

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN121321\  
 Data File : VN070052.D  
 Acq On : 14 Dec 2021 00:59  
 Operator : JC/MD  
 Sample : M5007-06  
 Misc : 5.00mL/MSVOA\_N/WATER  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 TOLL-MW-07

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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\_N\methods\82N120221W.M  
 Title : SW846 8260

Signal : TIC: VN070052.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         | 2.446       | 164           | 170         | 184          | rVB3     | 83807          | 130689        | 1.59%           | 0.259%        |
| 2         | 5.085       | 1125          | 1154        | 1176         | rBV5     | 44097          | 174399        | 2.12%           | 0.346%        |
| 3         | 5.618       | 1327          | 1353        | 1385         | rBV3     | 108434         | 385124        | 4.67%           | 0.763%        |
| 4         | 7.045       | 1861          | 1885        | 1907         | rBV5     | 53932          | 158879        | 1.93%           | 0.315%        |
| 5         | 7.324       | 1969          | 1989        | 2009         | rBV7     | 35117          | 101344        | 1.23%           | 0.201%        |
| 6         | 8.024       | 2225          | 2250        | 2261         | rBV      | 894859         | 2185251       | 26.52%          | 4.329%        |
| 7         | 8.086       | 2261          | 2273        | 2292         | rVV      | 1481585        | 3404952       | 41.33%          | 6.746%        |
| 8         | 8.174       | 2292          | 2306        | 2330         | rVB3     | 310599         | 783845        | 9.51%           | 1.553%        |
| 9         | 8.440       | 2381          | 2405        | 2433         | rBV      | 1026745        | 2374258       | 28.82%          | 4.704%        |
| 10        | 8.617       | 2449          | 2471        | 2496         | rBV      | 1056610        | 2532998       | 30.75%          | 5.018%        |
| 11        | 8.968       | 2582          | 2602        | 2637         | rBV      | 2534519        | 5344667       | 64.87%          | 10.589%       |
| 12        | 9.593       | 2818          | 2835        | 2852         | rBV3     | 84718          | 177525        | 2.15%           | 0.352%        |
| 13        | 9.883       | 2922          | 2943        | 2969         | rBV      | 696230         | 1401343       | 17.01%          | 2.776%        |
| 14        | 10.014      | 2969          | 2992        | 3021         | rBV      | 1030624        | 2151729       | 26.12%          | 4.263%        |
| 15        | 10.371      | 3112          | 3125        | 3135         | rBV3     | 79426          | 143647        | 1.74%           | 0.285%        |
| 16        | 10.443      | 3135          | 3152        | 3184         | rVV      | 4196913        | 7825786       | 94.99%          | 15.505%       |
| 17        | 10.862      | 3297          | 3308        | 3328         | rVB8     | 45209          | 121674        | 1.48%           | 0.241%        |
| 18        | 11.744      | 3618          | 3637        | 3673         | rBV      | 4480270        | 8238701       | 100.00%         | 16.323%       |
| 19        | 12.734      | 3987          | 4006        | 4029         | rBV      | 3436157        | 6101722       | 74.06%          | 12.089%       |
| 20        | 13.675      | 4340          | 4357        | 4389         | rBV      | 3786062        | 6630586       | 80.48%          | 13.137%       |
| 21        | 14.150      | 4519          | 4534        | 4549         | rBV3     | 60904          | 104825        | 1.27%           | 0.208%        |

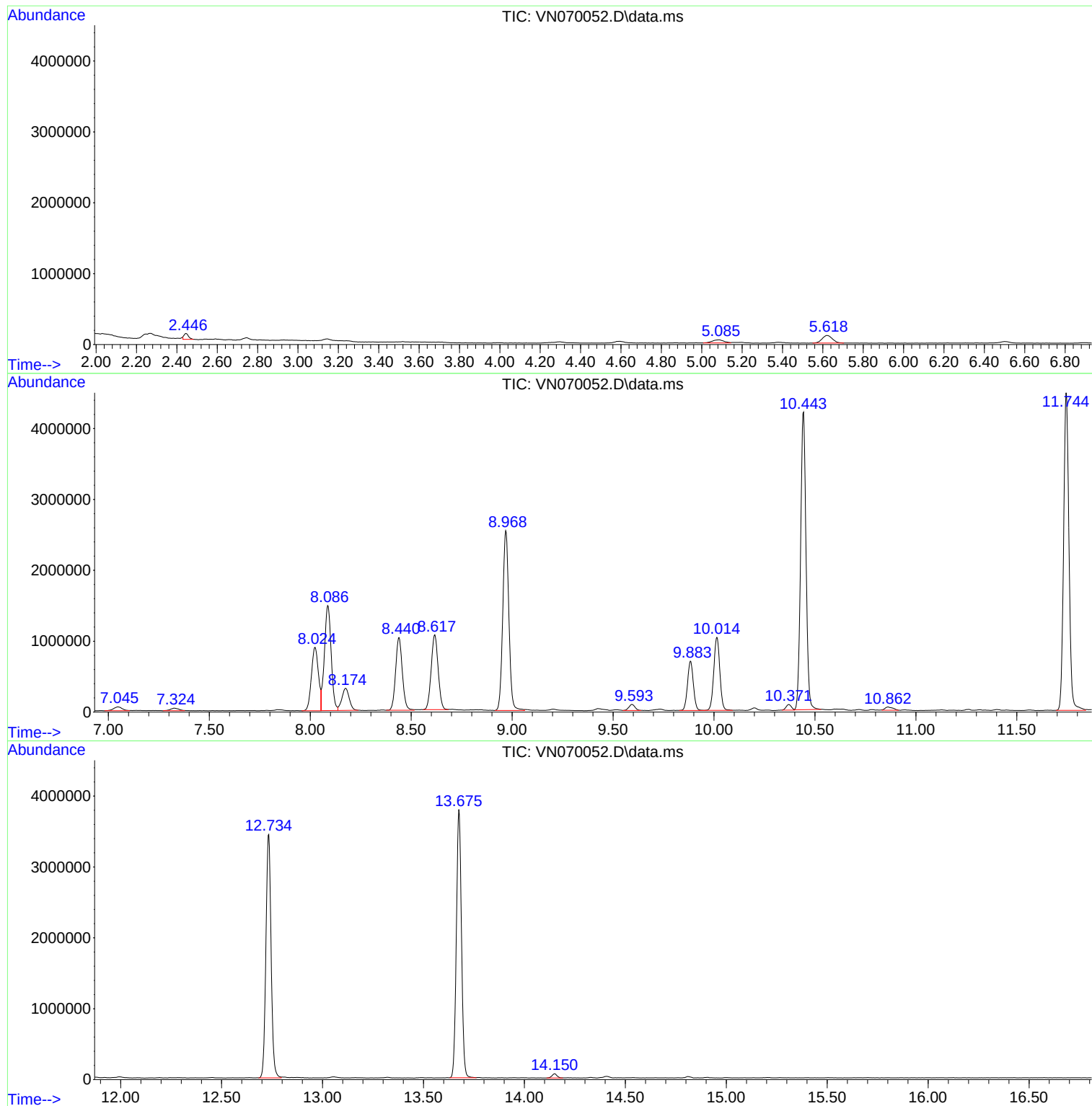
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ALS Vial : 32 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
TOLL-MW-07

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N120221W.M  
Quant Title : SW846 8260

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



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Instrument :  
MSVOA\_N  
ClientSampleId :  
TOLL-MW-07

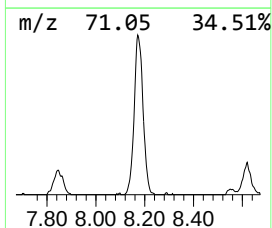
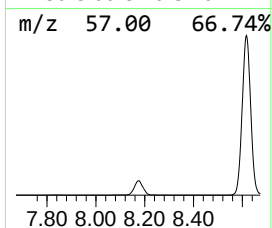
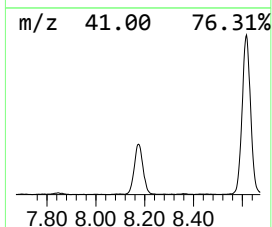
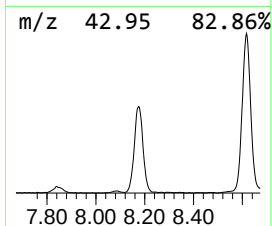
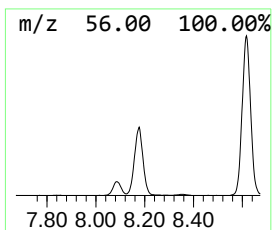
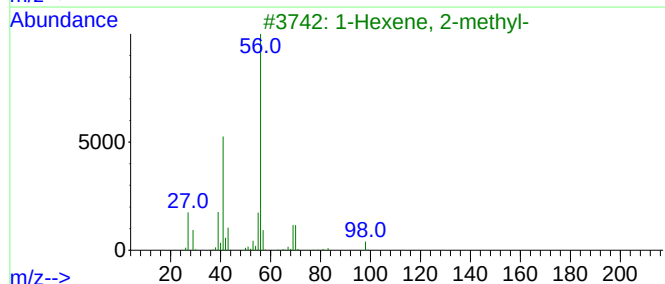
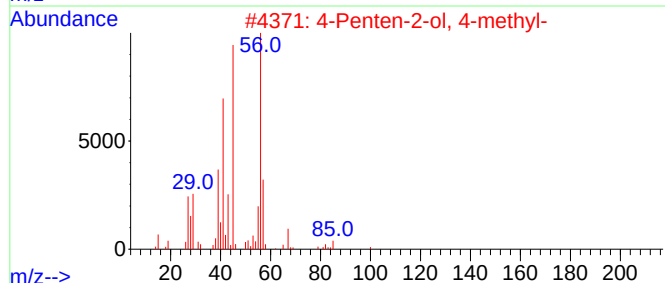
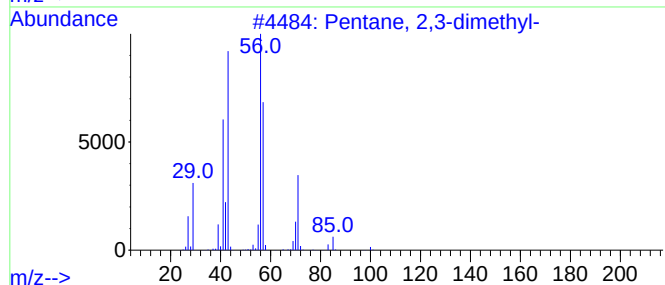
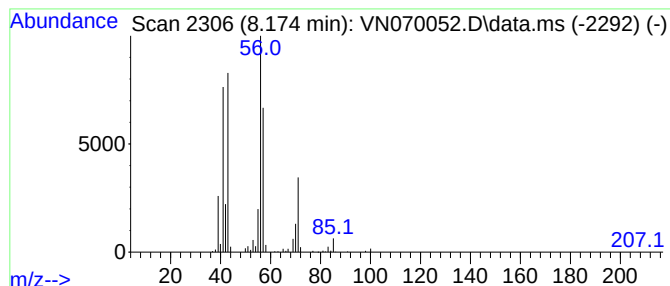
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N120221W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 8.174 | 11.51 ug/l | 783845 | Pentafluorobenzene | 8.088 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 2,3-dimethyl-   | 100 | C7H16   | 000565-59-3 | 94   |
| 2    |    |   | 4-Penten-2-ol, 4-methyl- | 100 | C6H12O  | 002004-67-3 | 47   |
| 3    |    |   | 1-Hexene, 2-methyl-      | 98  | C7H14   | 006094-02-6 | 47   |
| 4    |    |   | Hexane, 3,4-dimethyl-    | 114 | C8H18   | 000583-48-2 | 40   |
| 5    |    |   | Butane, 2,2,3-trimethyl- | 100 | C7H16   | 000464-06-2 | 40   |



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ALS Vial : 32 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
TOLL-MW-07

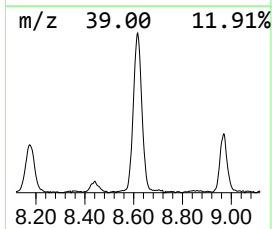
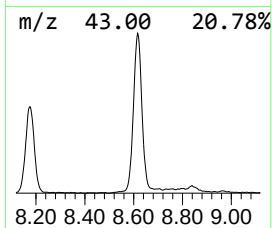
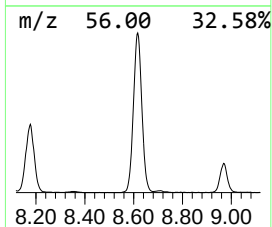
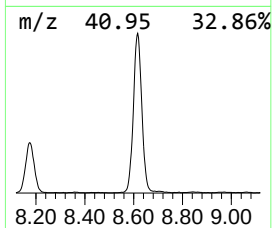
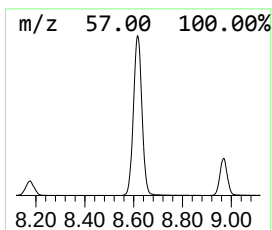
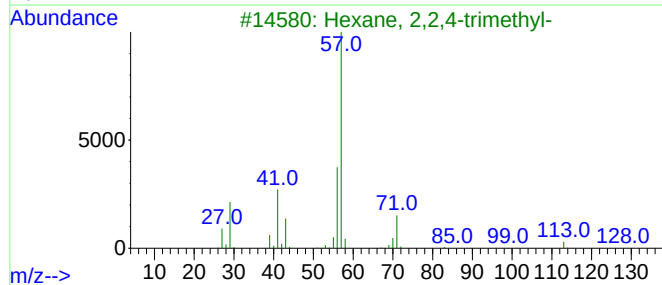
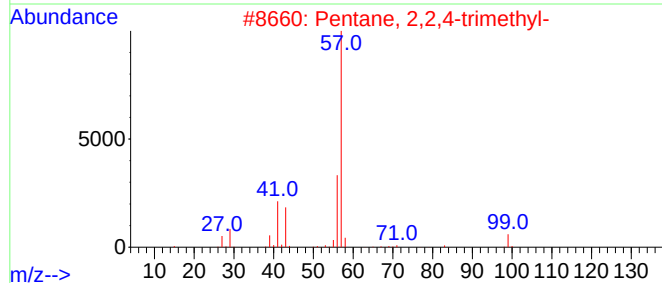
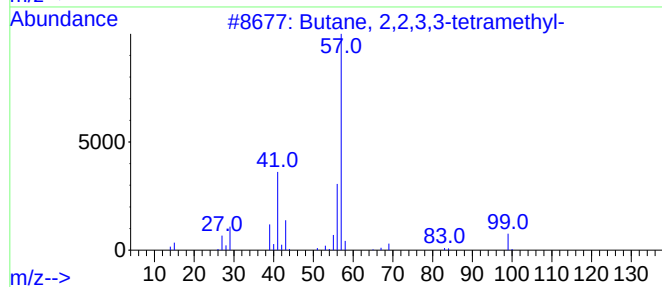
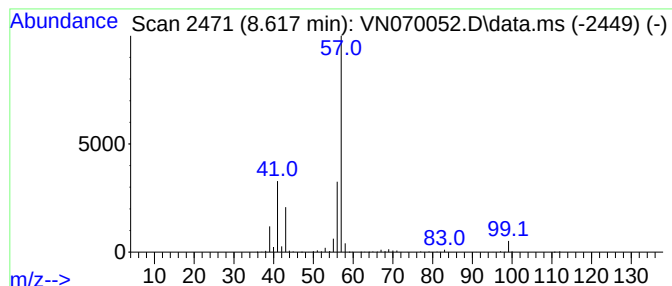
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N120221W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 8.617 | 23.70 ug/l | 2533000 | 1,4-Difluorobenzene | 8.968 |

| Hit# | of | 5 | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2,2,3,3-tetramethyl-    | 114 | C8H18   | 000594-82-1 | 72   |
| 2    |    |   | Pentane, 2,2,4-trimethyl-       | 114 | C8H18   | 000540-84-1 | 72   |
| 3    |    |   | Hexane, 2,2,4-trimethyl-        | 128 | C9H20   | 016747-26-5 | 59   |
| 4    |    |   | Hexane, 2,2-dimethyl-           | 114 | C8H18   | 000590-73-8 | 59   |
| 5    |    |   | Heptane, 2,2,4,6,6-pentamethyl- | 170 | C12H26  | 013475-82-6 | 56   |



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Misc : 5.00mL/MSVOA\_N/WATER  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
TOLL-MW-07

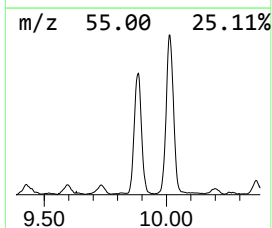
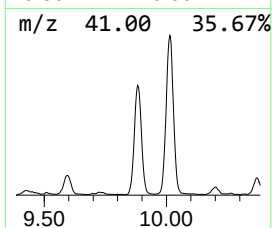
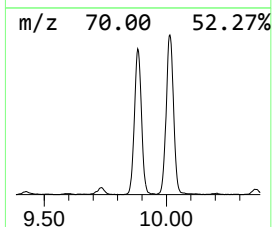
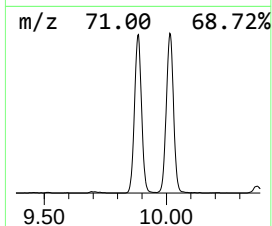
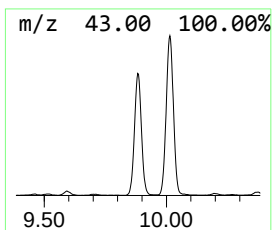
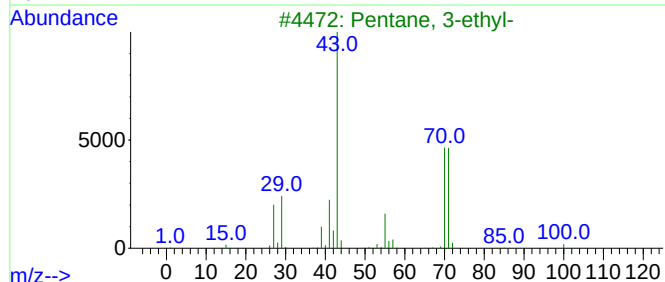
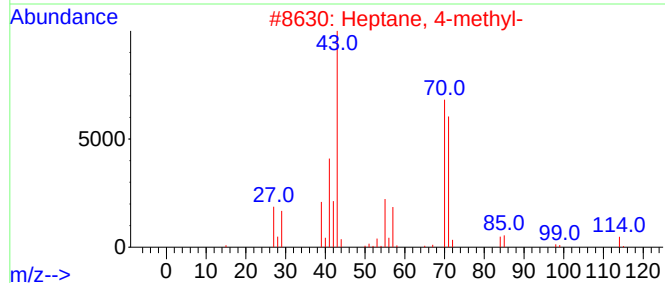
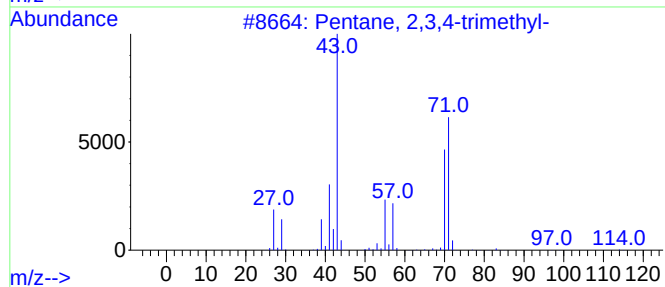
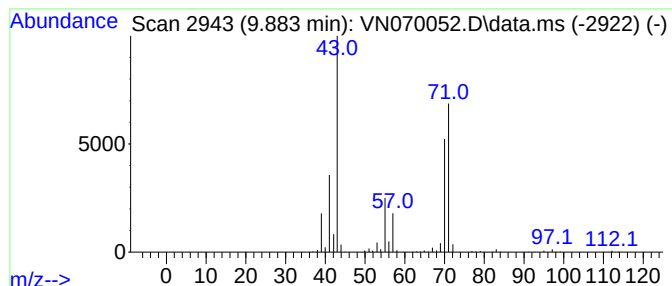
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N120221W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 3

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 9.883 | 13.11 ug/l | 1401340 | 1,4-Difluorobenzene | 8.968 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Pentane, 2,3,4-trimethyl-           | 114 | C8H18    | 000565-75-3 | 90   |
| 2    |    |   | Heptane, 4-methyl-                  | 114 | C8H18    | 000589-53-7 | 78   |
| 3    |    |   | Pentane, 3-ethyl-                   | 100 | C7H16    | 000617-78-7 | 72   |
| 4    |    |   | Ethanedioic acid, bis(3-methylbu... | 230 | C12H22O4 | 002051-00-5 | 59   |
| 5    |    |   | Diisooamyl ether                    | 158 | C10H22O  | 000544-01-4 | 56   |



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ALS Vial : 32 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
TOLL-MW-07

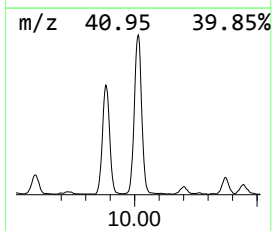
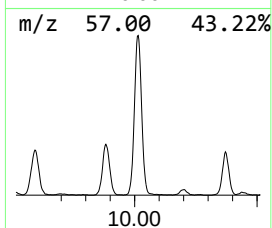
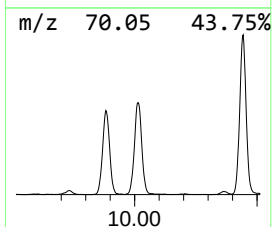
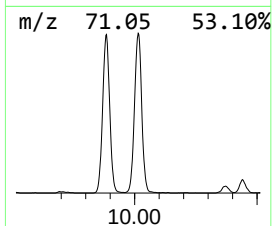
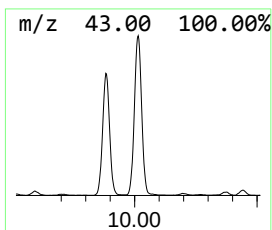
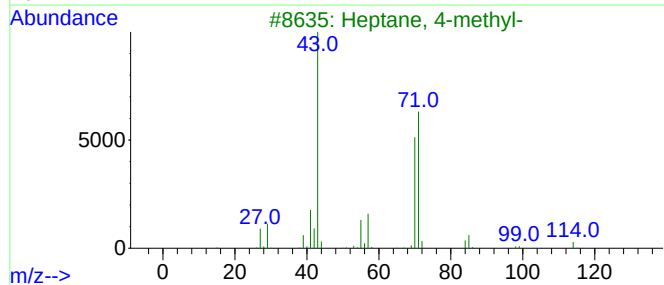
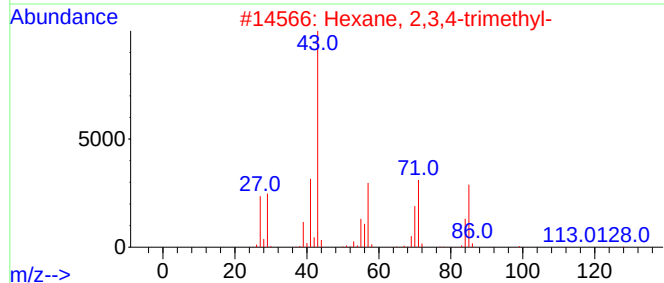
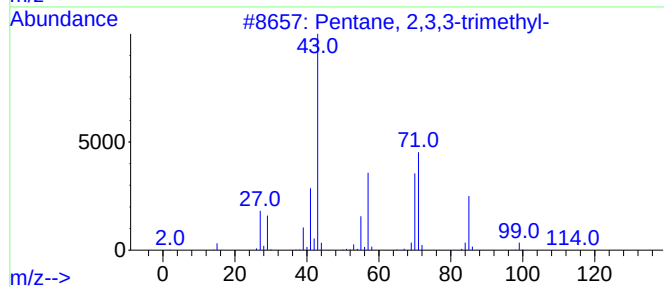
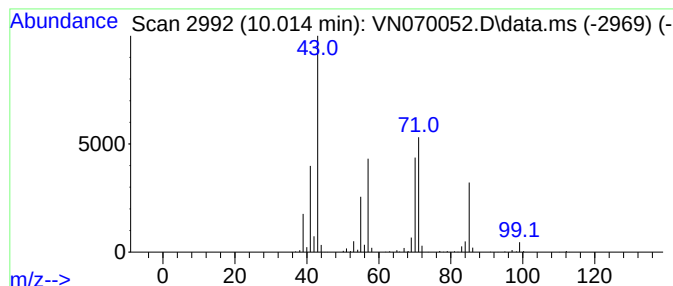
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N120221W.M  
Quant Title : SW846 8260

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

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Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 2

| R.T.   | EstConc    | Area    | Relative to ISTD    | R.T.  |
|--------|------------|---------|---------------------|-------|
| 10.014 | 20.13 ug/l | 2151730 | 1,4-Difluorobenzene | 8.968 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 2,3,3-trimethyl- | 114 | C8H18   | 000560-21-4 | 83   |
| 2    |    |   | Hexane, 2,3,4-trimethyl-  | 128 | C9H20   | 000921-47-1 | 64   |
| 3    |    |   | Heptane, 4-methyl-        | 114 | C8H18   | 000589-53-7 | 64   |
| 4    |    |   | Hexane, 3-methyl-         | 100 | C7H16   | 000589-34-4 | 59   |
| 5    |    |   | Hexane, 3,3-dimethyl-     | 114 | C8H18   | 000563-16-6 | 59   |



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Quant Title : SW846 8260

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|-------|---------|------|
|                    |        |         |       |          | #                     | RT    | Resp    | Conc |
| Pentane, 2,3-di... | 8.174  | 11.5    | ug/l  | 783845   | 1                     | 8.088 | 3404950 | 50.0 |
| Butane, 2,2,3,3... | 8.617  | 23.7    | ug/l  | 2533000  | 2                     | 8.968 | 5344670 | 50.0 |
| Pentane, 2,3,4-... | 9.883  | 13.1    | ug/l  | 1401340  | 2                     | 8.968 | 5344670 | 50.0 |
| Pentane, 2,3,3-... | 10.014 | 20.1    | ug/l  | 2151730  | 2                     | 8.968 | 5344670 | 50.0 |