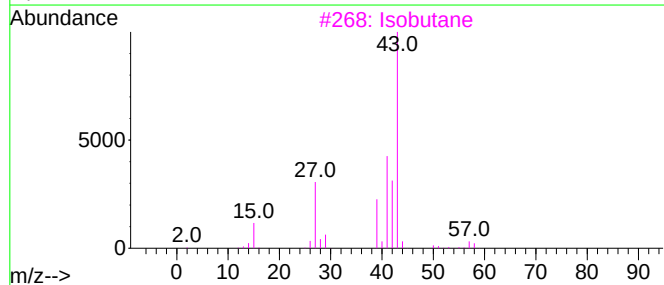
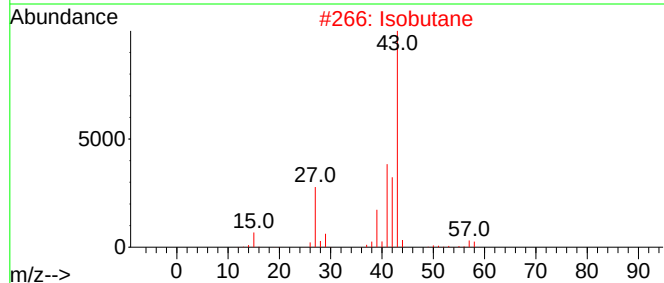
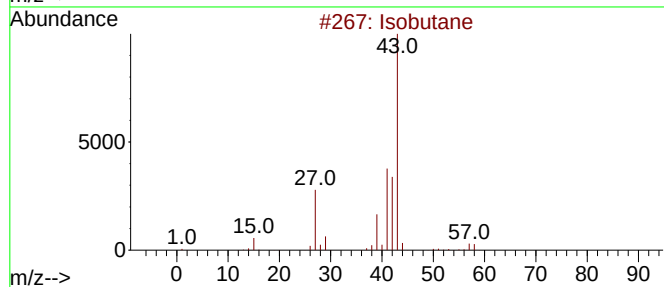
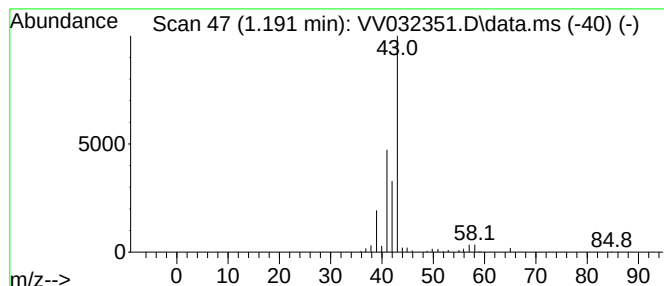
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR092923WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.191 | 1.58 ug/L | 74214 | 1,4-Difluorobenzene | 5.538 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------|-----|---------|-------------|------|
| 1    |    |   | Isobutane                    | 58  | C4H10   | 000075-28-5 | 72   |
| 2    |    |   | Isobutane                    | 58  | C4H10   | 000075-28-5 | 64   |
| 3    |    |   | Isobutane                    | 58  | C4H10   | 000075-28-5 | 50   |
| 4    |    |   | 3-Butenoic acid, ethyl ester | 114 | C6H10O2 | 001617-18-1 | 9    |
| 5    |    |   | Oxirane, trimethyl-          | 86  | C5H10O  | 005076-19-7 | 9    |



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Misc : 25.0mL/MSVOA\_V/WATER  
ALS Vial : 39 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
EX867

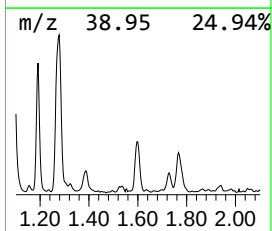
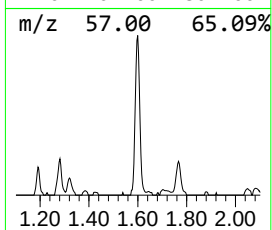
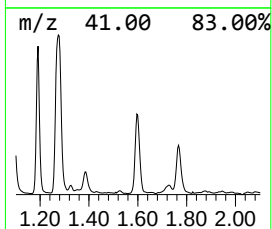
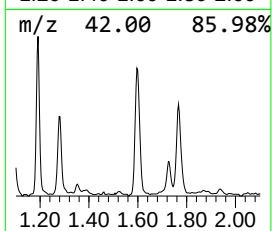
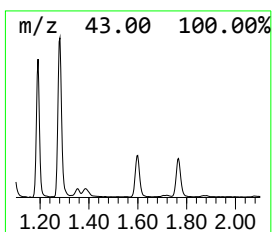
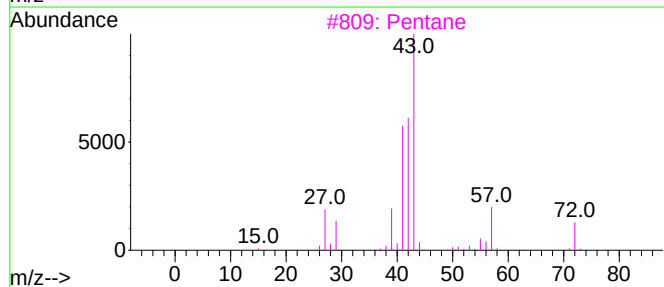
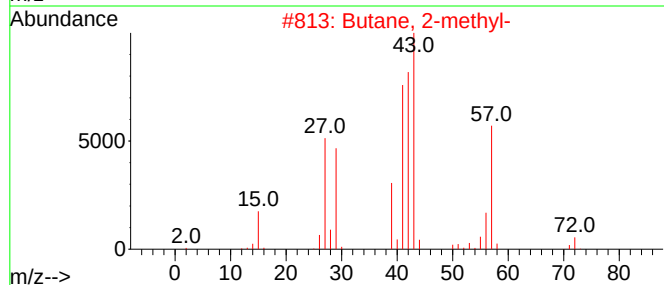
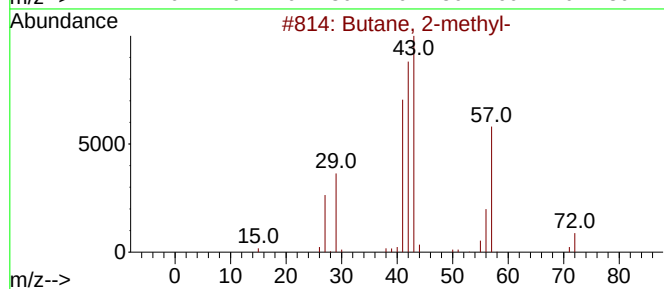
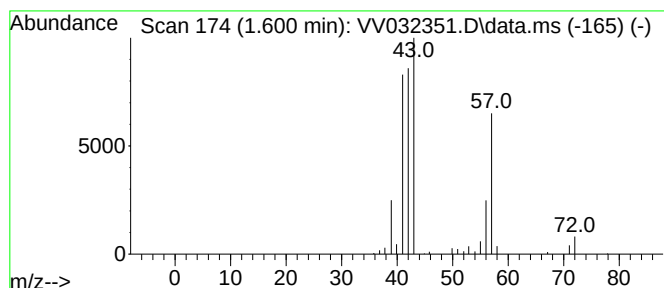
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR092923WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.600 | 1.25 ug/L | 58573 | 1,4-Difluorobenzene | 5.538 |

| Hit# | of 5 | Tentative ID         | MW | MolForm | CAS#        | Qual |
|------|------|----------------------|----|---------|-------------|------|
| 1    |      | Butane, 2-methyl-    | 72 | C5H12   | 000078-78-4 | 90   |
| 2    |      | Butane, 2-methyl-    | 72 | C5H12   | 000078-78-4 | 90   |
| 3    |      | Pentane              | 72 | C5H12   | 000109-66-0 | 38   |
| 4    |      | 3-Buten-1-ol         | 72 | C4H8O   | 000627-27-0 | 37   |
| 5    |      | 1-Propene, 2-methyl- | 56 | C4H8    | 000115-11-7 | 10   |



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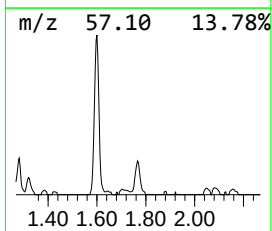
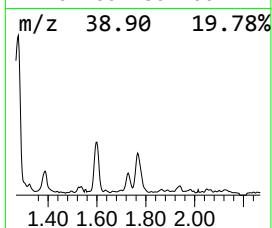
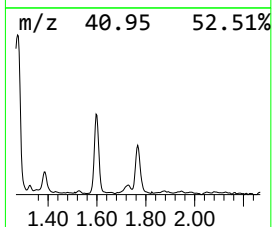
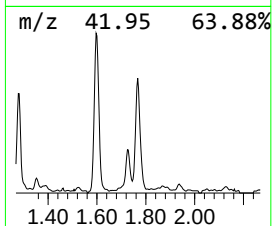
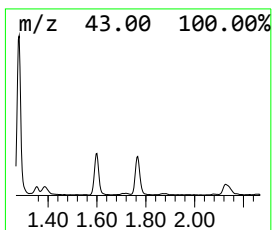
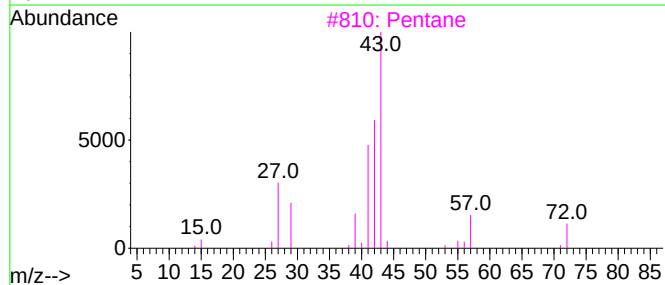
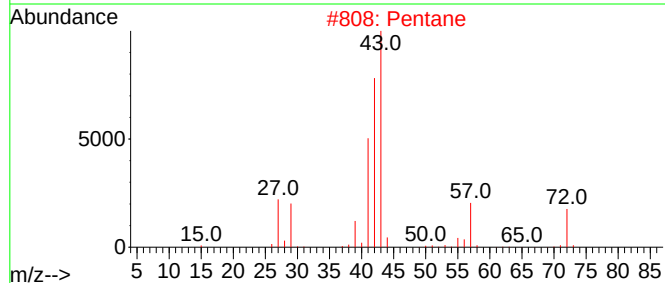
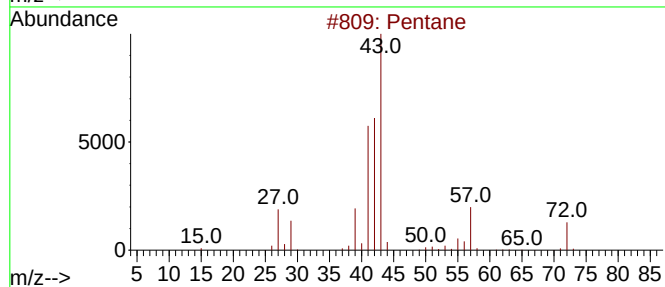
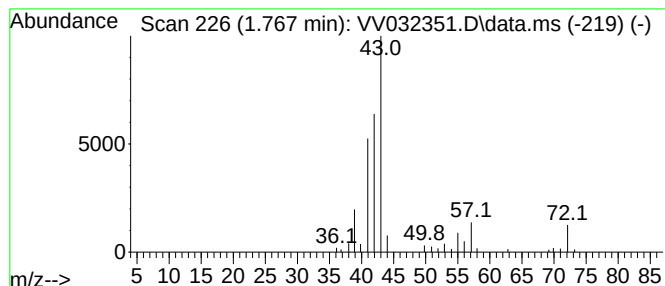
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVTR092923WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.767 | 0.94 ug/L | 43874 | 1,4-Difluorobenzene | 5.538 |

| Hit# | of      | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|---------|---|--------------|----|---------|-------------|------|
| 1    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 87   |
| 2    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |
| 3    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |
| 4    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |
| 5    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |



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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 |
| unknown-01         | 1.085 | 5.7     | ug/L  | 266430   | 1                     | 5.538 | 234511 | 5.0  |
| (DEL) Alkane: S... | 1.191 | 1.6     | ug/L  | 74214    | 1                     | 5.538 | 234511 | 5.0  |
| (DEL) Alkane: S... | 1.600 | 1.3     | ug/L  | 58573    | 1                     | 5.538 | 234511 | 5.0  |
| (DEL) Alkane: S... | 1.767 | 0.9     | ug/L  | 43874    | 1                     | 5.538 | 234511 | 5.0  |