

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU020525\  
 Data File : VU063178.D  
 Acq On : 06 Feb 2025 00:07  
 Operator : MD/SY  
 Sample : Q1226-24  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DCZN2

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\SFAMUTR020425WMA.M  
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU063178.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         | 1.592       | 84            | 94          | 109          | rBV      | 35447          | 43265         | 6.65%           | 1.009%        |
| 2         | 1.727       | 116           | 136         | 141          | rBV6     | 5712           | 17353         | 2.67%           | 0.405%        |
| 3         | 1.904       | 184           | 191         | 201          | rVB      | 32763          | 40681         | 6.25%           | 0.949%        |
| 4         | 2.557       | 383           | 394         | 407          | rBV      | 57050          | 92982         | 14.30%          | 2.169%        |
| 5         | 4.615       | 1020          | 1034        | 1039         | rBV      | 51418          | 99690         | 15.33%          | 2.326%        |
| 6         | 5.049       | 1155          | 1169        | 1199         | rBV      | 56749          | 127522        | 19.61%          | 2.975%        |
| 7         | 5.711       | 1357          | 1375        | 1413         | rBV2     | 116500         | 320222        | 49.23%          | 7.471%        |
| 8         | 6.235       | 1527          | 1538        | 1572         | rBV      | 115580         | 225794        | 34.72%          | 5.268%        |
| 9         | 6.534       | 1622          | 1631        | 1644         | rVB3     | 5574           | 10451         | 1.61%           | 0.244%        |
| 10        | 6.679       | 1660          | 1676        | 1693         | rBV2     | 73400          | 143786        | 22.11%          | 3.354%        |
| 11        | 7.557       | 1935          | 1949        | 1973         | rBV      | 33215          | 59388         | 9.13%           | 1.386%        |
| 12        | 7.888       | 2040          | 2052        | 2073         | rBV      | 131037         | 231354        | 35.57%          | 5.397%        |
| 13        | 8.174       | 2131          | 2141        | 2158         | rBV      | 18805          | 32390         | 4.98%           | 0.756%        |
| 14        | 8.624       | 2271          | 2281        | 2317         | rBV      | 177331         | 339763        | 52.24%          | 7.927%        |
| 15        | 9.409       | 2508          | 2525        | 2545         | rBV      | 159636         | 303333        | 46.64%          | 7.077%        |
| 16        | 10.746      | 2930          | 2941        | 2963         | rBV      | 57367          | 92556         | 14.23%          | 2.159%        |
| 17        | 10.994      | 3005          | 3018        | 3024         | rBV3     | 4738           | 8113          | 1.25%           | 0.189%        |
| 18        | 11.460      | 3154          | 3163        | 3174         | rBV      | 6526           | 9510          | 1.46%           | 0.222%        |
| 19        | 11.801      | 3258          | 3269        | 3289         | rBV      | 144998         | 244470        | 37.59%          | 5.703%        |
| 20        | 12.087      | 3348          | 3358        | 3366         | rBV2     | 4883           | 7250          | 1.11%           | 0.169%        |
| 21        | 12.183      | 3377          | 3388        | 3408         | rBV      | 122573         | 211881        | 32.58%          | 4.943%        |
| 22        | 12.466      | 3462          | 3476        | 3501         | rBV      | 110598         | 197326        | 30.34%          | 4.604%        |
| 23        | 12.634      | 3519          | 3528        | 3539         | rBV4     | 6283           | 9947          | 1.53%           | 0.232%        |
| 24        | 12.797      | 3570          | 3579        | 3590         | rVB5     | 4974           | 7464          | 1.15%           | 0.174%        |
| 25        | 12.974      | 3626          | 3634        | 3646         | rBV3     | 9370           | 14456         | 2.22%           | 0.337%        |
| 26        | 13.920      | 3914          | 3928        | 3936         | rBV      | 139497         | 212421        | 32.66%          | 4.956%        |
| 27        | 13.968      | 3936          | 3943        | 3965         | rVB2     | 90501          | 150482        | 23.14%          | 3.511%        |
| 28        | 14.305      | 4040          | 4048        | 4057         | rBV3     | 18700          | 30997         | 4.77%           | 0.723%        |
| 29        | 14.354      | 4057          | 4063        | 4076         | rVB      | 17238          | 27492         | 4.23%           | 0.641%        |
| 30        | 14.695      | 4159          | 4169        | 4179         | rBV2     | 24590          | 37923         | 5.83%           | 0.885%        |
| 31        | 14.775      | 4185          | 4194        | 4204         | rVB3     | 13142          | 19884         | 3.06%           | 0.464%        |
| 32        | 14.833      | 4204          | 4212        | 4223         | rVB5     | 7519           | 11646         | 1.79%           | 0.272%        |
| 33        | 14.939      | 4236          | 4245        | 4262         | rBV3     | 18498          | 29950         | 4.60%           | 0.699%        |
| 34        | 15.167      | 4303          | 4316        | 4328         | rBV      | 406819         | 650413        | 100.00%         | 15.174%       |
| 35        | 15.251      | 4337          | 4342        | 4356         | rVB      | 22785          | 37998         | 5.84%           | 0.886%        |
| 36        | 15.392      | 4374          | 4386        | 4408         | rVB3     | 26537          | 63494         | 9.76%           | 1.481%        |

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ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

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\SFAMUTR020425WMA.M  
Title : TRACE VOA SFAM1.0

|    |        |      |      |      |       |       |       |       |        |
|----|--------|------|------|------|-------|-------|-------|-------|--------|
| 37 | 15.521 | 4417 | 4426 | 4444 | rBV3  | 17702 | 36694 | 5.64% | 0.856% |
| 38 | 15.637 | 4453 | 4462 | 4469 | rBV2  | 11206 | 19774 | 3.04% | 0.461% |
| 39 | 15.733 | 4484 | 4492 | 4501 | rBV4  | 4043  | 6863  | 1.06% | 0.160% |
| 40 | 15.788 | 4501 | 4509 | 4519 | rVV6  | 6027  | 9804  | 1.51% | 0.229% |
| 41 | 15.981 | 4552 | 4569 | 4580 | rBV10 | 4254  | 10223 | 1.57% | 0.238% |
| 42 | 16.106 | 4595 | 4608 | 4615 | rBV8  | 6413  | 11924 | 1.83% | 0.278% |
| 43 | 16.373 | 4682 | 4691 | 4698 | rBV6  | 6349  | 11127 | 1.71% | 0.260% |
| 44 | 16.653 | 4764 | 4778 | 4786 | rBV5  | 5980  | 9294  | 1.43% | 0.217% |
| 45 | 17.418 | 5008 | 5016 | 5027 | rBV6  | 3902  | 7042  | 1.08% | 0.164% |

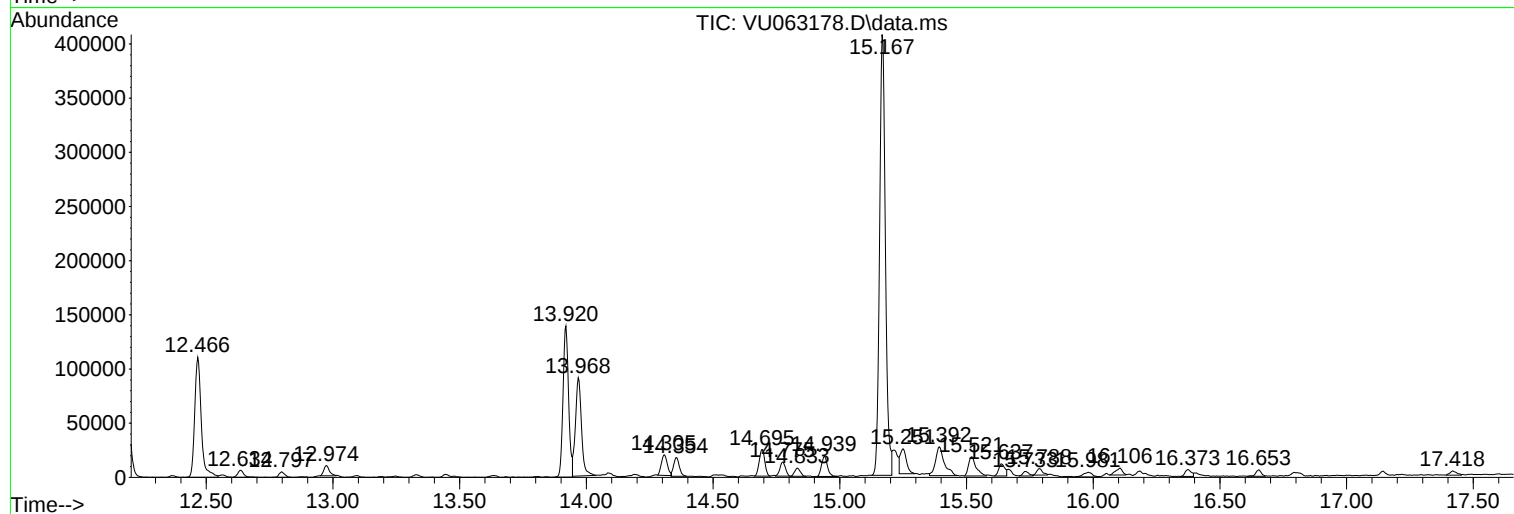
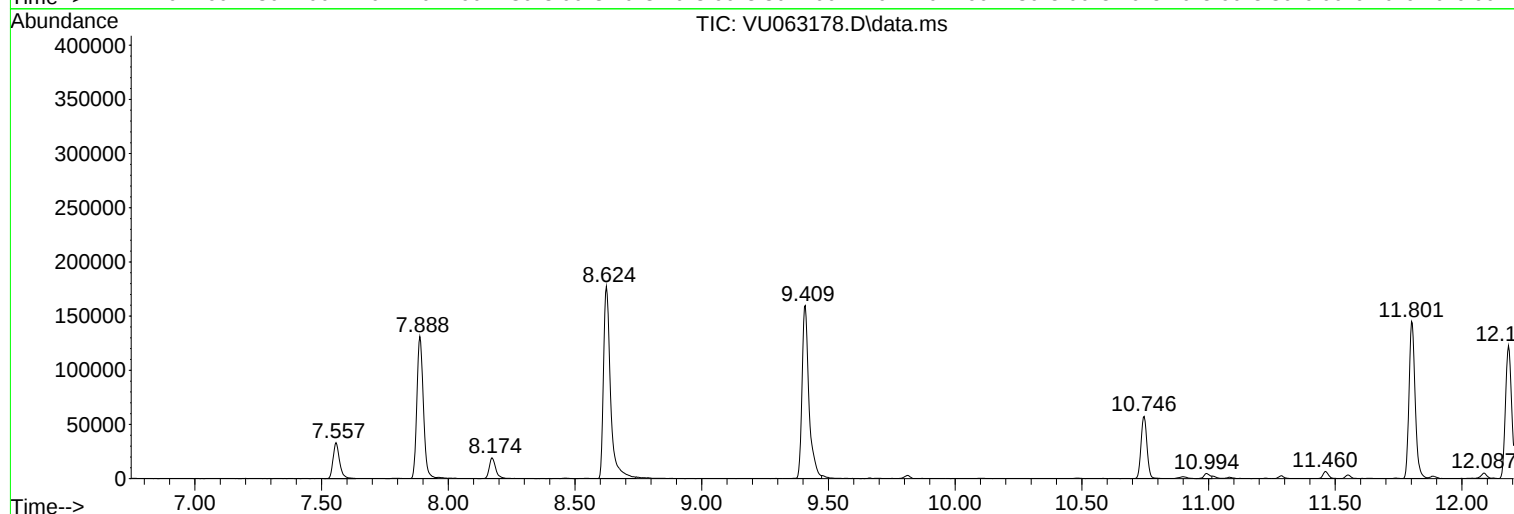
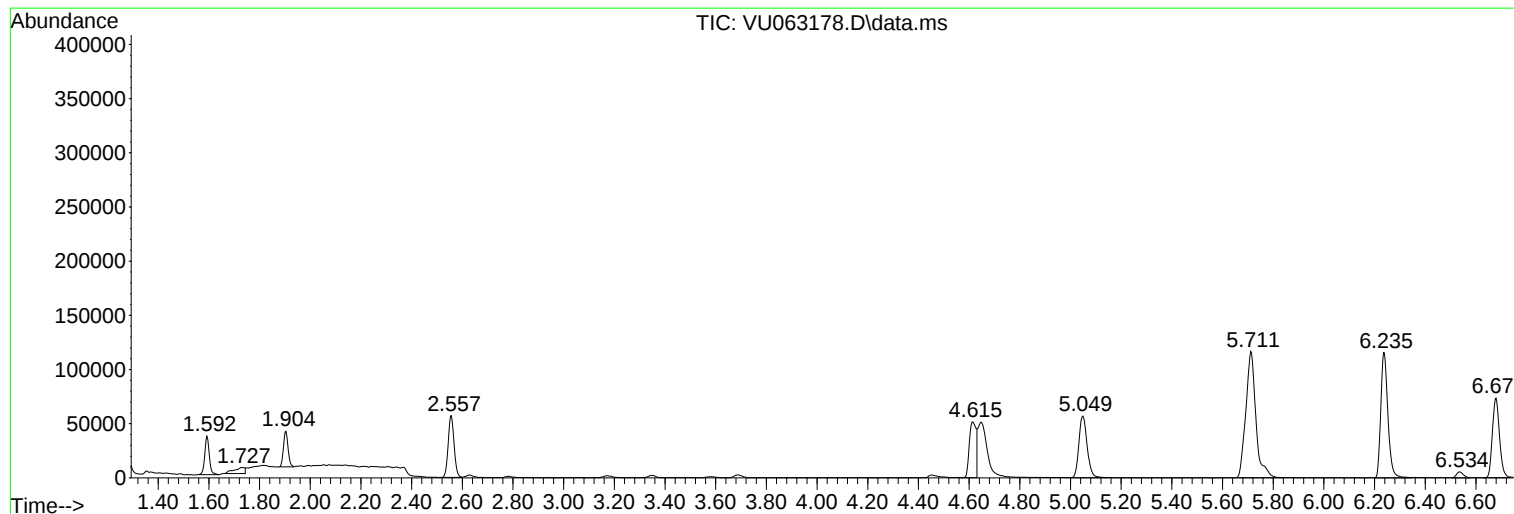
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ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR020425WMA.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\VU020525\  
Data File : VU063178.D  
Acq On : 06 Feb 2025 00:07  
Operator : MD/SY  
Sample : Q1226-24  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

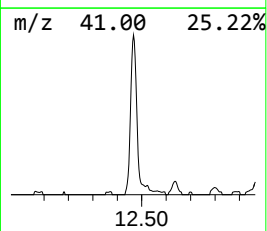
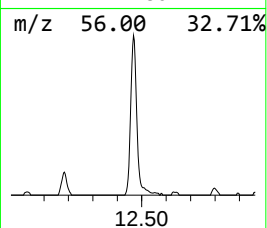
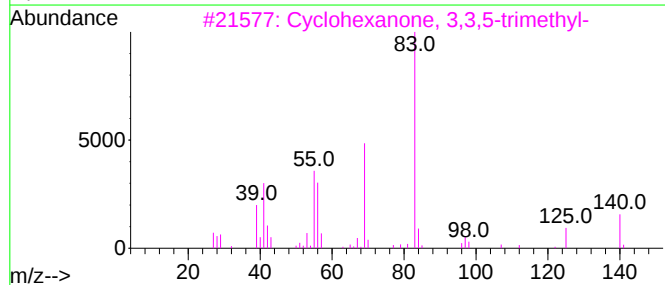
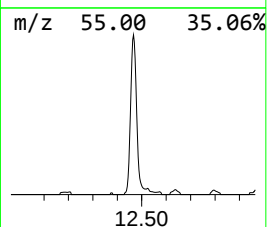
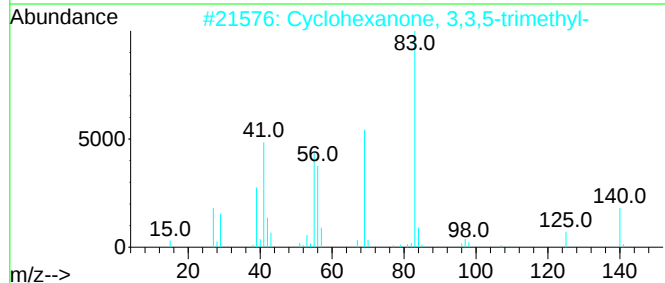
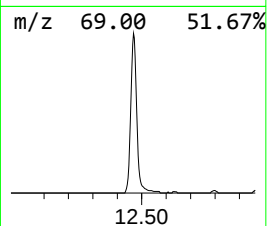
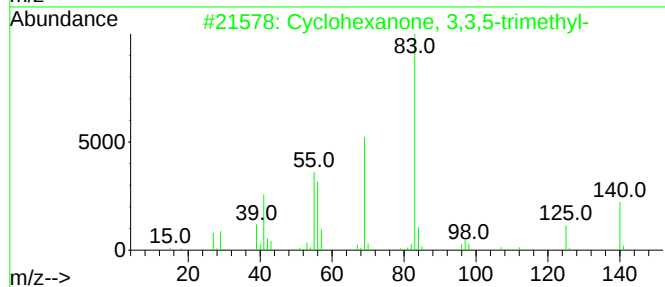
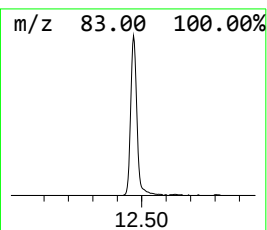
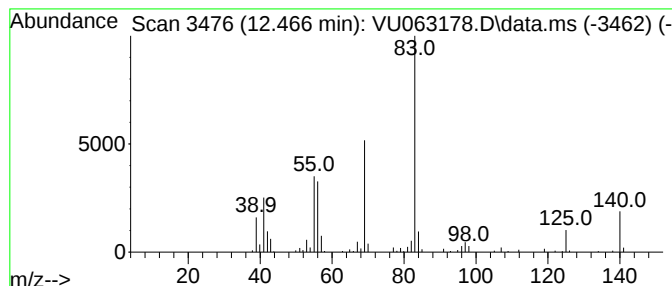
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR020425WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.466 | 4.04 ug/L | 197326 | 1,4-Dichlorobenzene-d4 | 11.804 |

| Hit# | of | 5 | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexanone, 3,3,5-trimethyl- | 140 | C9H16O  | 000873-94-9 | 95   |
| 2    |    |   | Cyclohexanone, 3,3,5-trimethyl- | 140 | C9H16O  | 000873-94-9 | 94   |
| 3    |    |   | Cyclohexanone, 3,3,5-trimethyl- | 140 | C9H16O  | 000873-94-9 | 94   |
| 4    |    |   | Cyclohexanone, 3,3,5-trimethyl- | 140 | C9H16O  | 000873-94-9 | 91   |
| 5    |    |   | 3-Acetamidofuran                | 125 | C6H7NO2 | 059445-85-1 | 53   |



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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

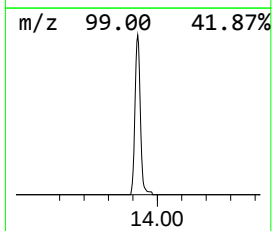
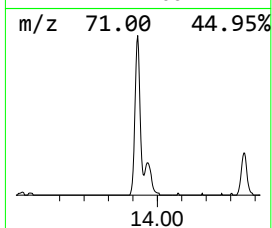
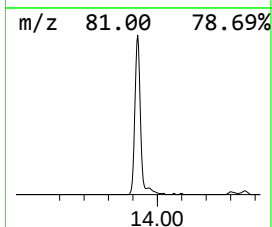
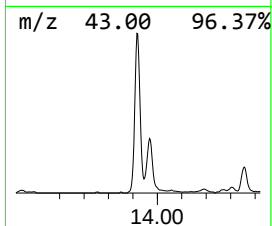
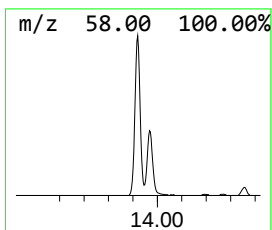
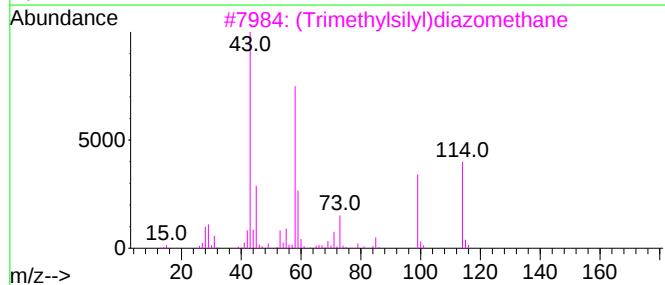
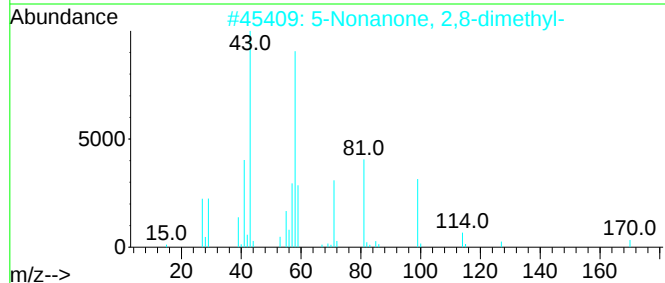
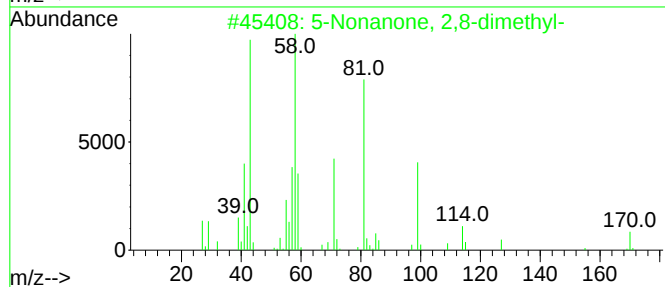
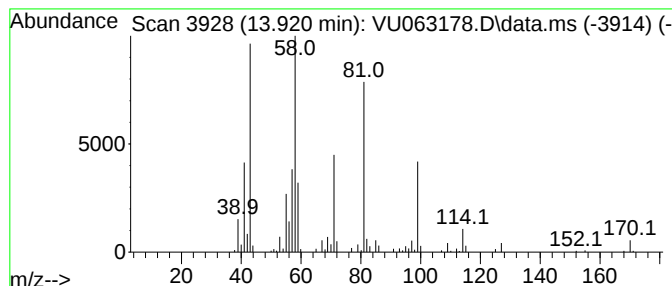
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR020425WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 3 5-Nonanone, 2,8-dimethyl- Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.920 | 4.34 ug/L | 212421 | 1,4-Dichlorobenzene-d4 | 11.804 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm   | CAS#        | Qual |
|------|----|---|------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 5-Nonanone, 2,8-dimethyl-    | 170 | C11H22O   | 002050-99-9 | 94   |
| 2    |    |   | 5-Nonanone, 2,8-dimethyl-    | 170 | C11H22O   | 002050-99-9 | 64   |
| 3    |    |   | (Trimethylsilyl)diazomethane | 114 | C4H10N2Si | 018107-18-1 | 38   |
| 4    |    |   | 2-Hexanone, 5-methyl-        | 114 | C7H14O    | 000110-12-3 | 38   |
| 5    |    |   | 2-Hexanone, 5-methyl-        | 114 | C7H14O    | 000110-12-3 | 35   |



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ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

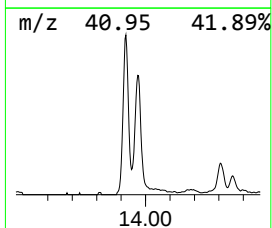
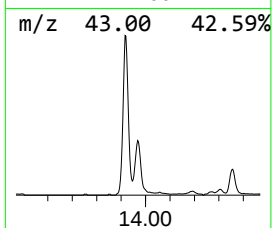
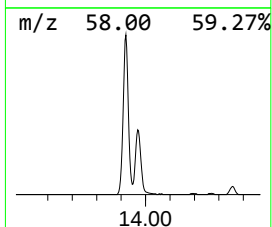
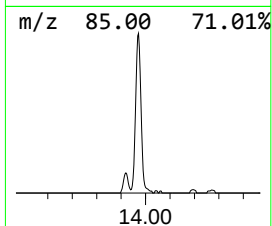
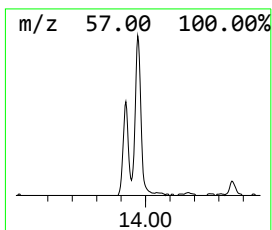
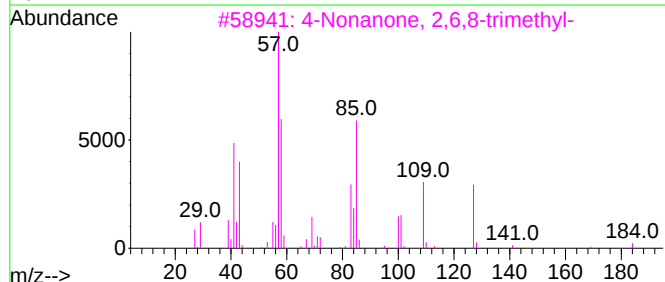
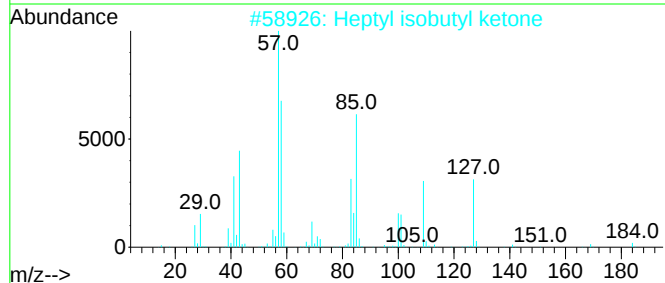
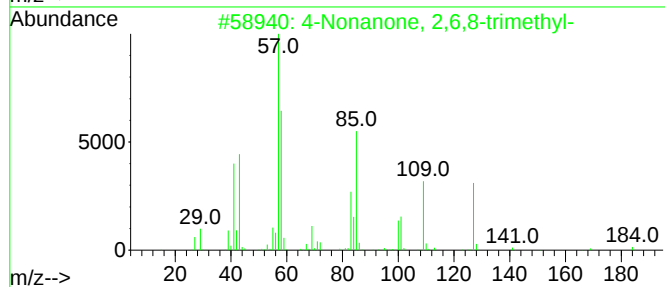
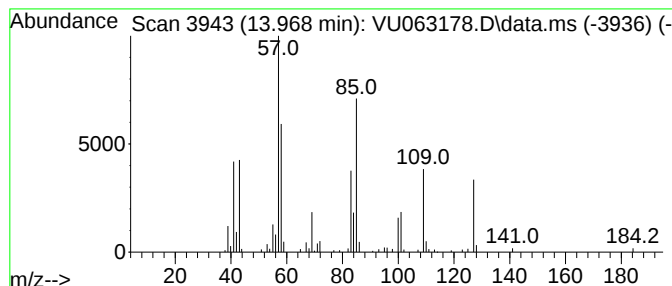
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR020425WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

\*\*\*\*\*  
Peak Number 4 4-Nonanone, 2,6,8-trimethyl- Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.968 | 3.08 ug/L | 150482 | 1,4-Dichlorobenzene-d4 | 11.804 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Nonanone, 2,6,8-trimethyl- | 184 | C12H24O | 000123-18-2 | 96   |
| 2    |    |   | Heptyl isobutyl ketone       | 184 | C12H24O | 019594-40-2 | 94   |
| 3    |    |   | 4-Nonanone, 2,6,8-trimethyl- | 184 | C12H24O | 000123-18-2 | 90   |
| 4    |    |   | 5-Nonanone                   | 142 | C9H18O  | 000502-56-7 | 38   |
| 5    |    |   | 4-Octanone, 2-methyl-        | 142 | C9H18O  | 007492-38-8 | 38   |



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ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
DCZN2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR020425WMA.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 |
| Cyclohexanone, ... | 12.466 | 4.0     | ug/L  | 197326   | 3                     | 11.804 | 244470 | 5.0  |
| 5-Nonanone, 2,8... | 13.920 | 4.3     | ug/L  | 212421   | 3                     | 11.804 | 244470 | 5.0  |
| 4-Nonanone, 2,6... | 13.968 | 3.1     | ug/L  | 150482   | 3                     | 11.804 | 244470 | 5.0  |