

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU122321\  
 Data File : VU046584.D  
 Acq On : 23 Dec 2021 22:37  
 Operator : SY/MD  
 Sample : M5170-06  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 H0AO4

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\SFAMUTR122121WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046584.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         | 1.366       | 3             | 8           | 10           | rBV      | 33484          | 33665         | 7.58%           | 1.040%        |
| 2         | 1.491       | 38            | 47          | 66           | rVB      | 27129          | 31157         | 7.02%           | 0.962%        |
| 3         | 1.604       | 72            | 82          | 94           | rVB      | 47215          | 56472         | 12.72%          | 1.744%        |
| 4         | 1.919       | 172           | 180         | 197          | rVV      | 24595          | 32363         | 7.29%           | 0.999%        |
| 5         | 1.999       | 197           | 205         | 218          | rVB2     | 10621          | 14835         | 3.34%           | 0.458%        |
| 6         | 2.208       | 262           | 270         | 280          | rVB2     | 5301           | 7349          | 1.66%           | 0.227%        |
| 7         | 2.572       | 372           | 383         | 397          | rVB      | 48678          | 78820         | 17.76%          | 2.434%        |
| 8         | 2.691       | 408           | 420         | 433          | rBV5     | 4681           | 10122         | 2.28%           | 0.313%        |
| 9         | 2.800       | 446           | 454         | 467          | rVB2     | 6898           | 12353         | 2.78%           | 0.381%        |
| 10        | 4.671       | 1016          | 1036        | 1097         | rBV      | 32554          | 174717        | 39.36%          | 5.396%        |
| 11        | 5.070       | 1144          | 1160        | 1185         | rVB2     | 50517          | 115001        | 25.91%          | 3.552%        |
| 12        | 5.729       | 1345          | 1365        | 1375         | rBV2     | 95275          | 252133        | 56.80%          | 7.786%        |
| 13        | 6.253       | 1513          | 1528        | 1544         | rBV      | 112252         | 211348        | 47.61%          | 6.527%        |
| 14        | 6.546       | 1608          | 1619        | 1632         | rBB      | 21287          | 38845         | 8.75%           | 1.200%        |
| 15        | 6.694       | 1652          | 1665        | 1686         | rBV      | 61609          | 119326        | 26.88%          | 3.685%        |
| 16        | 7.568       | 1925          | 1937        | 1952         | rBV      | 30219          | 52629         | 11.86%          | 1.625%        |
| 17        | 7.796       | 1998          | 2008        | 2028         | rBV3     | 12655          | 25448         | 5.73%           | 0.786%        |
| 18        | 7.899       | 2028          | 2040        | 2053         | rVV      | 112199         | 190834        | 42.99%          | 5.893%        |
| 19        | 7.970       | 2053          | 2062        | 2077         | rVB      | 45079          | 76472         | 17.23%          | 2.362%        |
| 20        | 8.182       | 2118          | 2128        | 2143         | rBV3     | 20101          | 34104         | 7.68%           | 1.053%        |
| 21        | 8.555       | 2234          | 2244        | 2254         | rBB2     | 18542          | 29515         | 6.65%           | 0.911%        |
| 22        | 8.639       | 2258          | 2270        | 2301         | rBV      | 221315         | 443919        | 100.00%         | 13.709%       |
| 23        | 9.417       | 2501          | 2512        | 2529         | rBV      | 162050         | 268634        | 60.51%          | 8.296%        |
| 24        | 9.571       | 2550          | 2560        | 2577         | rVB2     | 12976          | 21443         | 4.83%           | 0.662%        |
| 25        | 9.693       | 2584          | 2598        | 2611         | rVB      | 22328          | 37087         | 8.35%           | 1.145%        |
| 26        | 10.102      | 2714          | 2725        | 2733         | rBV2     | 7882           | 12277         | 2.77%           | 0.379%        |
| 27        | 10.237      | 2757          | 2767        | 2778         | rBV3     | 5340           | 8676          | 1.95%           | 0.268%        |
| 28        | 10.758      | 2917          | 2929        | 2943         | rBV      | 65587          | 104027        | 23.43%          | 3.213%        |
| 29        | 10.909      | 2964          | 2976        | 2985         | rVB3     | 3046           | 5116          | 1.15%           | 0.158%        |
| 30        | 10.999      | 2989          | 3004        | 3010         | rBV3     | 9488           | 16111         | 3.63%           | 0.498%        |
| 31        | 11.295      | 3086          | 3096        | 3106         | rVB3     | 3451           | 4815          | 1.08%           | 0.149%        |
| 32        | 11.468      | 3138          | 3150        | 3162         | rBV      | 23005          | 34102         | 7.68%           | 1.053%        |
| 33        | 11.812      | 3245          | 3257        | 3274         | rVB      | 167173         | 264975        | 59.69%          | 8.183%        |
| 34        | 11.896      | 3274          | 3283        | 3294         | rBV      | 7697           | 11036         | 2.49%           | 0.341%        |
| 35        | 12.060      | 3324          | 3334        | 3340         | rBV2     | 18251          | 28924         | 6.52%           | 0.893%        |
| 36        | 12.192      | 3364          | 3375        | 3391         | rVB      | 134386         | 218494        | 49.22%          | 6.748%        |

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 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 H0AO4

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\SFAMUTR122121WMA.M  
 Title : TRACE VOA SFAM1.0

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 37 | 12.468 | 3447 | 3461 | 3465 | rBV4 | 3883  | 6506  | 1.47% | 0.201% |
| 38 | 12.497 | 3465 | 3470 | 3479 | rVB3 | 3746  | 5565  | 1.25% | 0.172% |
| 39 | 12.571 | 3485 | 3493 | 3500 | rBV  | 7095  | 9691  | 2.18% | 0.299% |
| 40 | 12.677 | 3519 | 3526 | 3538 | rBV2 | 4018  | 7044  | 1.59% | 0.218% |
| 41 | 12.880 | 3581 | 3589 | 3599 | rVB6 | 3787  | 5918  | 1.33% | 0.183% |
| 42 | 12.973 | 3609 | 3618 | 3626 | rBV2 | 6226  | 9227  | 2.08% | 0.285% |
| 43 | 13.025 | 3626 | 3634 | 3646 | rVB  | 9718  | 14230 | 3.21% | 0.439% |
| 44 | 13.291 | 3707 | 3717 | 3727 | rVB3 | 10186 | 14957 | 3.37% | 0.462% |
| 45 | 13.452 | 3758 | 3767 | 3782 | rVB4 | 14765 | 24340 | 5.48% | 0.752% |
| 46 | 13.623 | 3812 | 3820 | 3829 | rVB2 | 6225  | 8630  | 1.94% | 0.267% |
| 47 | 14.089 | 3950 | 3965 | 3977 | rBV  | 17852 | 27793 | 6.26% | 0.858% |
| 48 | 14.687 | 4140 | 4151 | 4160 | rVB3 | 3717  | 6398  | 1.44% | 0.198% |
| 49 | 15.224 | 4309 | 4318 | 4329 | rVB4 | 8500  | 14632 | 3.30% | 0.452% |
| 50 | 15.410 | 4367 | 4376 | 4387 | rVB3 | 3889  | 6011  | 1.35% | 0.186% |

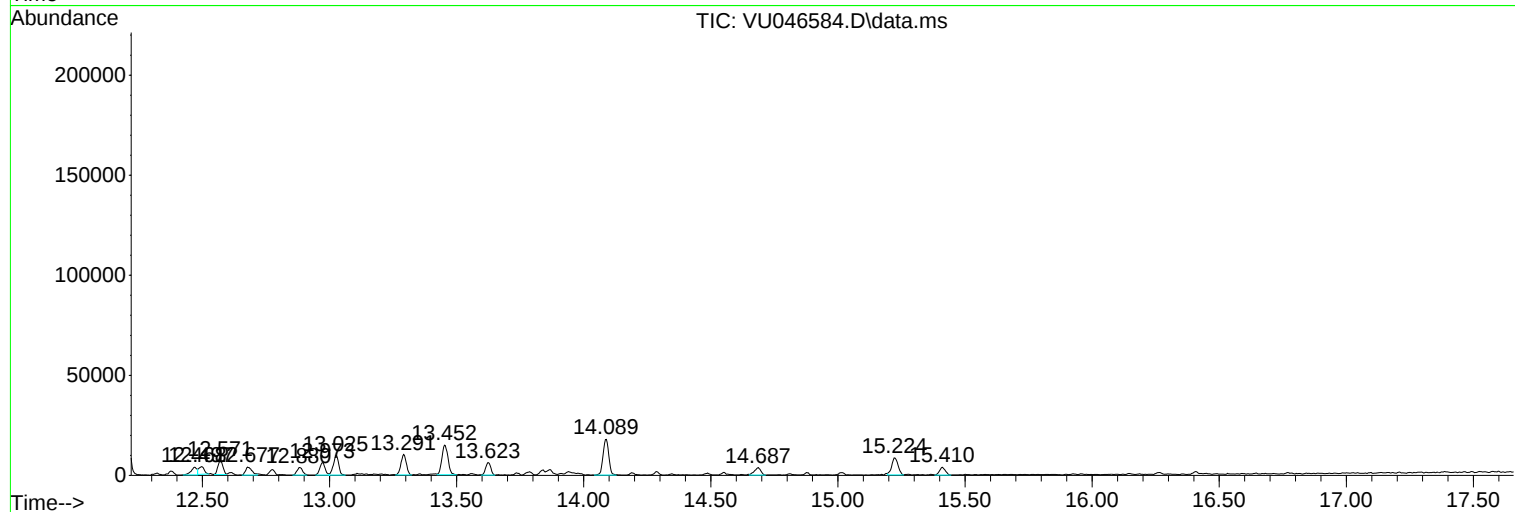
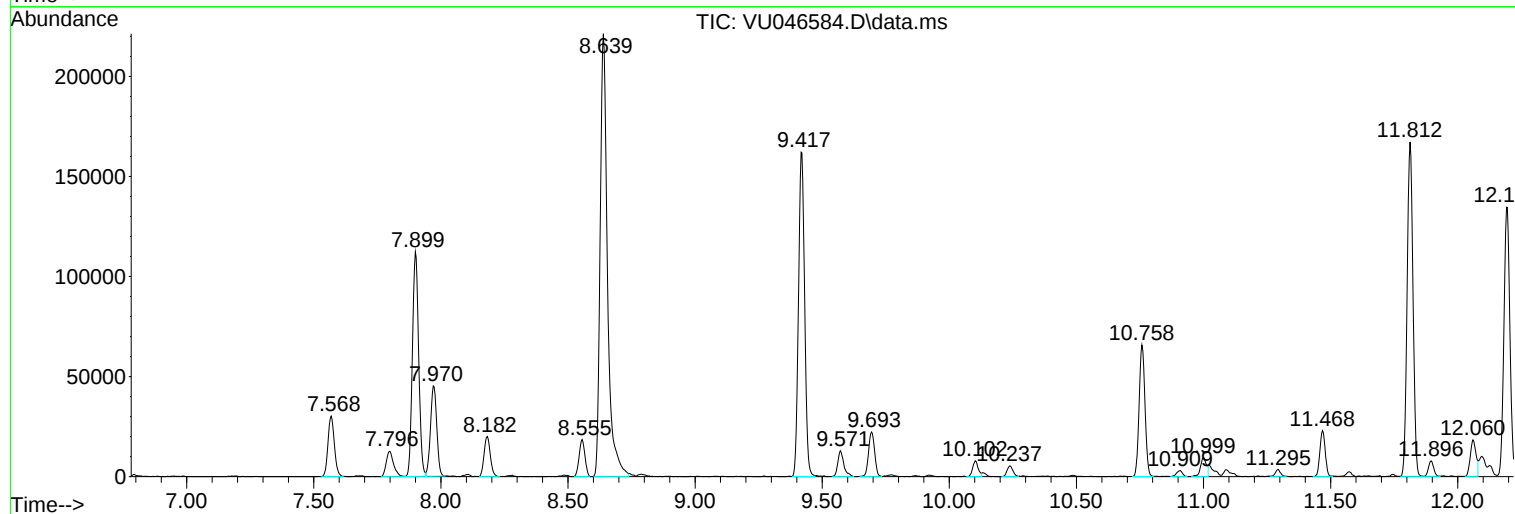
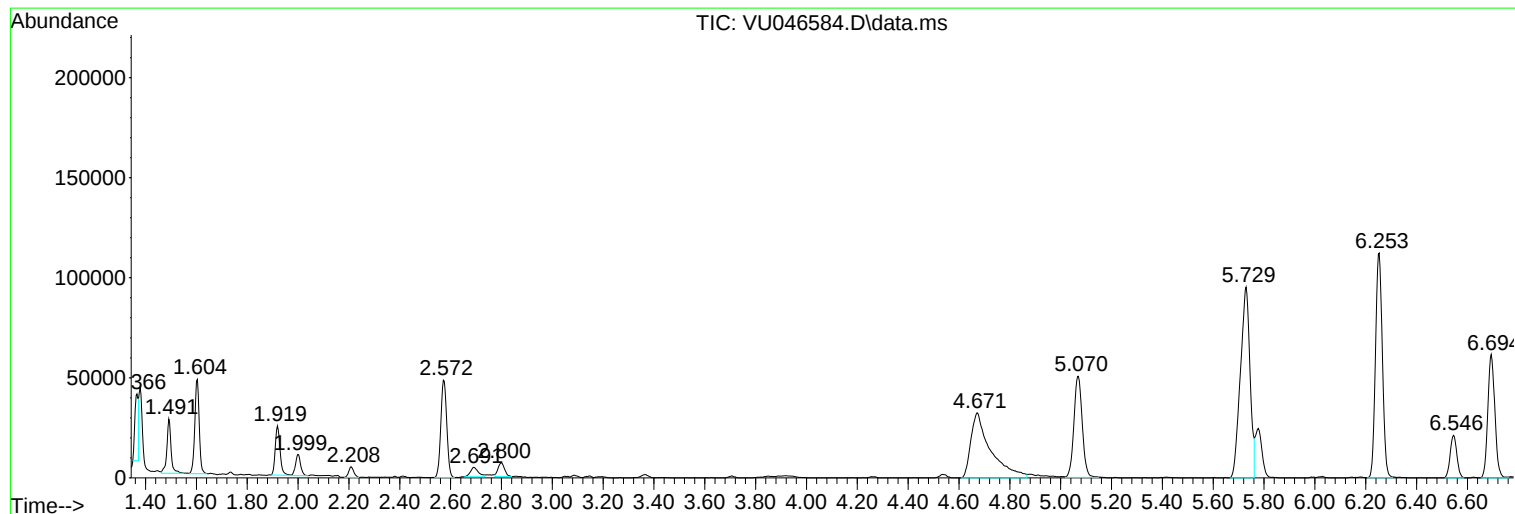
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Sample : M5170-06  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
H0AO4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.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\VU122321\  
Data File : VU046584.D  
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Sample : M5170-06  
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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
H0AO4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

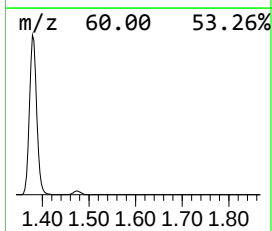
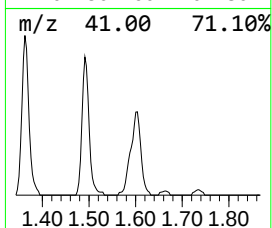
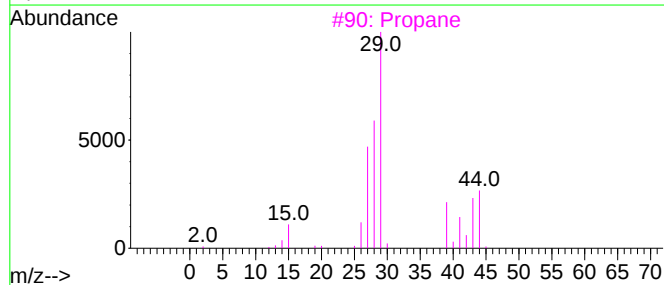
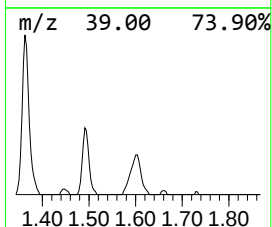
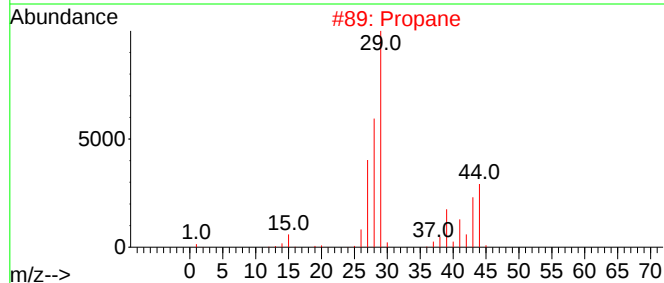
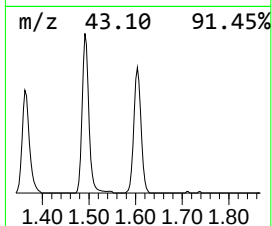
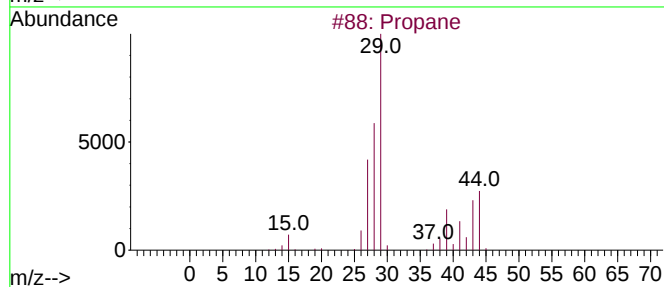
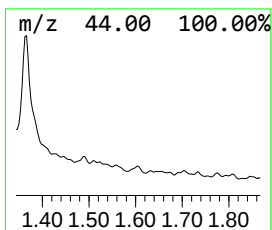
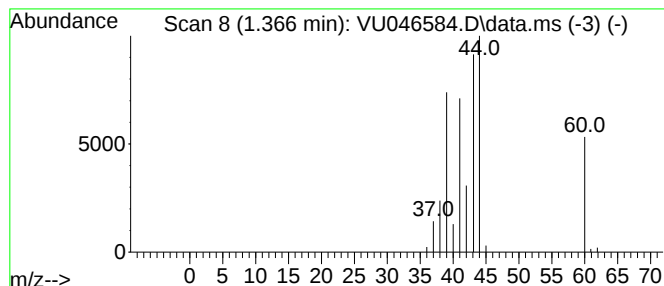
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.366 | 0.80 ug/L | 33665 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of | 5 | Tentative ID    | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------|----|---------|-------------|------|
| 1    |    |   | Propane         | 44 | C3H8    | 000074-98-6 | 78   |
| 2    |    |   | Propane         | 44 | C3H8    | 000074-98-6 | 64   |
| 3    |    |   | Propane         | 44 | C3H8    | 000074-98-6 | 9    |
| 4    |    |   | Propene         | 42 | C3H6    | 000115-07-1 | 9    |
| 5    |    |   | Ethylenediamine | 60 | C2H8N2  | 000107-15-3 | 4    |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
H0AO4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

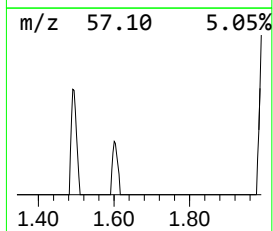
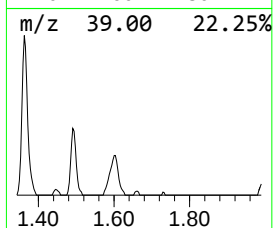
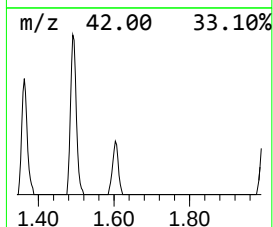
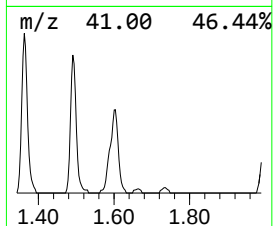
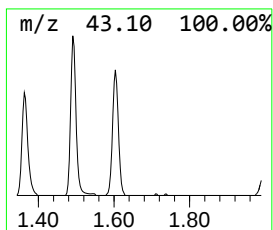
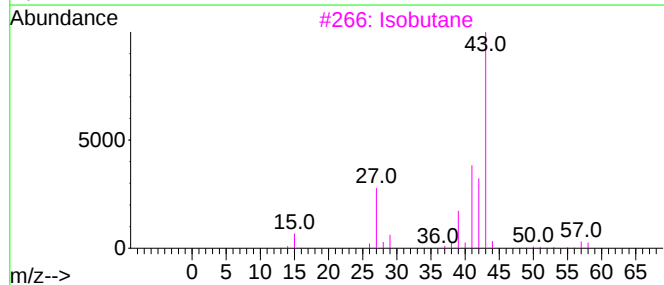
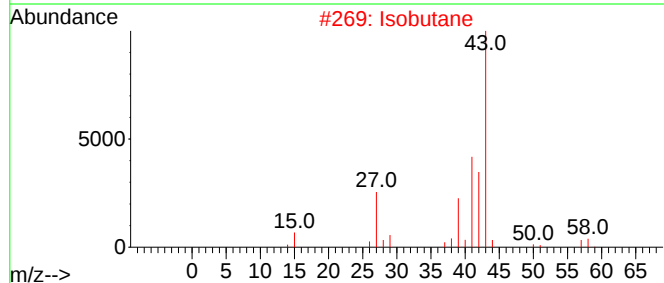
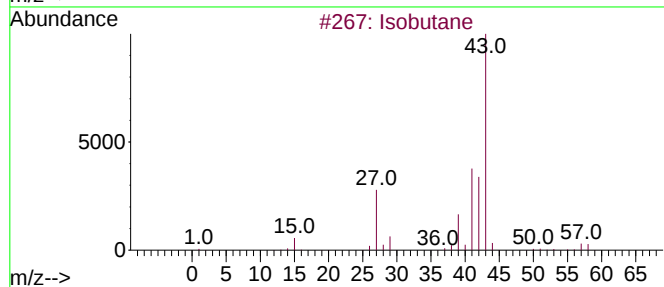
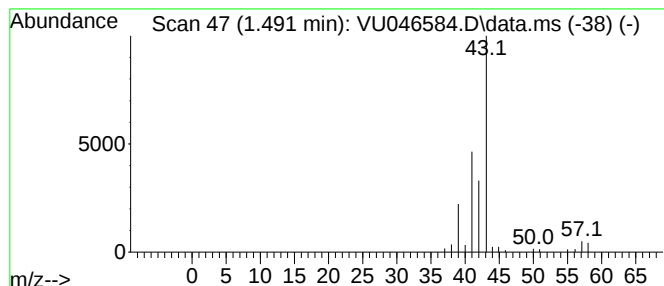
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.491 | 0.74 ug/L | 31157 | 1,4-Difluorobenzene | 6.253 |

| Hit# | of 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|------|--------------|----|---------|-------------|------|
| 1    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 64   |
| 2    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 58   |
| 3    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 53   |
| 4    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 50   |
| 5    |      | Isobutane    | 58 | C4H10   | 000075-28-5 | 50   |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
H0AO4

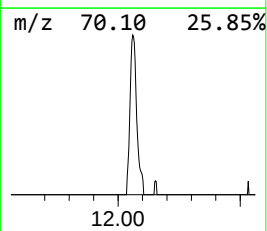
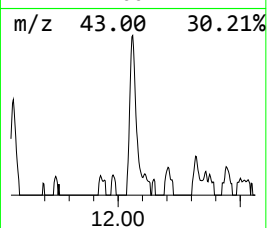
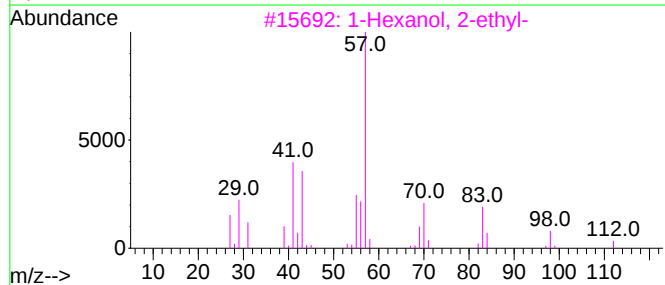
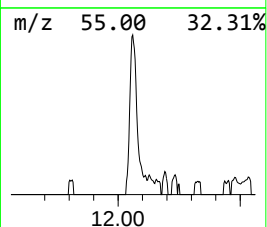
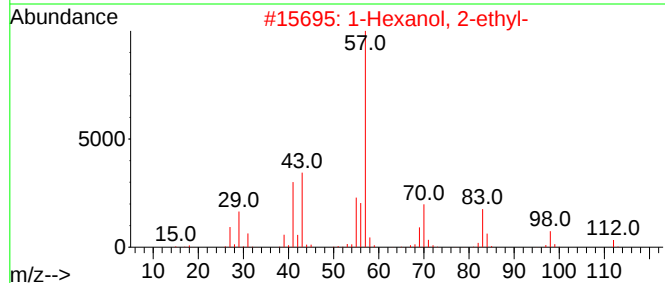
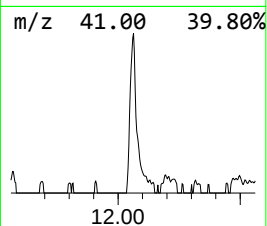
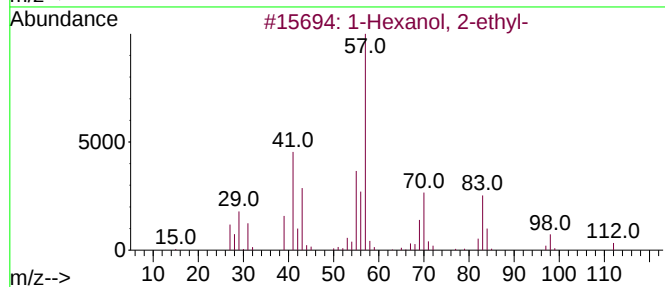
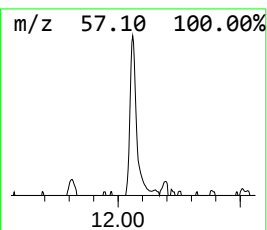
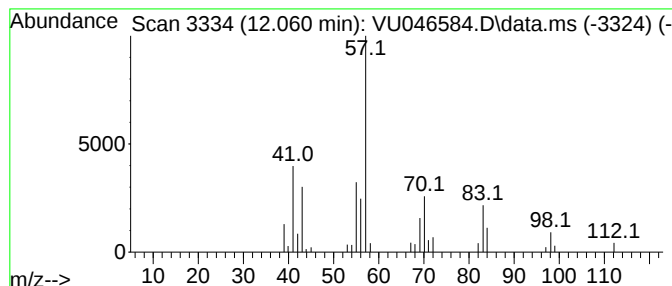
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.060 | 0.55 ug/L | 28924 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------|-----|---------|-------------|------|
| 1    |      | 1-Hexanol, 2-ethyl- | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    |      | 1-Hexanol, 2-ethyl- | 130 | C8H18O  | 000104-76-7 | 83   |
| 3    |      | 1-Hexanol, 2-ethyl- | 130 | C8H18O  | 000104-76-7 | 83   |
| 4    |      | 1-Hexanol, 2-ethyl- | 130 | C8H18O  | 000104-76-7 | 78   |
| 5    |      | 1-Hexanol, 2-ethyl- | 130 | C8H18O  | 000104-76-7 | 72   |



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Instrument :  
MSVOA\_U  
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H0AO4

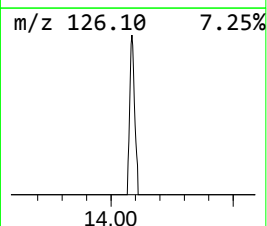
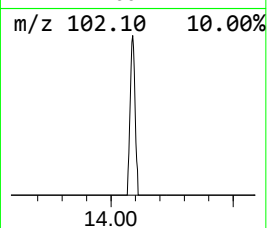
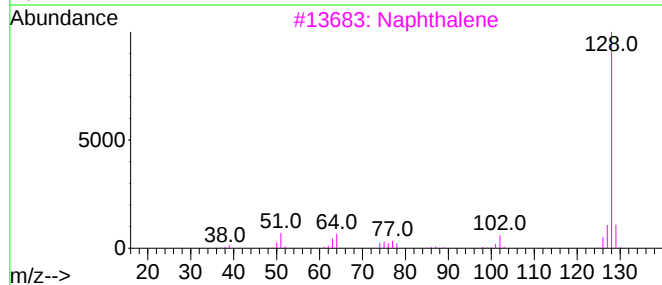
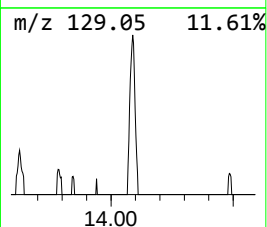
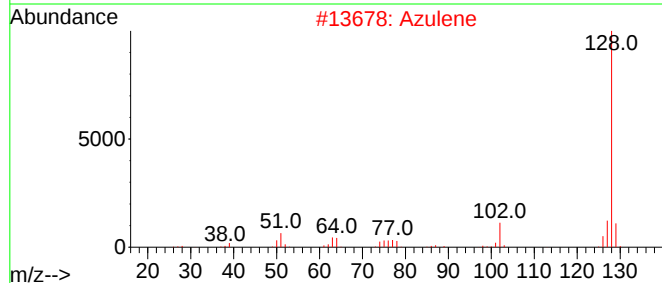
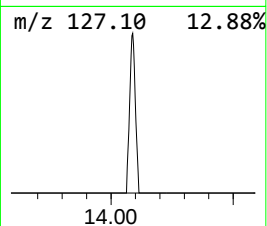
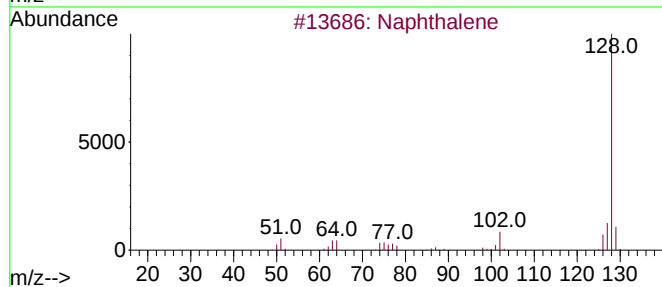
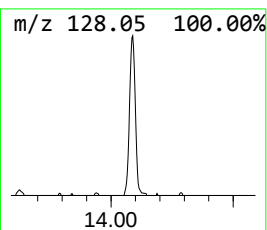
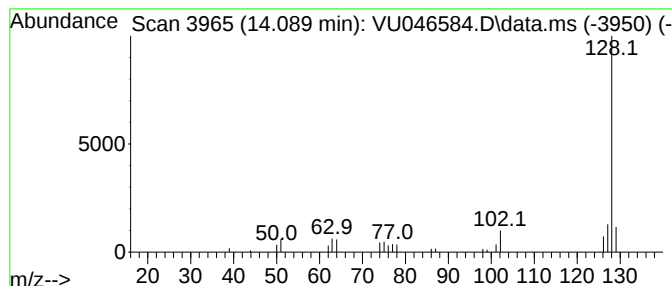
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 5 Azulene Concentration Rank 5

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 14.089 | 0.52 ug/L | 27793 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 95   |
| 2    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 94   |
| 3    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 94   |
| 4    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 94   |
| 5    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU122321\  
Data File : VU046584.D  
Acq On : 23 Dec 2021 22:37  
Operator : SY/MD  
Sample : M5170-06  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
H0AO4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR122121WMA.M  
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| (DEL) Alkane: S... | 1.366  | 0.8     | ug/L  | 33665    | 1                     | 6.253  | 211348 | 5.0  |
| (DEL) Alkane: S... | 1.491  | 0.7     | ug/L  | 31157    | 1                     | 6.253  | 211348 | 5.0  |
| 1-Hexanol, 2-et... | 12.060 | 0.6     | ug/L  | 28924    | 3                     | 11.812 | 264975 | 5.0  |
| Azulene            | 14.089 | 0.5     | ug/L  | 27793    | 3                     | 11.812 | 264975 | 5.0  |