

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX102022\  
 Data File : VX032271.D  
 Acq On : 20 Oct 2022 18:24  
 Operator : JC/MD  
 Sample : N5185-05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MW-04

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\_X\Method\82X101922W.M  
 Title : SW846 8260

Signal : TIC: VX032271.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         | 1.264       | 26            | 29          | 41           | rBV2     | 24424          | 36104         | 5.04%           | 0.669%        |
| 2         | 1.368       | 43            | 46          | 52           | rVB      | 90262          | 89862         | 12.56%          | 1.666%        |
| 3         | 1.752       | 103           | 109         | 120          | rBV      | 359898         | 490264        | 68.51%          | 9.090%        |
| 4         | 1.953       | 137           | 142         | 152          | rVB      | 10420          | 15986         | 2.23%           | 0.296%        |
| 5         | 2.337       | 200           | 205         | 210          | rBV      | 10645          | 20516         | 2.87%           | 0.380%        |
| 6         | 2.782       | 271           | 278         | 282          | rBV      | 30598          | 66665         | 9.32%           | 1.236%        |
| 7         | 2.825       | 282           | 285         | 290          | rVV      | 30515          | 61099         | 8.54%           | 1.133%        |
| 8         | 2.867       | 290           | 292         | 303          | rVB      | 14239          | 22457         | 3.14%           | 0.416%        |
| 9         | 3.105       | 322           | 331         | 342          | rBV2     | 33366          | 74853         | 10.46%          | 1.388%        |
| 10        | 4.221       | 504           | 514         | 519          | rBV3     | 4101           | 11726         | 1.64%           | 0.217%        |
| 11        | 4.306       | 519           | 528         | 542          | rVB      | 37436          | 107502        | 15.02%          | 1.993%        |
| 12        | 5.385       | 694           | 705         | 715          | rBV      | 83297          | 245592        | 34.32%          | 4.554%        |
| 13        | 5.471       | 715           | 719         | 723          | rVV3     | 7854           | 19948         | 2.79%           | 0.370%        |
| 14        | 5.550       | 723           | 732         | 757          | rVB      | 157627         | 477795        | 66.76%          | 8.859%        |
| 15        | 5.830       | 770           | 778         | 788          | rVB7     | 3475           | 9725          | 1.36%           | 0.180%        |
| 16        | 5.958       | 788           | 799         | 808          | rBV      | 94051          | 248159        | 34.68%          | 4.601%        |
| 17        | 6.044       | 808           | 813         | 824          | rVV2     | 7784           | 19487         | 2.72%           | 0.361%        |
| 18        | 6.166       | 824           | 833         | 839          | rVV4     | 4435           | 12713         | 1.78%           | 0.236%        |
| 19        | 6.257       | 839           | 848         | 856          | rVV5     | 7779           | 23681         | 3.31%           | 0.439%        |
| 20        | 6.361       | 856           | 865         | 872          | rVB5     | 3205           | 8625          | 1.21%           | 0.160%        |
| 21        | 6.763       | 922           | 931         | 946          | rBV      | 228230         | 539305        | 75.36%          | 10.000%       |
| 22        | 7.373       | 1020          | 1031        | 1040         | rBV6     | 7832           | 22569         | 3.15%           | 0.418%        |
| 23        | 8.104       | 1145          | 1151        | 1160         | rBV3     | 6238           | 12039         | 1.68%           | 0.223%        |
| 24        | 8.647       | 1234          | 1240        | 1249         | rBV      | 452403         | 715660        | 100.00%         | 13.270%       |
| 25        | 10.055      | 1465          | 1471        | 1480         | rBV      | 458237         | 608988        | 85.09%          | 11.292%       |
| 26        | 10.195      | 1489          | 1494        | 1502         | rVB      | 92443          | 118099        | 16.50%          | 2.190%        |
| 27        | 10.305      | 1507          | 1512        | 1518         | rBV      | 17894          | 24244         | 3.39%           | 0.450%        |
| 28        | 10.964      | 1615          | 1620        | 1626         | rVB      | 12310          | 14942         | 2.09%           | 0.277%        |
| 29        | 11.079      | 1634          | 1639        | 1652         | rBV      | 372994         | 484541        | 67.71%          | 8.984%        |
| 30        | 11.305      | 1671          | 1676        | 1683         | rVB      | 23793          | 28994         | 4.05%           | 0.538%        |
| 31        | 11.616      | 1722          | 1727        | 1733         | rBV      | 36883          | 46505         | 6.50%           | 0.862%        |
| 32        | 12.024      | 1788          | 1794        | 1800         | rBV      | 463228         | 573355        | 80.12%          | 10.631%       |
| 33        | 12.091      | 1800          | 1805        | 1811         | rVB      | 22411          | 29674         | 4.15%           | 0.550%        |
| 34        | 12.244      | 1825          | 1830        | 1836         | rBV2     | 45088          | 56828         | 7.94%           | 1.054%        |
| 35        | 12.463      | 1861          | 1866        | 1871         | rBV2     | 7073           | 8755          | 1.22%           | 0.162%        |
| 36        | 12.616      | 1887          | 1891        | 1894         | rBV      | 5625           | 7213          | 1.01%           | 0.134%        |

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Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

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\_X\Method\82X101922W.M  
Title : SW846 8260

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 37 | 12.701 | 1900 | 1905 | 1912 | rBV2 | 10917 | 15570 | 2.18% | 0.289% |
| 38 | 13.292 | 1998 | 2002 | 2008 | rVB2 | 8583  | 10776 | 1.51% | 0.200% |
| 39 | 13.780 | 2077 | 2082 | 2088 | rBV  | 9164  | 12397 | 1.73% | 0.230% |

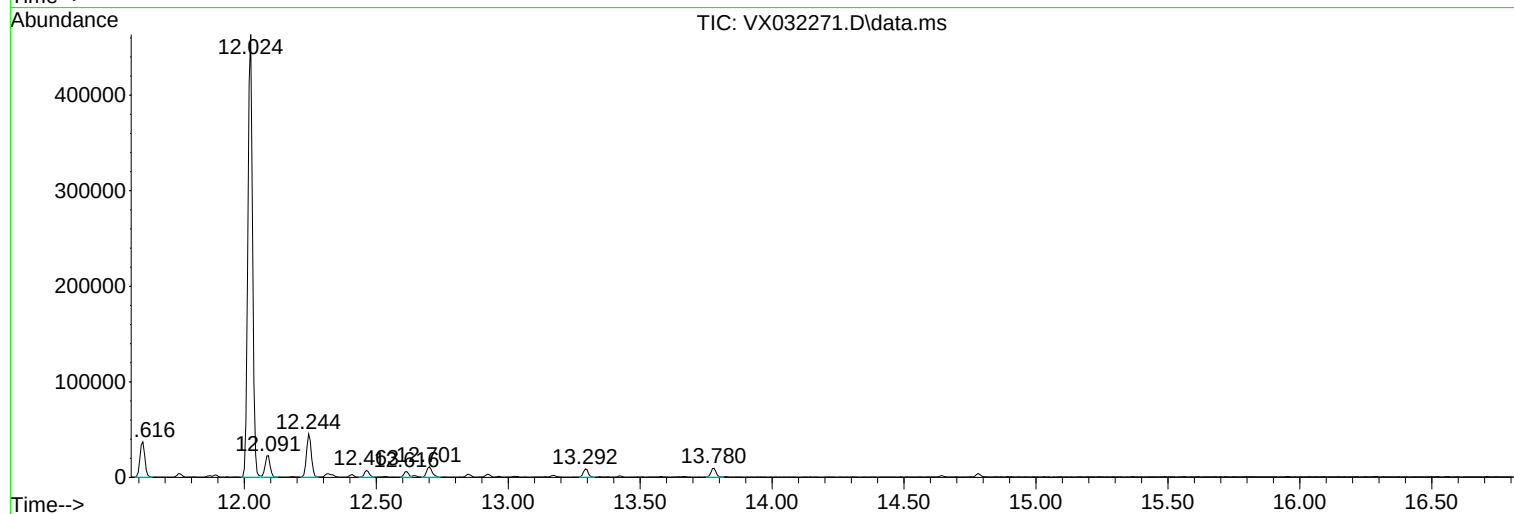
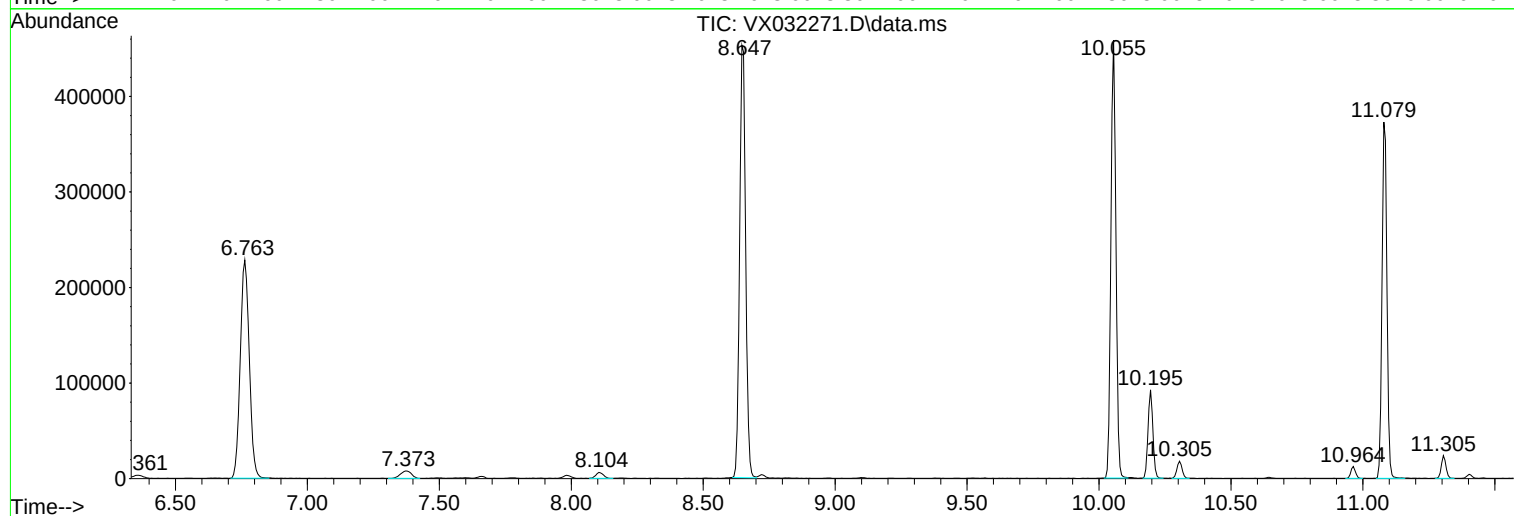
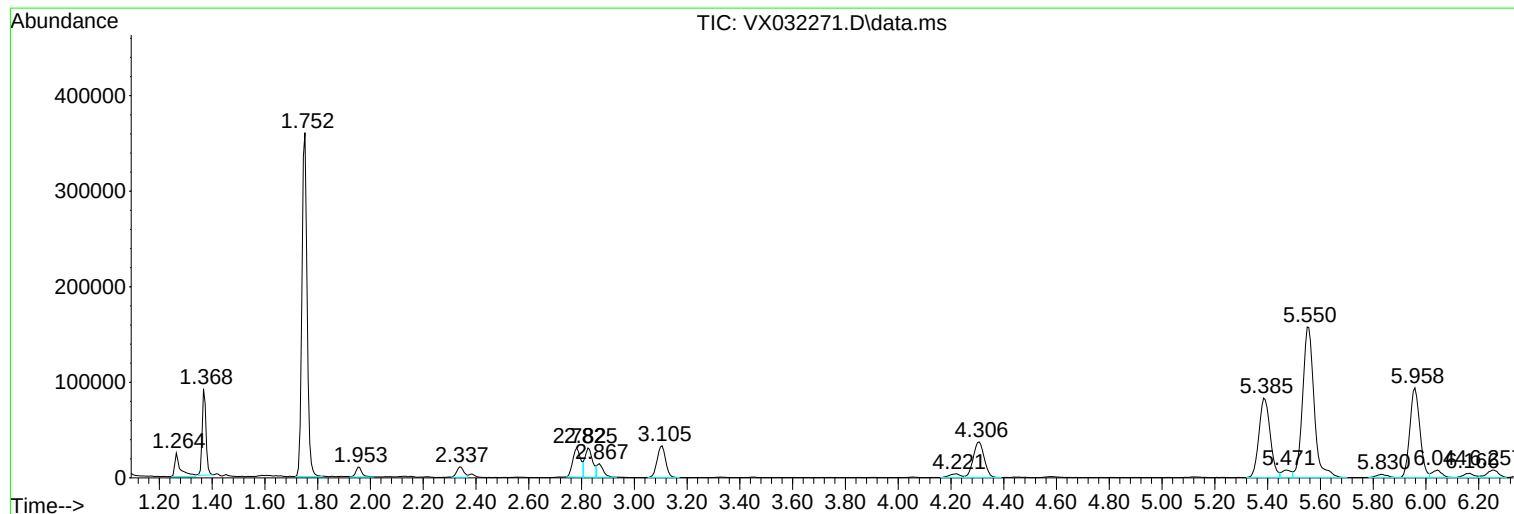
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ClientSampleId :  
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

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



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Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

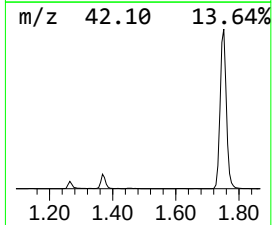
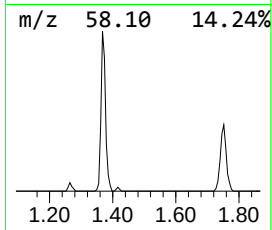
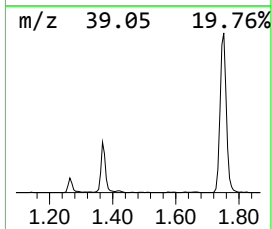
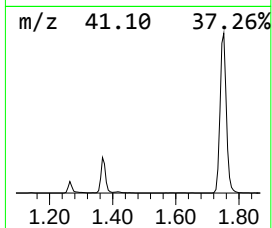
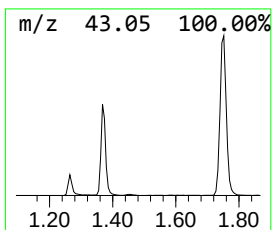
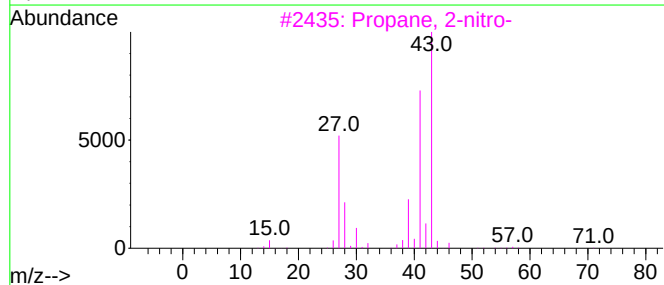
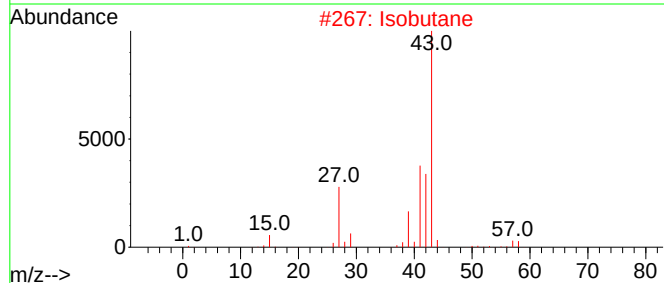
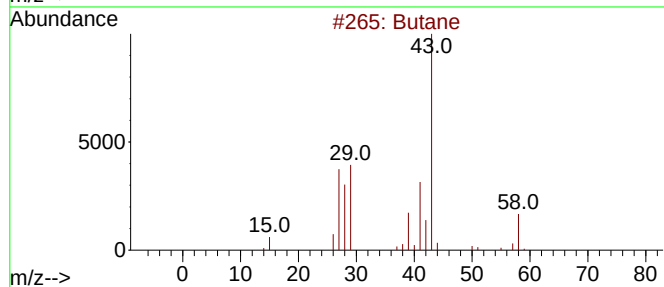
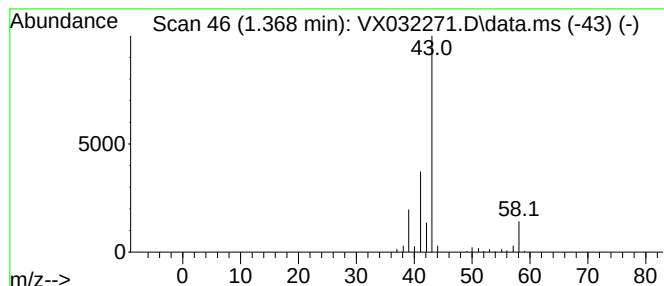
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.368 | 9.40 ug/l | 89862 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm   | CAS#        | Qual |
|------|----|---|----------------------------|-----|-----------|-------------|------|
| 1    |    |   | Butane                     | 58  | C4H10     | 000106-97-8 | 72   |
| 2    |    |   | Isobutane                  | 58  | C4H10     | 000075-28-5 | 9    |
| 3    |    |   | Propane, 2-nitro-          | 89  | C3H7NO2   | 000079-46-9 | 9    |
| 4    |    |   | Isopropylsulfonyl chloride | 142 | C3H7ClO2S | 010147-37-2 | 9    |
| 5    |    |   | Propane, 1-nitro-          | 89  | C3H7NO2   | 000108-03-2 | 9    |



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Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

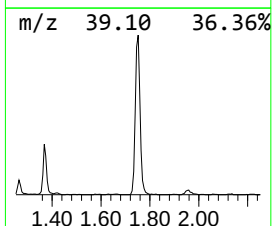
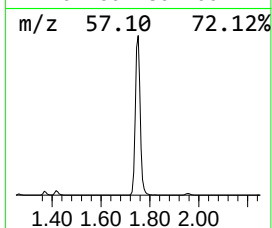
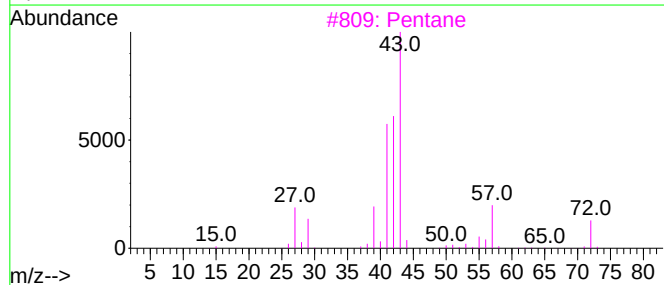
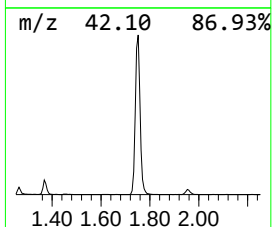
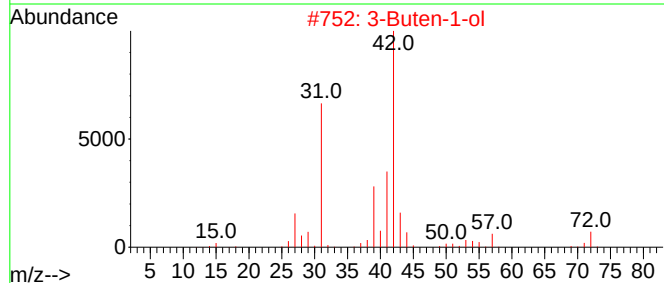
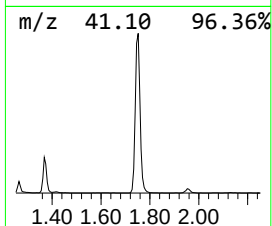
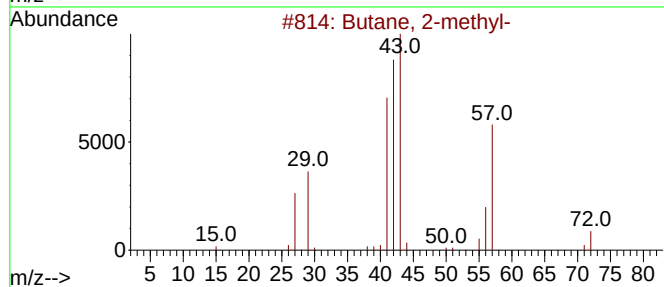
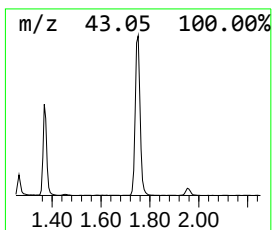
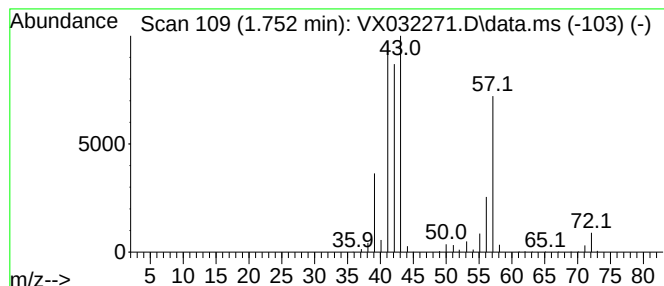
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Butane, 2-methyl- Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 1.752 | 51.30 ug/l | 490264 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID         | MW | MolForm | CAS#        | Qual |
|------|----|---|----------------------|----|---------|-------------|------|
| 1    |    |   | Butane, 2-methyl-    | 72 | C5H12   | 000078-78-4 | 86   |
| 2    |    |   | 3-Buten-1-ol         | 72 | C4H8O   | 000627-27-0 | 47   |
| 3    |    |   | Pentane              | 72 | C5H12   | 000109-66-0 | 36   |
| 4    |    |   | 1-Propene, 2-methyl- | 56 | C4H8    | 000115-11-7 | 14   |
| 5    |    |   | 3-Buten-2-ol         | 72 | C4H8O   | 000598-32-3 | 9    |



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Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

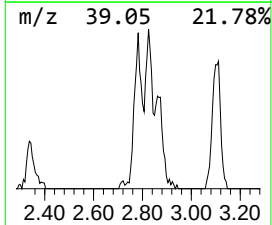
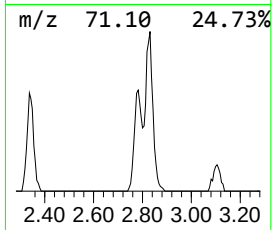
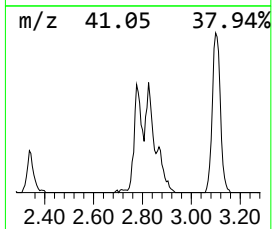
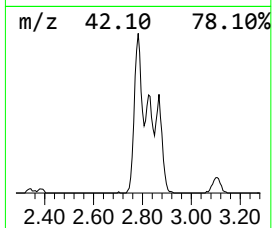
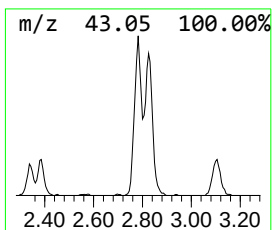
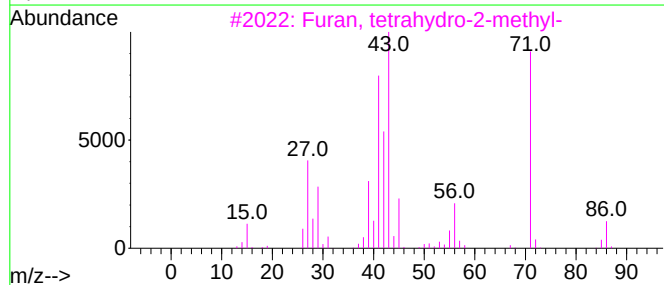
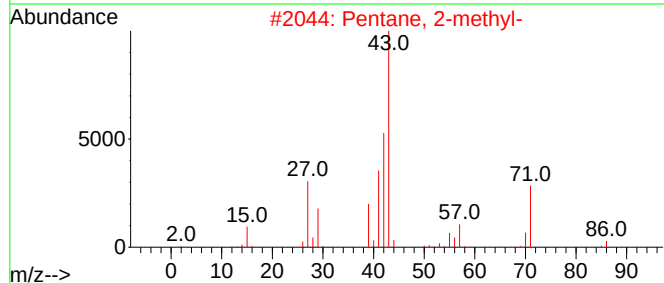
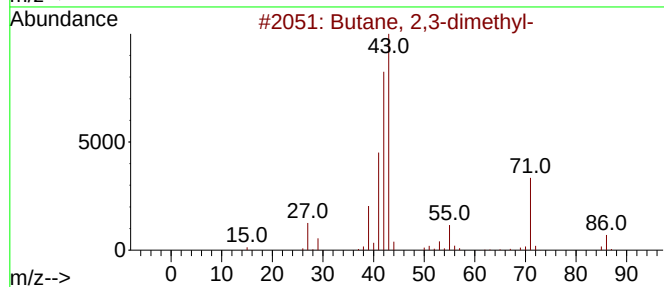
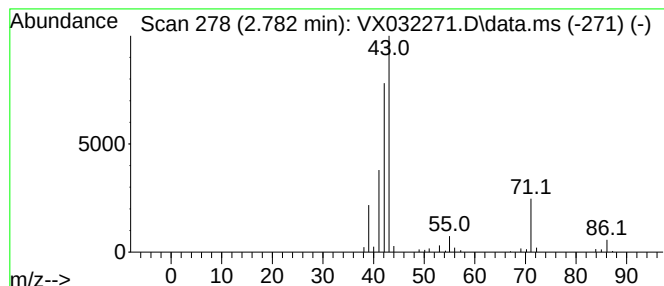
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 5

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.782 | 6.98 ug/l | 66665 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm  | CAS#         | Qual |
|------|----|---|----------------------------------|-----|----------|--------------|------|
| 1    |    |   | Butane, 2,3-dimethyl-            | 86  | C6H14    | 000079-29-8  | 87   |
| 2    |    |   | Pentane, 2-methyl-               | 86  | C6H14    | 000107-83-5  | 59   |
| 3    |    |   | Furan, tetrahydro-2-methyl-      | 86  | C5H10O   | 000096-47-9  | 14   |
| 4    |    |   | Oxalic acid, pentyl propyl ester | 202 | C10H18O4 | 1000309-25-7 | 10   |
| 5    |    |   | Propanoyl chloride, 2-methyl-    | 106 | C4H7ClO  | 000079-30-1  | 10   |



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ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

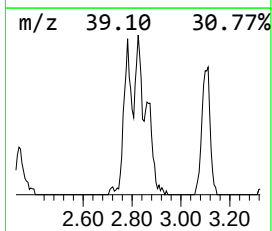
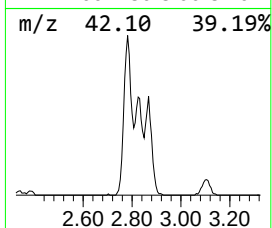
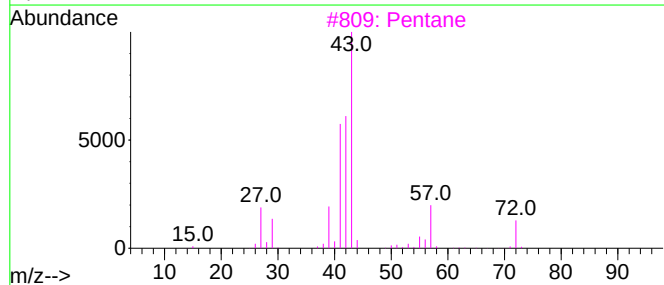
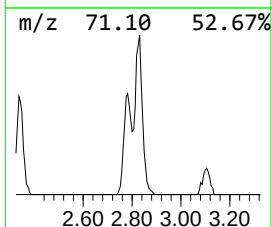
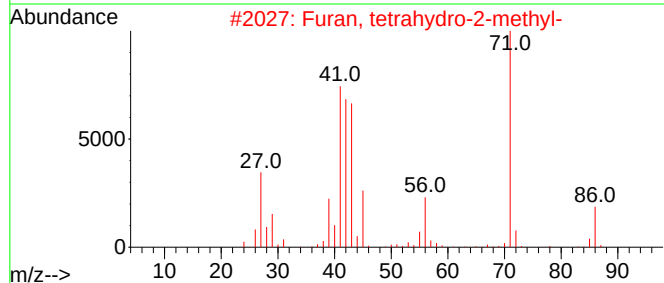
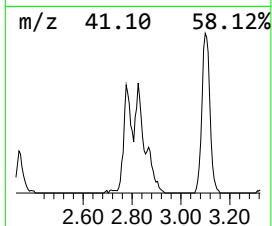
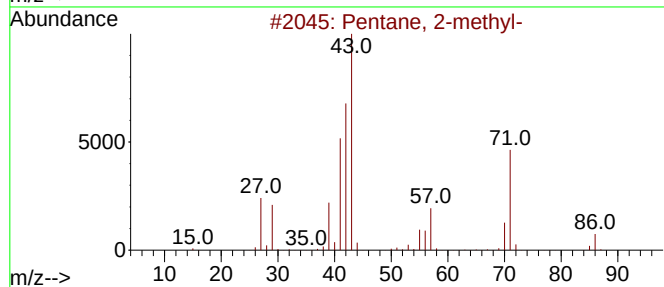
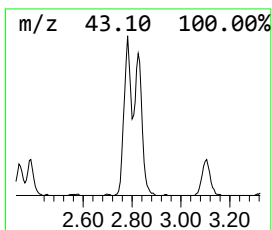
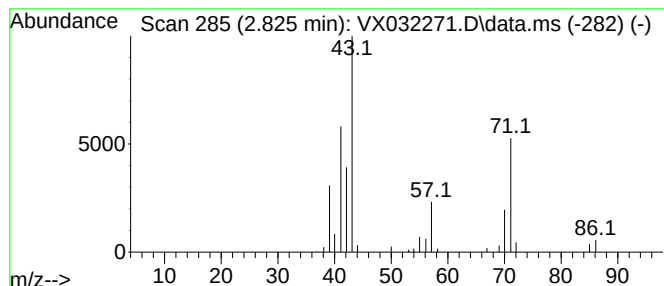
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

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

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Peak Number 4 Pentane, 2-methyl- Concentration Rank 6

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.825 | 6.39 ug/l | 61099 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 2-methyl-          | 86  | C6H14   | 000107-83-5 | 50   |
| 2    |    |   | Furan, tetrahydro-2-methyl- | 86  | C5H10O  | 000096-47-9 | 40   |
| 3    |    |   | Pentane                     | 72  | C5H12   | 000109-66-0 | 38   |
| 4    |    |   | Oxirane, butyl-             | 100 | C6H12O  | 001436-34-6 | 33   |
| 5    |    |   | Hexane, 2-methyl-           | 100 | C7H16   | 000591-76-4 | 32   |



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Operator : JC/MD  
Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

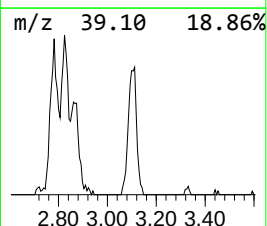
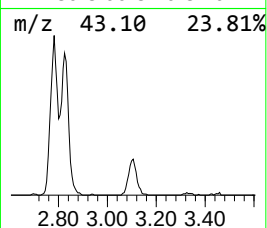
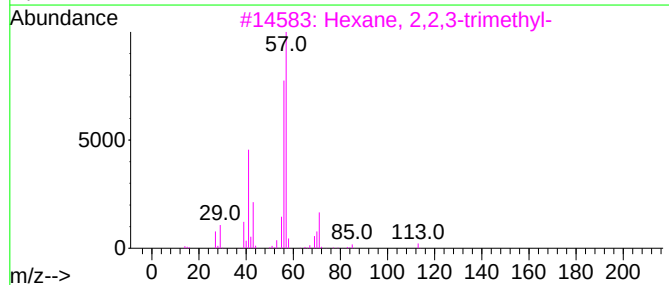
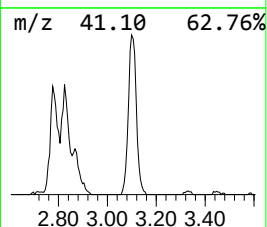
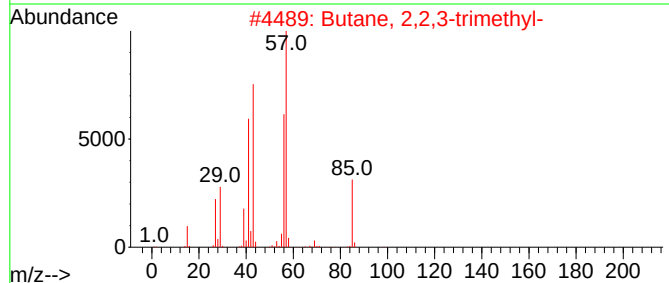
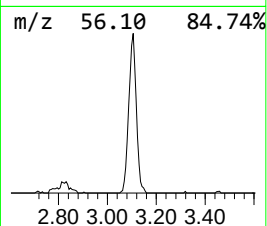
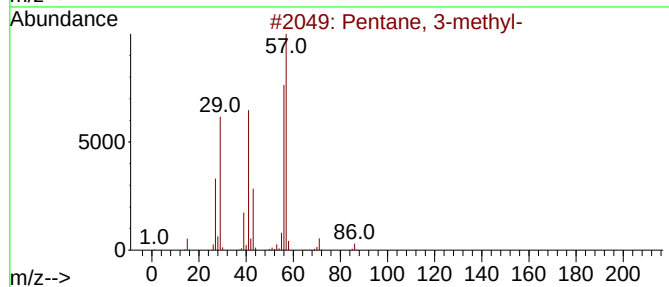
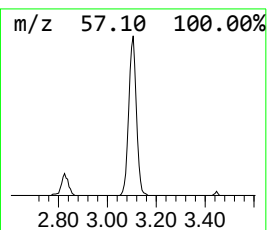
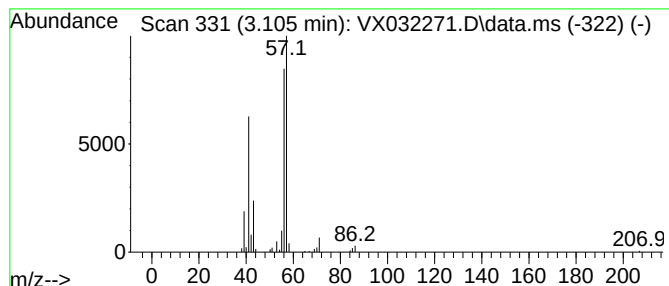
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Quant Title : SW846 8260

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

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Peak Number 5 Pentane, 3-methyl- Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 3.105 | 7.83 ug/l | 74853 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 3-methyl-             | 86  | C6H14   | 000096-14-0 | 91   |
| 2    |    |   | Butane, 2,2,3-trimethyl-       | 100 | C7H16   | 000464-06-2 | 78   |
| 3    |    |   | Hexane, 2,2,3-trimethyl-       | 128 | C9H20   | 016747-25-4 | 74   |
| 4    |    |   | Pentane, 2,2,3-trimethyl-      | 114 | C8H18   | 000564-02-3 | 64   |
| 5    |    |   | Pentane, 3-ethyl-2,2-dimethyl- | 128 | C9H20   | 016747-32-3 | 64   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX102022\  
Data File : VX032271.D  
Acq On : 20 Oct 2022 18:24  
Operator : JC/MD  
Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
Quant Title : SW846 8260

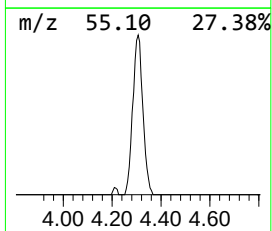
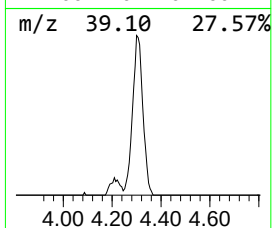
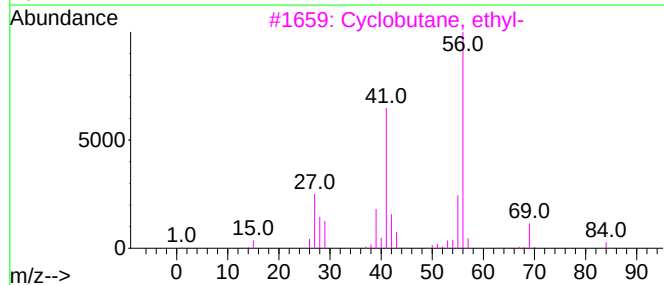
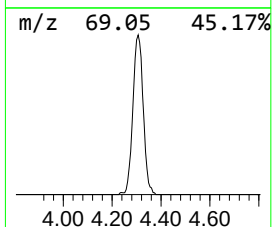
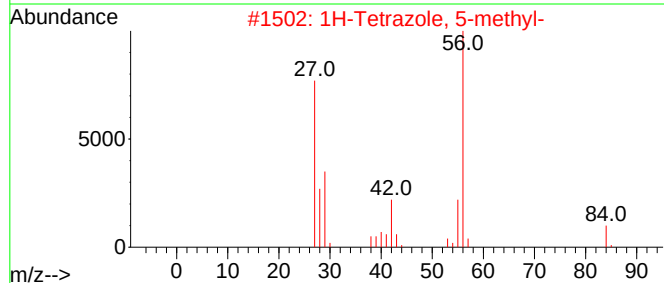
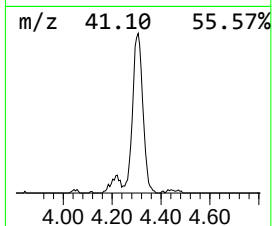
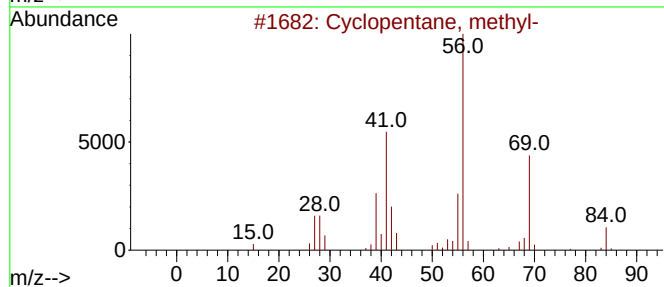
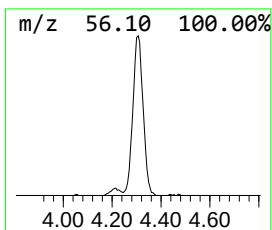
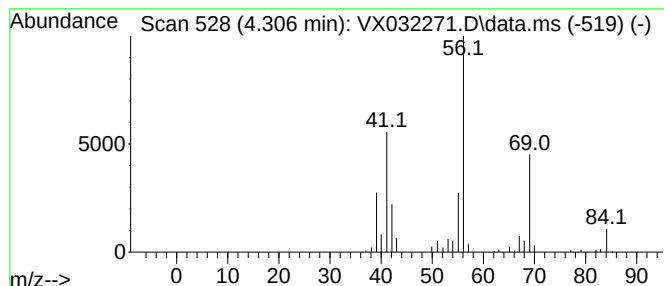
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Cyclopentane, methyl- Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 4.306 | 11.25 ug/l | 107502 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclopentane, methyl-               | 84  | C6H12   | 000096-37-7 | 94   |
| 2    |    |   | 1H-Tetrazole, 5-methyl-             | 84  | C2H4N4  | 004076-36-2 | 80   |
| 3    |    |   | Cyclobutane, ethyl-                 | 84  | C6H12   | 004806-61-5 | 64   |
| 4    |    |   | 2H-Pyran-2,6(3H)-dione, dihydro-... | 142 | C7H10O3 | 004160-82-1 | 59   |
| 5    |    |   | Cyclobutane                         | 56  | C4H8    | 000287-23-0 | 53   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX102022\  
Data File : VX032271.D  
Acq On : 20 Oct 2022 18:24  
Operator : JC/MD  
Sample : N5185-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X101922W.M  
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 |
| Butane             | 1.368 | 9.4     | ug/l  | 89862    | 1                     | 5.556 | 477795 | 50.0 |
| Butane, 2-methyl-  | 1.752 | 51.3    | ug/l  | 490264   | 1                     | 5.556 | 477795 | 50.0 |
| Butane, 2,3-dim... | 2.782 | 7.0     | ug/l  | 66665    | 1                     | 5.556 | 477795 | 50.0 |
| Pentane, 2-methyl- | 2.825 | 6.4     | ug/l  | 61099    | 1                     | 5.556 | 477795 | 50.0 |
| Pentane, 3-methyl- | 3.105 | 7.8     | ug/l  | 74853    | 1                     | 5.556 | 477795 | 50.0 |
| Cyclopentane, m... | 4.306 | 11.3    | ug/l  | 107502   | 1                     | 5.556 | 477795 | 50.0 |