

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
 Data File : VU054653.D  
 Acq On : 22 Jun 2023 14:00  
 Operator : MD/SY  
 Sample : 03326-03  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GCA33

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\SFAMUTR060723WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054653.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         | 1.361       | 16            | 22          | 41           | rVB      | 273984         | 301219        | 29.66%          | 2.785%        |
| 2         | 1.444       | 43            | 48          | 56           | rVB2     | 37587          | 41588         | 4.09%           | 0.385%        |
| 3         | 1.493       | 56            | 63          | 78           | rVB      | 182083         | 183903        | 18.11%          | 1.700%        |
| 4         | 1.599       | 86            | 96          | 111          | rBV4     | 294033         | 404748        | 39.85%          | 3.742%        |
| 5         | 1.692       | 119           | 125         | 132          | rBV2     | 17893          | 25515         | 2.51%           | 0.236%        |
| 6         | 1.914       | 186           | 194         | 210          | rVB      | 118098         | 186354        | 18.35%          | 1.723%        |
| 7         | 1.994       | 211           | 219         | 233          | rVB      | 145863         | 197047        | 19.40%          | 1.822%        |
| 8         | 2.152       | 263           | 268         | 275          | rVB3     | 18811          | 24170         | 2.38%           | 0.223%        |
| 9         | 2.203       | 276           | 284         | 301          | rVB3     | 67163          | 117546        | 11.57%          | 1.087%        |
| 10        | 2.409       | 339           | 348         | 357          | rVB7     | 11828          | 23891         | 2.35%           | 0.221%        |
| 11        | 2.563       | 384           | 396         | 411          | rBV      | 199473         | 337794        | 33.26%          | 3.123%        |
| 12        | 2.682       | 422           | 433         | 447          | rVB2     | 30957          | 59889         | 5.90%           | 0.554%        |
| 13        | 2.856       | 477           | 487         | 502          | rVB4     | 11252          | 21026         | 2.07%           | 0.194%        |
| 14        | 3.042       | 535           | 545         | 548          | rBV7     | 7845           | 12461         | 1.23%           | 0.115%        |
| 15        | 3.078       | 549           | 556         | 568          | rVB3     | 21976          | 44298         | 4.36%           | 0.410%        |
| 16        | 3.357       | 625           | 643         | 659          | rVB2     | 18685          | 41359         | 4.07%           | 0.382%        |
| 17        | 3.701       | 733           | 750         | 761          | rBV3     | 16626          | 47338         | 4.66%           | 0.438%        |
| 18        | 4.528       | 994           | 1007        | 1015         | rBV3     | 8083           | 17713         | 1.74%           | 0.164%        |
| 19        | 4.637       | 1028          | 1041        | 1084         | rBV      | 118805         | 418477        | 41.20%          | 3.869%        |
| 20        | 4.814       | 1087          | 1096        | 1116         | rVB3     | 11793          | 33003         | 3.25%           | 0.305%        |
| 21        | 5.058       | 1157          | 1172        | 1202         | rVB      | 179677         | 412249        | 40.59%          | 3.811%        |
| 22        | 5.377       | 1257          | 1271        | 1284         | rVB7     | 14300          | 35687         | 3.51%           | 0.330%        |
| 23        | 5.589       | 1323          | 1337        | 1347         | rBV6     | 9968           | 21786         | 2.14%           | 0.201%        |
| 24        | 5.721       | 1357          | 1378        | 1408         | rBV2     | 355644         | 969638        | 95.47%          | 8.965%        |
| 25        | 5.981       | 1447          | 1459        | 1471         | rBV2     | 7500           | 16242         | 1.60%           | 0.150%        |
| 26        | 6.132       | 1493          | 1506        | 1517         | rBV4     | 9509           | 20069         | 1.98%           | 0.186%        |
| 27        | 6.245       | 1528          | 1541        | 1561         | rBV      | 402692         | 786346        | 77.42%          | 7.270%        |
| 28        | 6.541       | 1621          | 1633        | 1647         | rVB9     | 9195           | 20485         | 2.02%           | 0.189%        |
| 29        | 6.685       | 1663          | 1678        | 1693         | rBV      | 233053         | 460023        | 45.29%          | 4.253%        |
| 30        | 6.756       | 1693          | 1700        | 1710         | rVB5     | 24695          | 47333         | 4.66%           | 0.438%        |
| 31        | 6.981       | 1758          | 1770        | 1784         | rVB5     | 4853           | 10738         | 1.06%           | 0.099%        |
| 32        | 7.563       | 1937          | 1951        | 1972         | rBV      | 110363         | 200176        | 19.71%          | 1.851%        |
| 33        | 7.852       | 2030          | 2041        | 2042         | rBV4     | 9265           | 11392         | 1.12%           | 0.105%        |
| 34        | 7.894       | 2043          | 2054        | 2067         | rVV      | 423725         | 731792        | 72.05%          | 6.766%        |
| 35        | 7.965       | 2067          | 2076        | 2089         | rVB2     | 66662          | 120008        | 11.82%          | 1.110%        |
| 36        | 8.177       | 2133          | 2142        | 2153         | rBV      | 66545          | 110720        | 10.90%          | 1.024%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
 Data File : VU054653.D  
 Acq On : 22 Jun 2023 14:00  
 Operator : MD/SY  
 Sample : 03326-03  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 GCA33

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\SFAMUTR060723WMA.M  
 Title : TRACE VOA SFAM1.0

|    |        |      |      |      |      |        |         |         |        |
|----|--------|------|------|------|------|--------|---------|---------|--------|
| 37 | 8.630  | 2270 | 2283 | 2316 | rBV2 | 500611 | 1015684 | 100.00% | 9.391% |
| 38 | 8.788  | 2324 | 2332 | 2344 | rVB7 | 14413  | 27742   | 2.73%   | 0.256% |
| 39 | 8.859  | 2348 | 2354 | 2363 | rVB3 | 7205   | 10323   | 1.02%   | 0.095% |
| 40 | 9.412  | 2512 | 2526 | 2551 | rBV  | 555069 | 988985  | 97.37%  | 9.144% |
| 41 | 9.566  | 2562 | 2574 | 2587 | rBV2 | 32772  | 54031   | 5.32%   | 0.500% |
| 42 | 9.688  | 2603 | 2612 | 2625 | rVV2 | 33244  | 57937   | 5.70%   | 0.536% |
| 43 | 10.097 | 2729 | 2739 | 2757 | rBV5 | 15425  | 30481   | 3.00%   | 0.282% |
| 44 | 10.347 | 2808 | 2817 | 2825 | rBV5 | 8445   | 14219   | 1.40%   | 0.131% |
| 45 | 10.460 | 2840 | 2852 | 2866 | rBV9 | 13660  | 28112   | 2.77%   | 0.260% |
| 46 | 10.749 | 2931 | 2942 | 2957 | rBV  | 172566 | 283090  | 27.87%  | 2.617% |
| 47 | 10.897 | 2977 | 2988 | 3000 | rBV4 | 9085   | 18481   | 1.82%   | 0.171% |
| 48 | 10.997 | 3009 | 3019 | 3032 | rBV3 | 8375   | 21583   | 2.12%   | 0.200% |
| 49 | 11.084 | 3040 | 3046 | 3054 | rBV  | 8330   | 11236   | 1.11%   | 0.104% |
| 50 | 11.463 | 3153 | 3164 | 3185 | rVB2 | 24880  | 43133   | 4.25%   | 0.399% |
| 51 | 11.685 | 3225 | 3233 | 3244 | rBV8 | 13439  | 22896   | 2.25%   | 0.212% |
| 52 | 11.743 | 3244 | 3251 | 3258 | rVV8 | 8845   | 12340   | 1.21%   | 0.114% |
| 53 | 11.807 | 3258 | 3271 | 3289 | rVV  | 554112 | 908149  | 89.41%  | 8.396% |
| 54 | 12.087 | 3342 | 3358 | 3368 | rBV  | 6545   | 17035   | 1.68%   | 0.157% |
| 55 | 12.187 | 3377 | 3389 | 3407 | rBV  | 399446 | 657672  | 64.75%  | 6.081% |
| 56 | 12.884 | 3595 | 3606 | 3619 | rBV5 | 39841  | 65572   | 6.46%   | 0.606% |
| 57 | 13.984 | 3940 | 3948 | 3956 | rVB8 | 8866   | 13351   | 1.31%   | 0.123% |

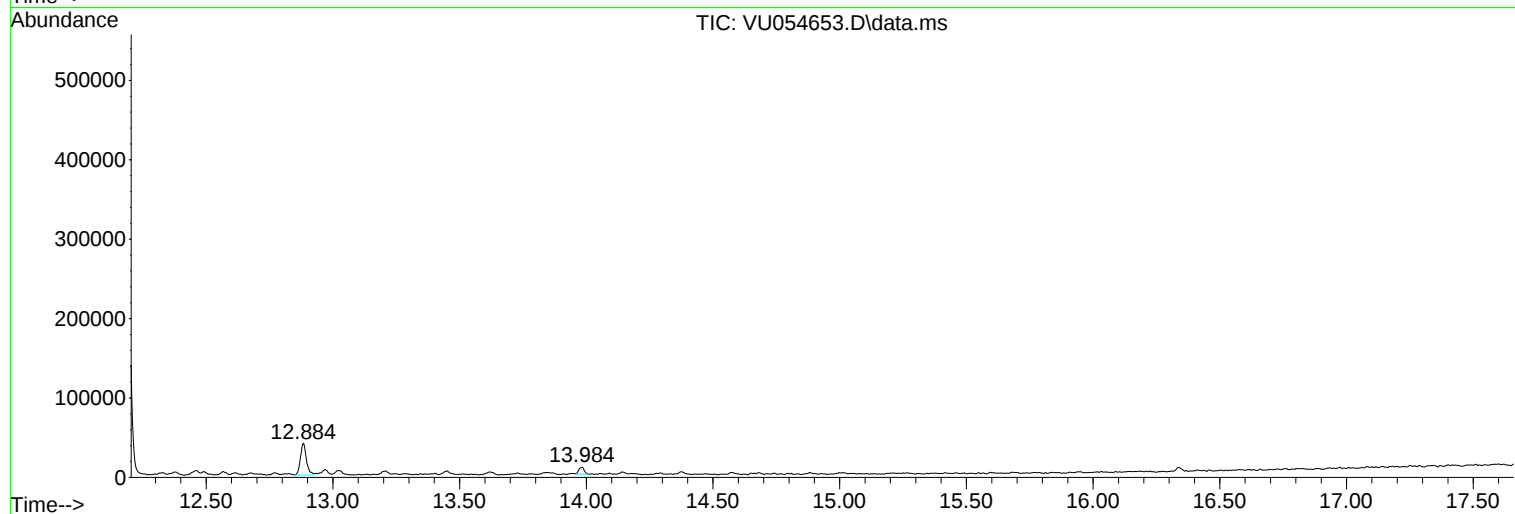
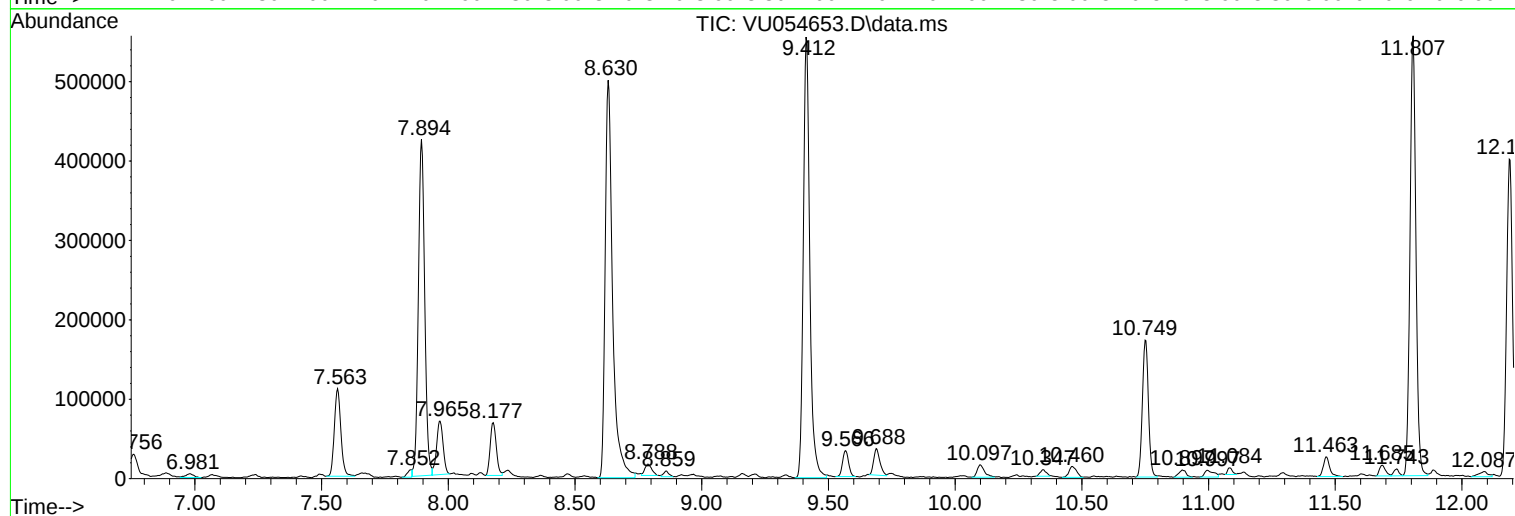
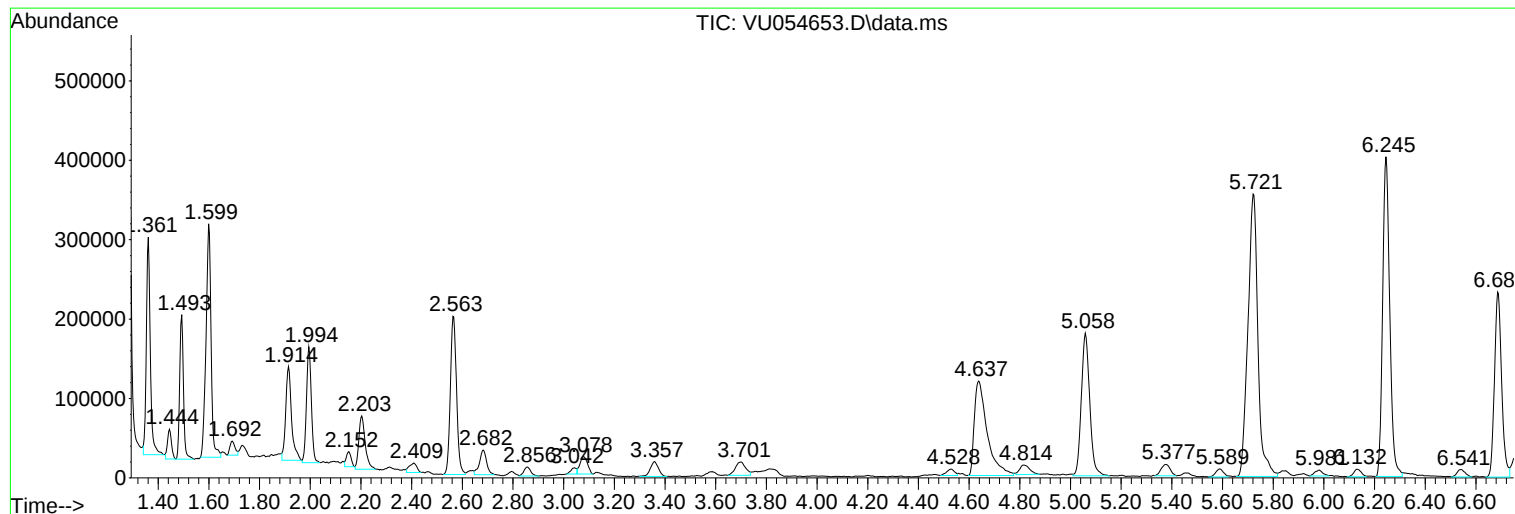
Sum of corrected areas: 10816075

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

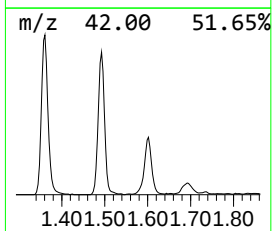
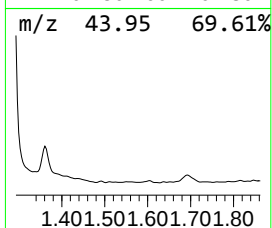
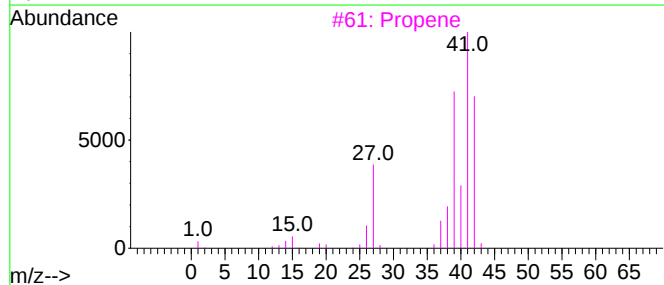
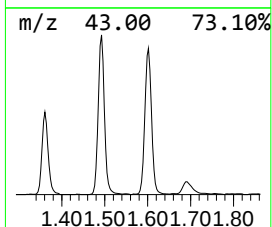
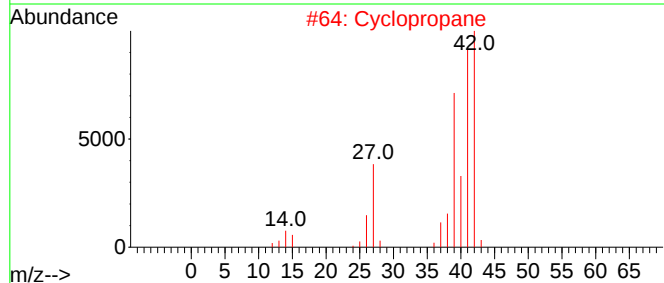
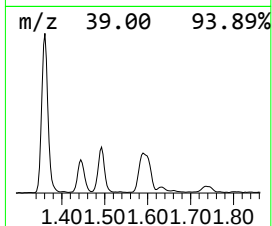
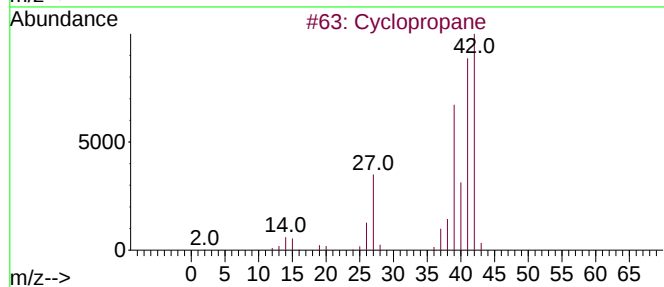
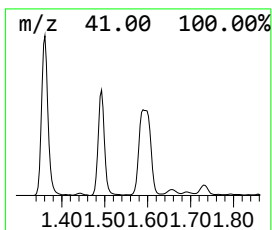
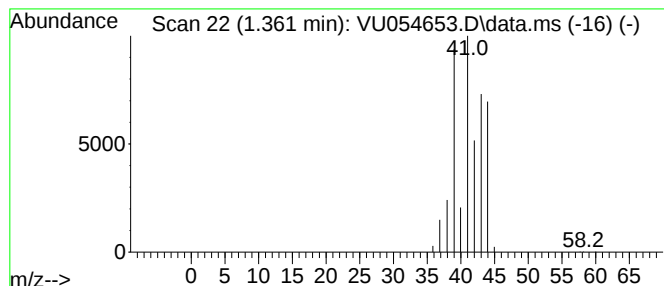
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 1 (DEL) Alkane: Cyclic1.361 Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.361 | 1.92 ug/L | 301219 | 1,4-Difluorobenzene | 6.245 |

| Hit# | of | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------|----|---------|-------------|------|
| 1    |    |   | Cyclopropane | 42 | C3H6    | 000075-19-4 | 39   |
| 2    |    |   | Cyclopropane | 42 | C3H6    | 000075-19-4 | 10   |
| 3    |    |   | Propene      | 42 | C3H6    | 000115-07-1 | 7    |
| 4    |    |   | Propane      | 44 | C3H8    | 000074-98-6 | 5    |
| 5    |    |   | Cyclopropene | 40 | C3H4    | 002781-85-3 | 4    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

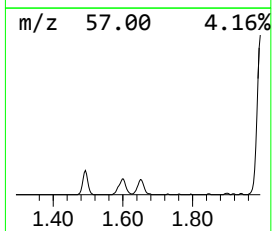
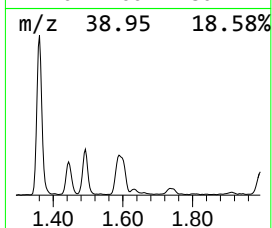
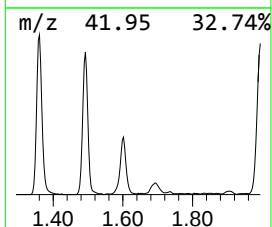
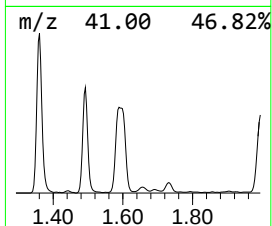
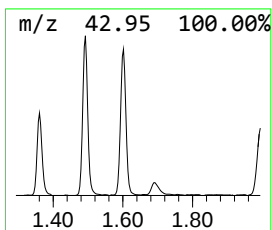
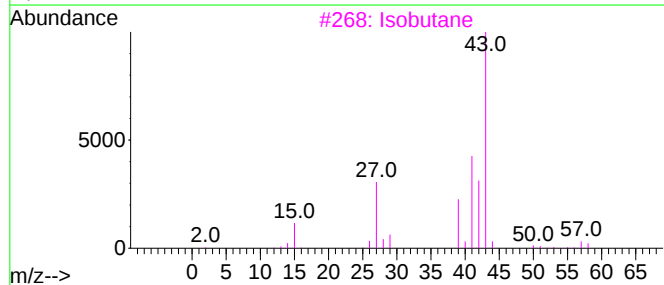
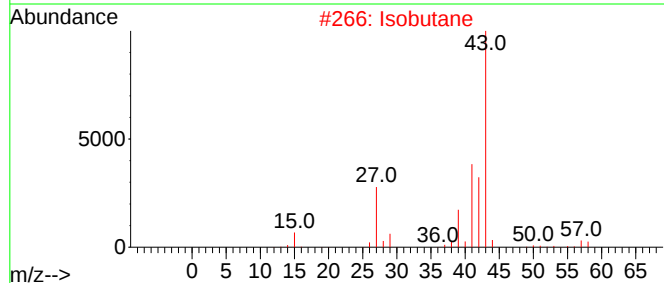
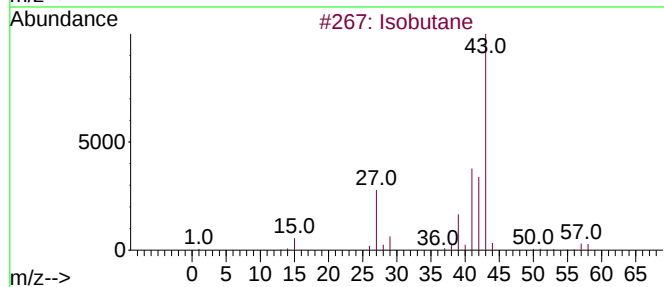
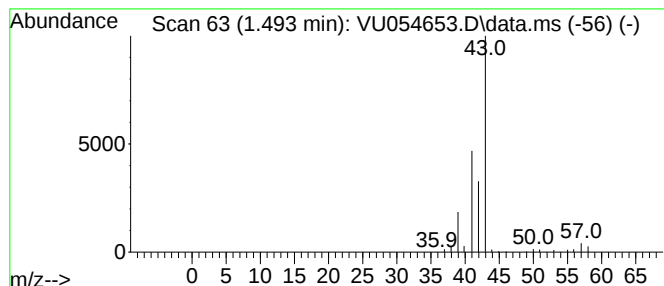
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.493 | 1.17 ug/L | 183903 | 1,4-Difluorobenzene | 6.245 |

| Hit# | of 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|------|--------------|----|---------|-------------|------|
| 1    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 72   |
| 2    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 59   |
| 3    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 50   |
| 4    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 9    |
| 5    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

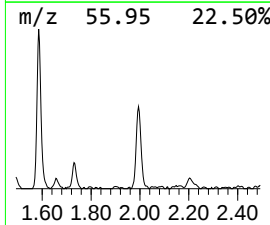
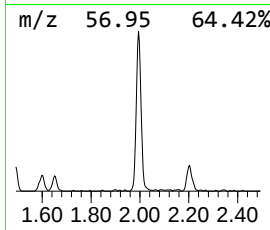
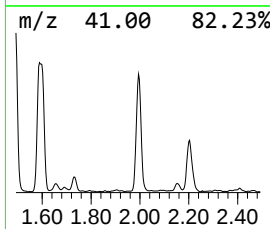
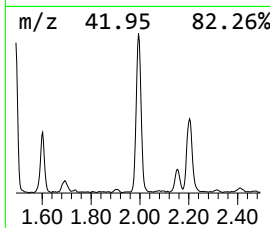
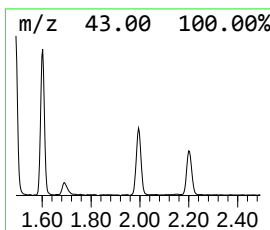
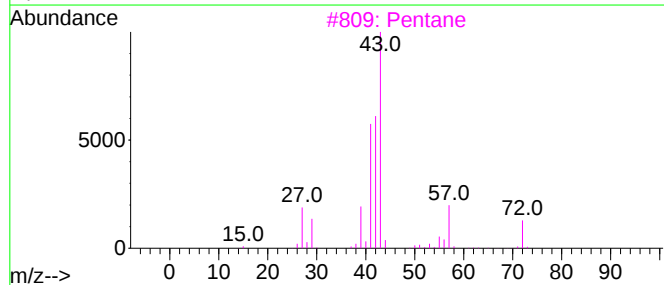
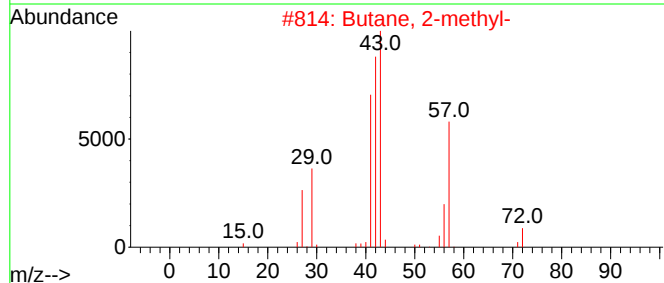
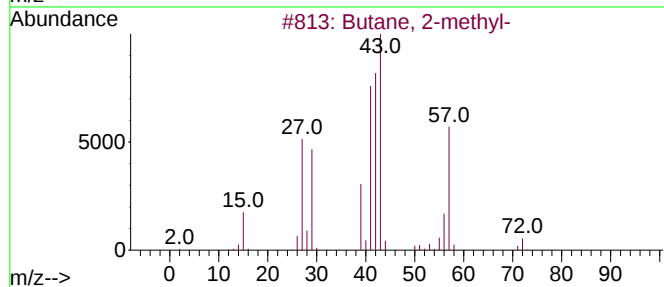
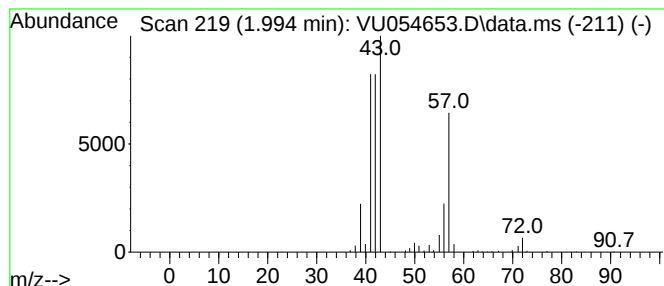
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 1.994 | 1.25 ug/L | 197047 | 1,4-Difluorobenzene | 6.245 |

| 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 | 80   |
| 3    |    |   | Pentane              | 72 | C5H12   | 000109-66-0 | 42   |
| 4    |    |   | 3-Buten-1-ol         | 72 | C4H8O   | 000627-27-0 | 25   |
| 5    |    |   | 1-Propene, 2-methyl- | 56 | C4H8    | 000115-11-7 | 10   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

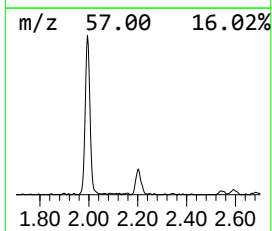
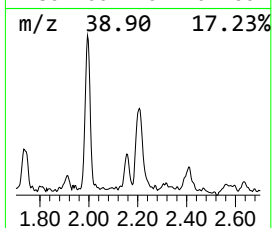
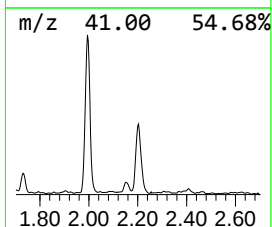
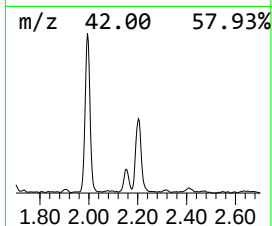
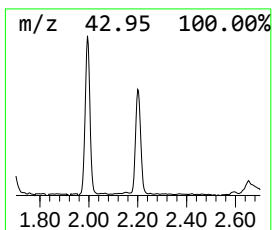
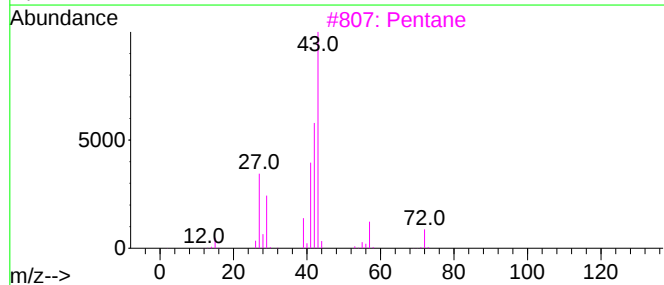
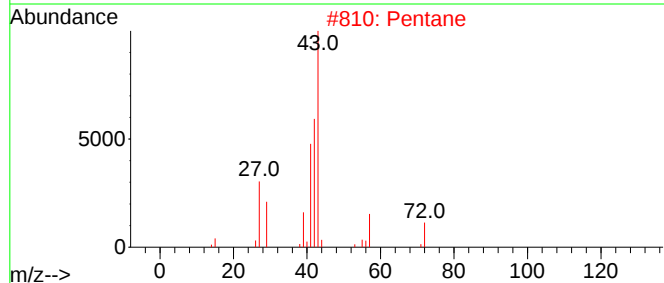
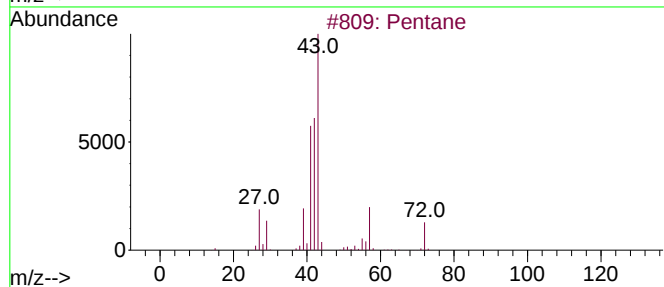
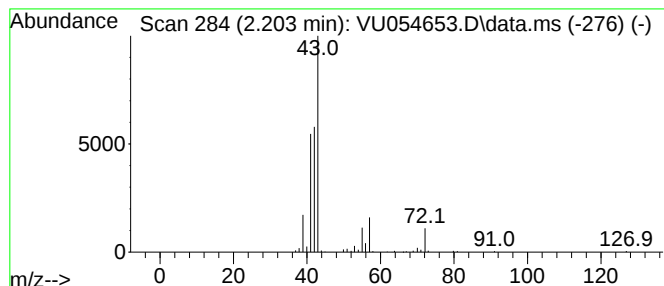
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 2.203 | 0.75 ug/L | 117546 | 1,4-Difluorobenzene | 6.245 |

| Hit# | of      | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|---------|---|--------------|----|---------|-------------|------|
| 1    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 87   |
| 2    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 86   |
| 3    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 86   |
| 4    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |
| 5    | Pentane |   |              | 72 | C5H12   | 000109-66-0 | 72   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU062223\  
Data File : VU054653.D  
Acq On : 22 Jun 2023 14:00  
Operator : MD/SY  
Sample : 03326-03  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
GCA33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR060723WMA.M  
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: C... | 1.361 | 1.9     | ug/L  | 301219   | 1                     | 6.245 | 786346 | 5.0  |
| (DEL) Alkane: S... | 1.493 | 1.2     | ug/L  | 183903   | 1                     | 6.245 | 786346 | 5.0  |
| (DEL) Alkane: S... | 1.994 | 1.3     | ug/L  | 197047   | 1                     | 6.245 | 786346 | 5.0  |
| (DEL) Alkane: S... | 2.203 | 0.8     | ug/L  | 117546   | 1                     | 6.245 | 786346 | 5.0  |