

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042122\  
 Data File : VX028253.D  
 Acq On : 21 Apr 2022 19:52  
 Operator : JC/MD  
 Sample : N2511-06 50X  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 1530

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\82X041922W.M

Title : SW846 8260

Signal : TIC: VX028253.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         | 1.276       | 24            | 31          | 41           | rBV3     | 14678          | 53642         | 2.26%           | 0.407%        |
| 2         | 1.569       | 71            | 79          | 83           | rBV5     | 17100          | 39256         | 1.65%           | 0.298%        |
| 3         | 2.947       | 296           | 305         | 315          | rVB      | 14737          | 34562         | 1.45%           | 0.263%        |
| 4         | 5.391       | 693           | 706         | 722          | rBV      | 291115         | 853184        | 35.90%          | 6.480%        |
| 5         | 5.556       | 722           | 733         | 752          | rVB      | 394635         | 1119775       | 47.12%          | 8.505%        |
| 6         | 5.958       | 788           | 799         | 816          | rBV      | 290187         | 776751        | 32.69%          | 5.900%        |
| 7         | 6.763       | 920           | 931         | 948          | rBV      | 628399         | 1477752       | 62.19%          | 11.224%       |
| 8         | 8.653       | 1233          | 1241        | 1251         | rBV      | 1534790        | 2376260       | 100.00%         | 18.048%       |
| 9         | 10.055      | 1465          | 1471        | 1491         | rBV      | 1381406        | 1833557       | 77.16%          | 13.926%       |
| 10        | 11.079      | 1634          | 1639        | 1651         | rBV      | 1258555        | 1657507       | 69.75%          | 12.589%       |
| 11        | 12.024      | 1788          | 1794        | 1802         | rBV      | 1544111        | 1820156       | 76.60%          | 13.824%       |
| 12        | 12.104      | 1802          | 1807        | 1813         | rVB2     | 26510          | 36690         | 1.54%           | 0.279%        |
| 13        | 13.128      | 1971          | 1975        | 1984         | rVB3     | 28170          | 56782         | 2.39%           | 0.431%        |
| 14        | 13.219      | 1985          | 1990        | 2009         | rBV      | 167578         | 316202        | 13.31%          | 2.402%        |
| 15        | 13.427      | 2019          | 2024        | 2036         | rBV      | 323584         | 558619        | 23.51%          | 4.243%        |
| 16        | 14.195      | 2145          | 2150        | 2166         | rBV      | 65441          | 155490        | 6.54%           | 1.181%        |

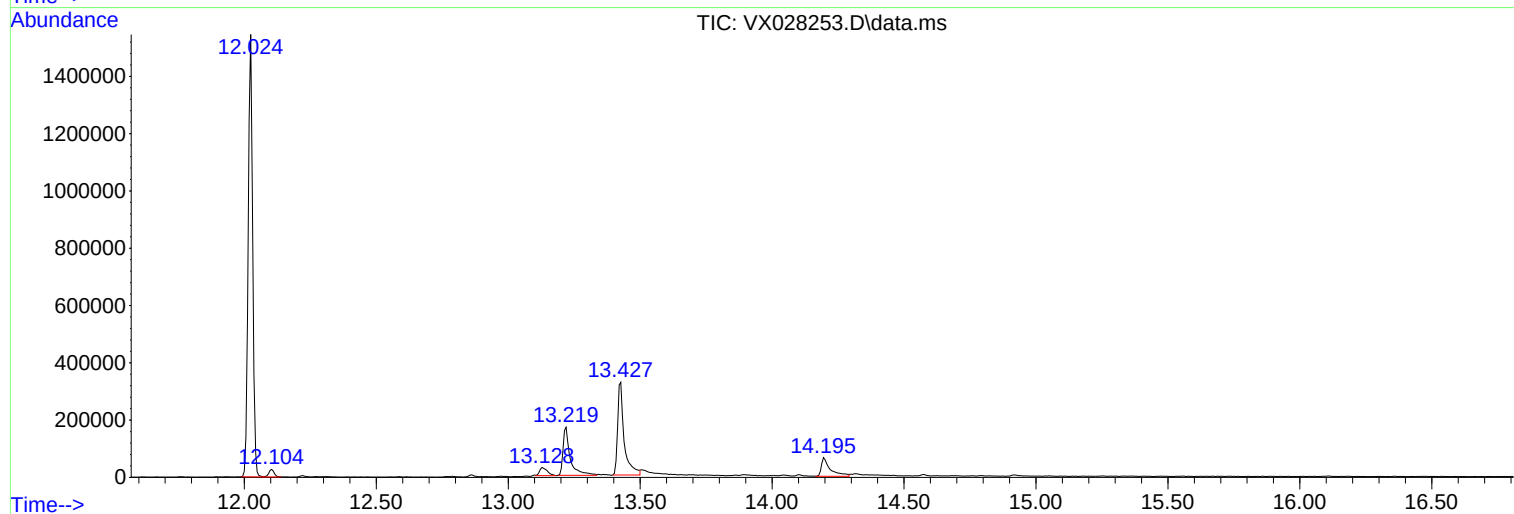
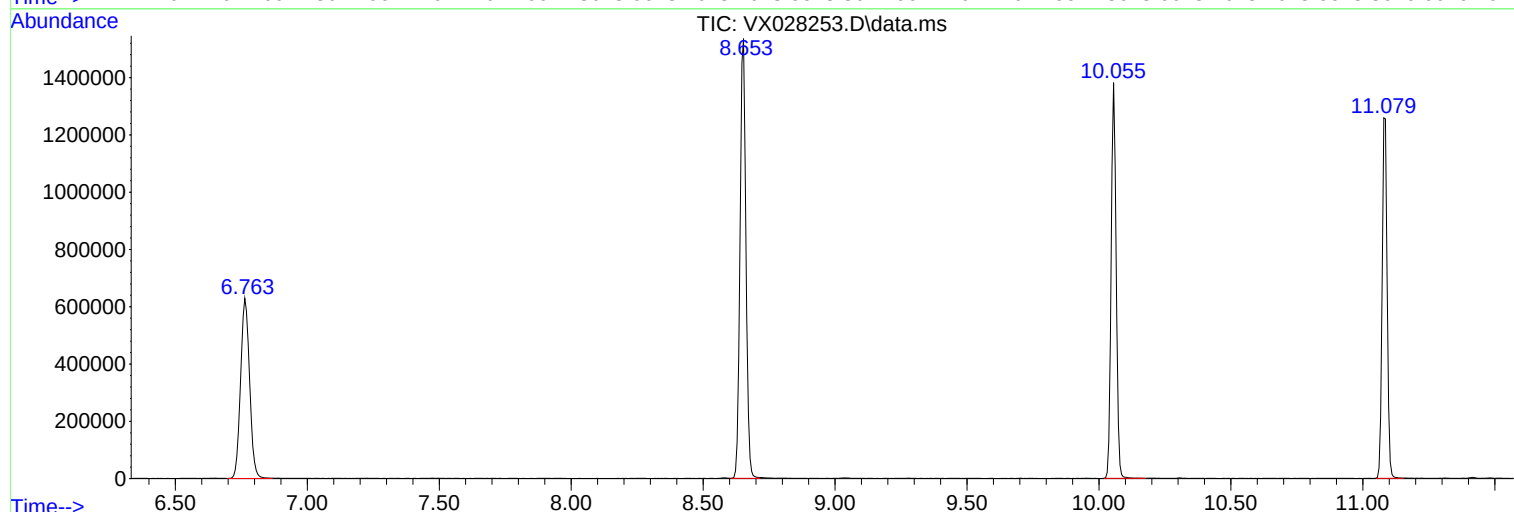
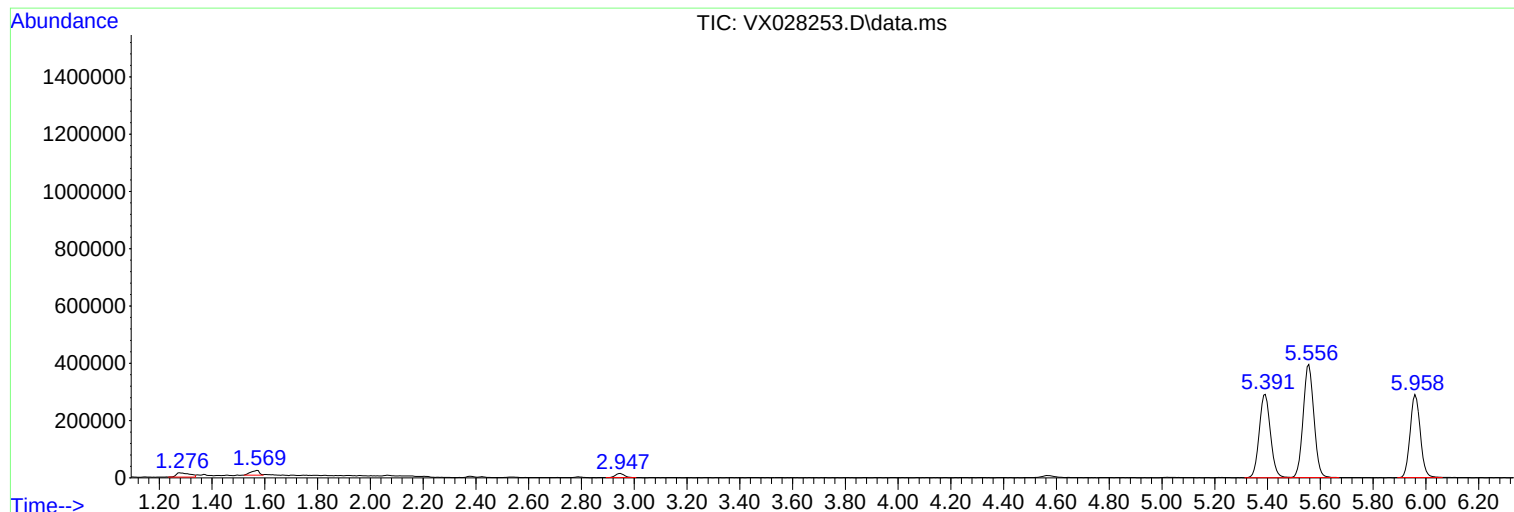
Sum of corrected areas: 13166185

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042122\  
Data File : VX028253.D  
Acq On : 21 Apr 2022 19:52  
Operator : JC/MD  
Sample : N2511-06 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1530

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041922W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042122\  
Data File : VX028253.D  
Acq On : 21 Apr 2022 19:52  
Operator : JC/MD  
Sample : N2511-06 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1530

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041922W.M  
Quant Title : SW846 8260

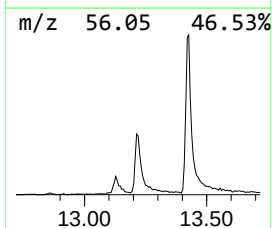
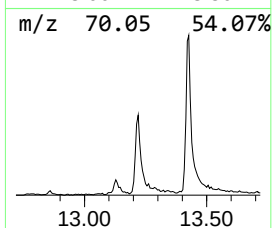
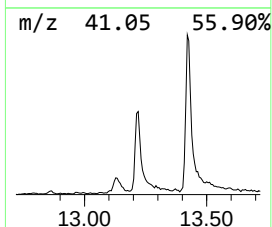
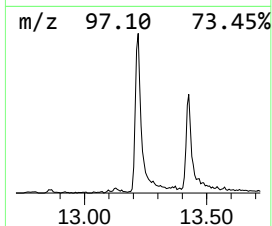
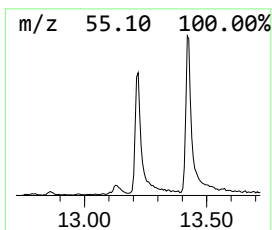
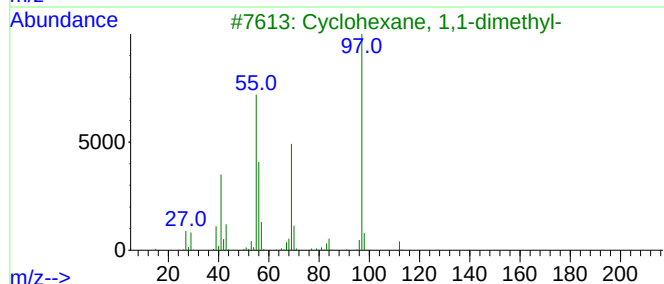
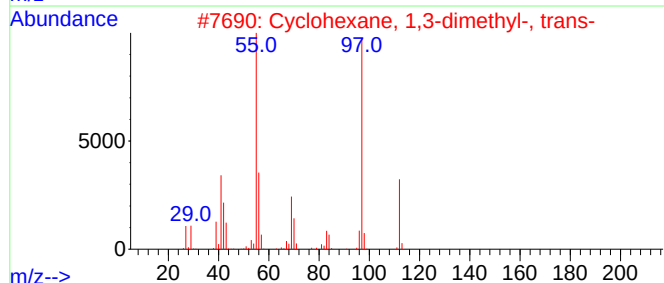
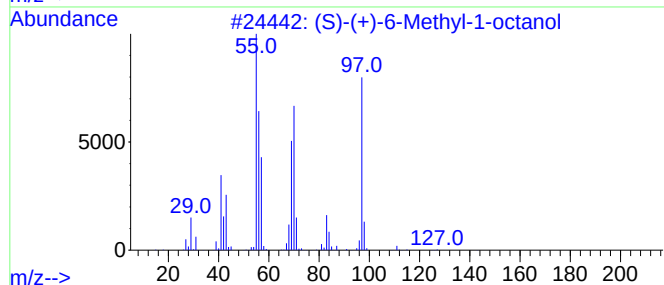
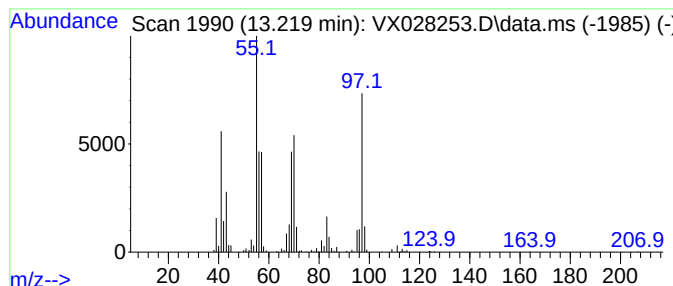
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 (S)-(+)-6-Methyl-1-octanol Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.219 | 8.69 ug/l | 316202 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | (S)-(+)-6-Methyl-1-octanol          | 144 | C9H20O       | 110453-78-6  | 87      |      |      |
| 2    | Cyclohexane, 1,3-dimethyl-, trans-  | 112 | C8H16        | 002207-03-6  | 59      |      |      |
| 3    | Cyclohexane, 1,1-dimethyl-          | 112 | C8H16        | 000590-66-9  | 53      |      |      |
| 4    | Cyclohexane, 1,2-dimethyl-, trans-  | 112 | C8H16        | 006876-23-9  | 50      |      |      |
| 5    | Sulfurous acid, cyclohexylmethyl... | 402 | C23H46O3S    | 1000309-22-4 | 43      |      |      |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042122\  
Data File : VX028253.D  
Acq On : 21 Apr 2022 19:52  
Operator : JC/MD  
Sample : N2511-06 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1530

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041922W.M  
Quant Title : SW846 8260

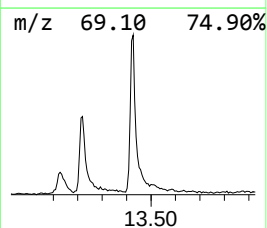
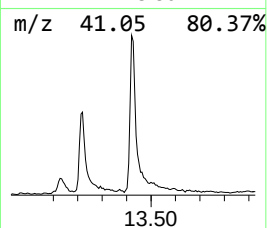
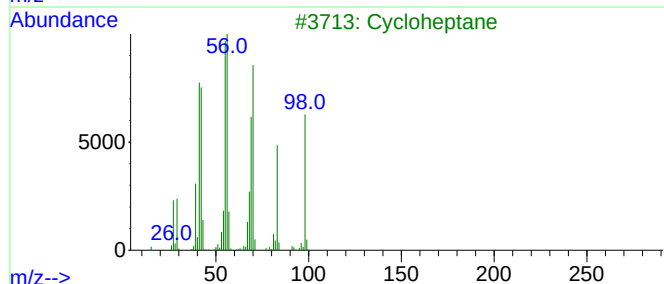
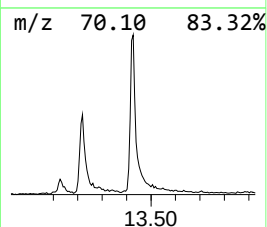
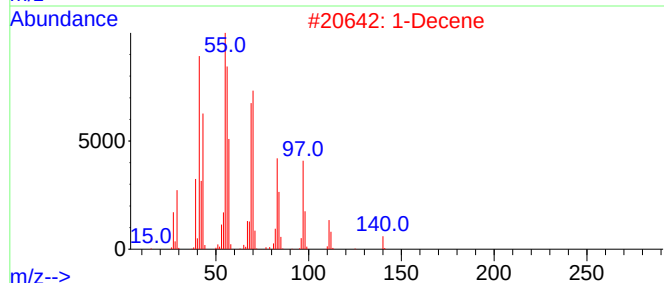
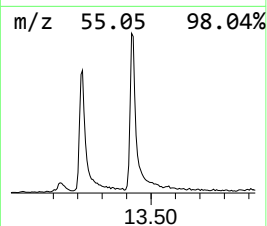
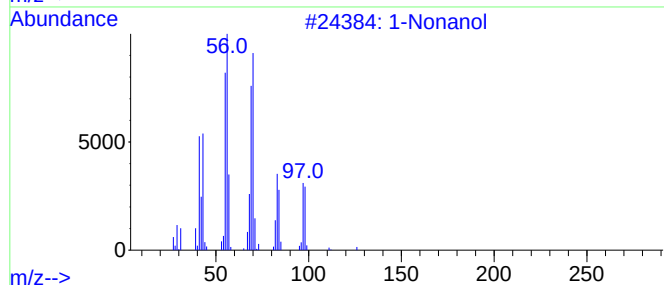
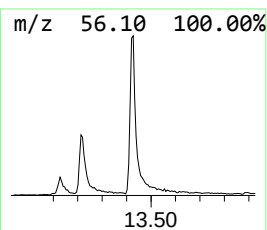
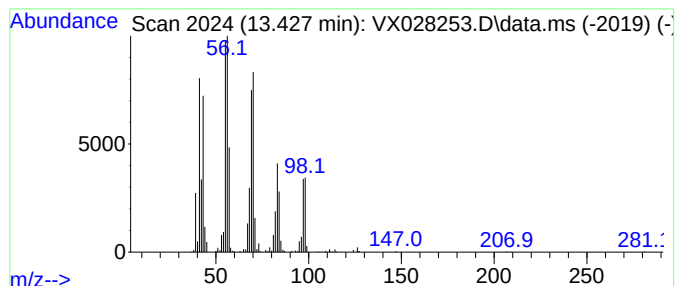
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 2 1-Nonanol Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.427 | 15.35 ug/l | 558619 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm    | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|------------|-------------|------|
| 1    | 1-Nonanol                           |   |              | 144 | C9H20O     | 000143-08-8 | 91   |
| 2    | 1-Decene                            |   |              | 140 | C10H20     | 000872-05-9 | 86   |
| 3    | Cycloheptane                        |   |              | 98  | C7H14      | 000291-64-5 | 83   |
| 4    | 1-Nonene                            |   |              | 126 | C9H18      | 000124-11-8 | 83   |
| 5    | Pentafluoropropionic acid, octyl... |   |              | 276 | C11H17F5O2 | 001867-95-4 | 64   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX042122\  
Data File : VX028253.D  
Acq On : 21 Apr 2022 19:52  
Operator : JC/MD  
Sample : N2511-06 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1530

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X041922W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| (S)-(+)-6-Methy... | 13.219 | 8.7     | ug/l  | 316202   | 4                     | 12.024 | 1820160 | 50.0 |
| 1-Nonanol          | 13.427 | 15.4    | ug/l  | 558619   | 4                     | 12.024 | 1820160 | 50.0 |