

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_D\Data\VD061923\  
 Data File : VD076476.D  
 Acq On : 19 Jun 2023 18:14  
 Operator : KP/SY  
 Sample : 03289-07  
 Misc : 5.01G/5.0ml/MSVOA\_D/SOIL  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_D  
 ClientSampleId :  
 SB-03-0-2.0

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\_D\Method\82D061623S.M  
 Title : SW846 8260

Signal : TIC: VD076476.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         | 1.728       | 18            | 24          | 33           | rVV      | 90571          | 165505        | 100.00%         | 45.913%       |
| 2         | 1.887       | 49            | 51          | 56           | rVB4     | 1889           | 2521          | 1.52%           | 0.699%        |
| 3         | 2.152       | 90            | 96          | 98           | rBV      | 4735           | 8258          | 4.99%           | 2.291%        |
| 4         | 2.193       | 101           | 103         | 105          | rVV2     | 2161           | 2313          | 1.40%           | 0.642%        |
| 5         | 2.228       | 105           | 109         | 112          | rVV4     | 3628           | 5648          | 3.41%           | 1.567%        |
| 6         | 2.258       | 112           | 114         | 117          | rVV3     | 2192           | 2331          | 1.41%           | 0.647%        |
| 7         | 2.287       | 117           | 119         | 121          | rVV2     | 1867           | 1763          | 1.07%           | 0.489%        |
| 8         | 2.511       | 155           | 157         | 160          | rVB2     | 1674           | 1946          | 1.18%           | 0.540%        |
| 9         | 2.887       | 218           | 221         | 223          | rVB2     | 1428           | 1685          | 1.02%           | 0.467%        |
| 10        | 3.681       | 350           | 356         | 358          | rBV2     | 1073           | 1681          | 1.02%           | 0.466%        |
| 11        | 4.793       | 539           | 545         | 547          | rBV4     | 2091           | 3572          | 2.16%           | 0.991%        |
| 12        | 4.940       | 565           | 570         | 573          | rVB2     | 1467           | 2638          | 1.59%           | 0.732%        |
| 13        | 4.975       | 573           | 576         | 579          | rBV2     | 1487           | 2459          | 1.49%           | 0.682%        |
| 14        | 5.116       | 596           | 600         | 601          | rBV2     | 1339           | 1670          | 1.01%           | 0.463%        |
| 15        | 5.675       | 691           | 695         | 698          | rBV2     | 1246           | 1843          | 1.11%           | 0.511%        |
| 16        | 7.034       | 919           | 926         | 927          | rBV3     | 2202           | 3011          | 1.82%           | 0.835%        |
| 17        | 7.057       | 927           | 930         | 932          | rVV3     | 2585           | 2629          | 1.59%           | 0.729%        |
| 18        | 7.663       | 1027          | 1033        | 1038         | rBV2     | 1238           | 2896          | 1.75%           | 0.803%        |
| 19        | 7.799       | 1051          | 1056        | 1064         | rBV3     | 3528           | 6578          | 3.97%           | 1.825%        |
| 20        | 7.875       | 1064          | 1069        | 1075         | rVB2     | 4805           | 8548          | 5.16%           | 2.371%        |
| 21        | 8.228       | 1122          | 1129        | 1133         | rBV3     | 4395           | 8370          | 5.06%           | 2.322%        |
| 22        | 8.463       | 1166          | 1169        | 1172         | rVB      | 1429           | 1698          | 1.03%           | 0.471%        |
| 23        | 8.769       | 1216          | 1221        | 1229         | rVB3     | 8334           | 16075         | 9.71%           | 4.459%        |
| 24        | 9.069       | 1266          | 1272        | 1275         | rBV2     | 1151           | 2710          | 1.64%           | 0.752%        |
| 25        | 9.422       | 1331          | 1332        | 1336         | rBV2     | 1555           | 1754          | 1.06%           | 0.487%        |
| 26        | 10.210      | 1462          | 1466        | 1468         | rBV      | 1518           | 2154          | 1.30%           | 0.598%        |
| 27        | 10.269      | 1470          | 1476        | 1481         | rVV3     | 11347          | 20749         | 12.54%          | 5.756%        |
| 28        | 10.657      | 1540          | 1542        | 1547         | rBV3     | 2901           | 3483          | 2.10%           | 0.966%        |
| 29        | 10.834      | 1567          | 1572        | 1575         | rVB2     | 1300           | 1881          | 1.14%           | 0.522%        |
| 30        | 11.587      | 1693          | 1700        | 1708         | rVB2     | 12682          | 23508         | 14.20%          | 6.521%        |
| 31        | 12.575      | 1862          | 1868        | 1875         | rBV5     | 9148           | 17237         | 10.41%          | 4.782%        |
| 32        | 12.734      | 1892          | 1895        | 1898         | rVB4     | 1667           | 2055          | 1.24%           | 0.570%        |
| 33        | 12.940      | 1927          | 1930        | 1933         | rVV2     | 1868           | 2157          | 1.30%           | 0.598%        |
| 34        | 13.516      | 2021          | 2028        | 2033         | rVV4     | 10879          | 19175         | 11.59%          | 5.319%        |
| 35        | 14.239      | 2148          | 2151        | 2152         | rBV2     | 2162           | 1671          | 1.01%           | 0.464%        |
| 36        | 15.492      | 2358          | 2364        | 2365         | rBV4     | 1399           | 2127          | 1.29%           | 0.590%        |

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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_D  
ClientSampleId :  
SB-03-0-2.0

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\_D\Method\82D061623S.M  
Title : SW846 8260

|    |        |      |      |      |      |      |      |       |        |
|----|--------|------|------|------|------|------|------|-------|--------|
| 37 | 16.063 | 2458 | 2461 | 2462 | rBV3 | 1892 | 2046 | 1.24% | 0.568% |
| 38 | 16.469 | 2528 | 2530 | 2533 | rBV3 | 1563 | 2131 | 1.29% | 0.591% |

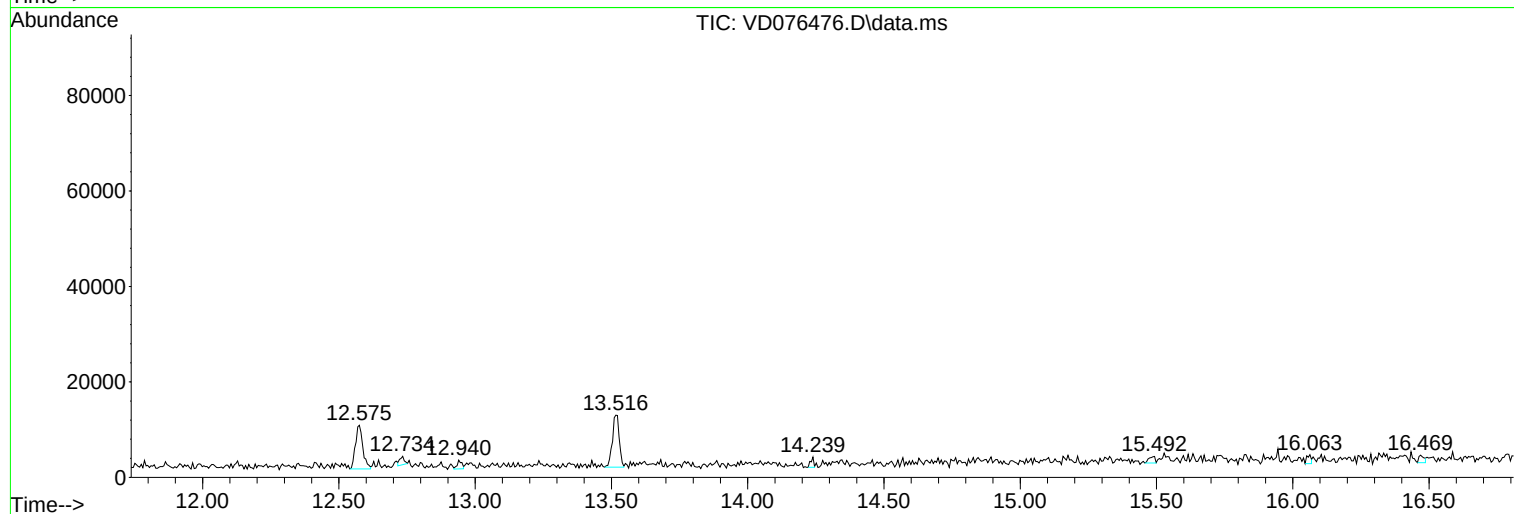
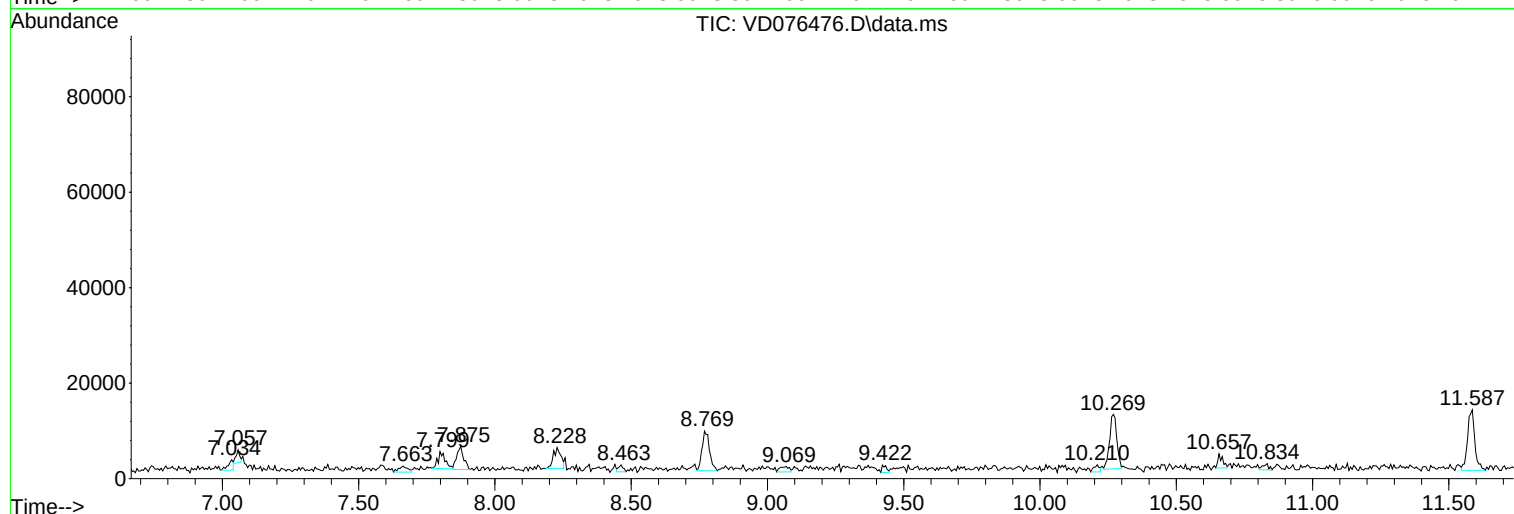
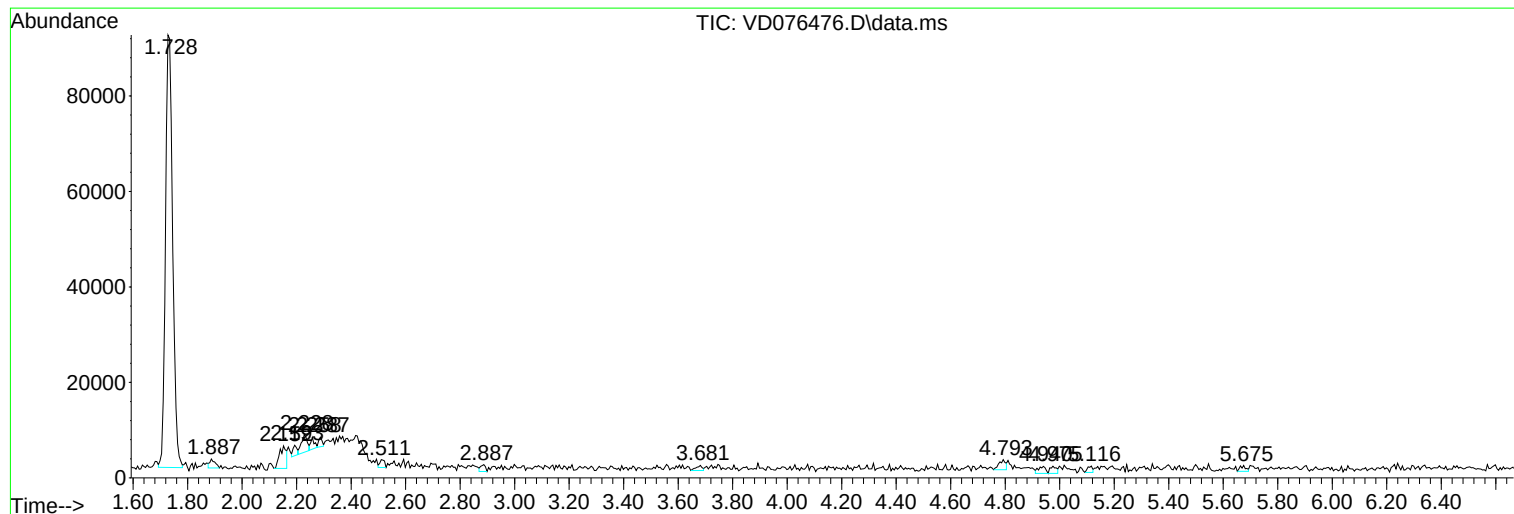
Sum of corrected areas: 360476

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_D\Method\82D061623S.M  
Quant Title : SW846 8260

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_D\Method\82D061623S.M  
Quant Title : SW846 8260

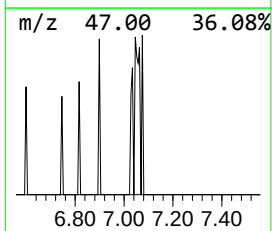
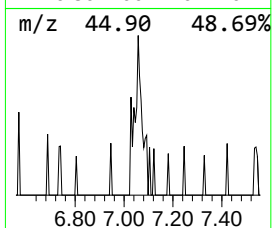
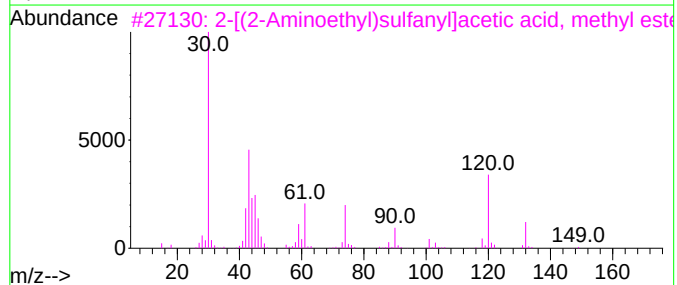
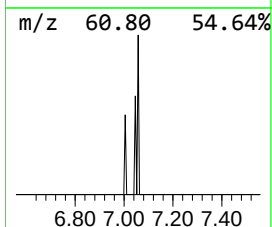
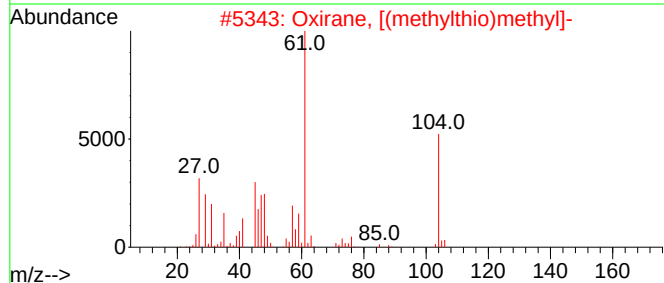
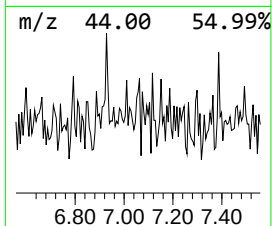
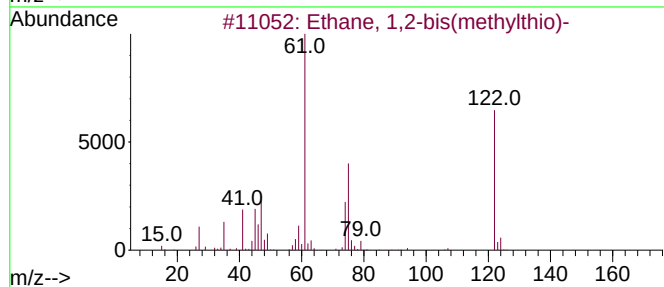
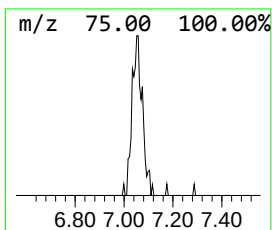
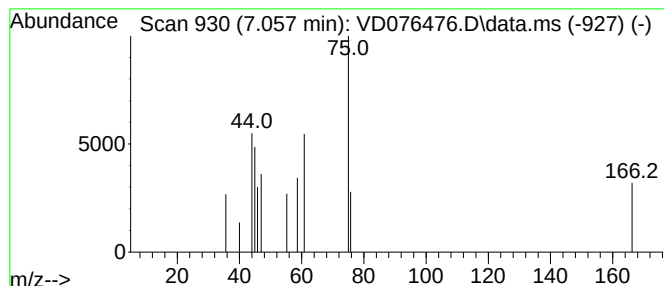
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 unknown7.057 Concentration Rank 8

| R.T.  | EstConc    | Area | Relative to ISTD   | R.T.  |
|-------|------------|------|--------------------|-------|
| 7.057 | 15.38 ug/l | 2629 | Pentafluorobenzene | 7.875 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Ethane, 1,2-bis(methylthio)-        | 122 | C4H10S2   | 006628-18-8 | 36   |
| 2    |    |   | Oxirane, [(methylthio)methyl]-      | 104 | C4H8OS    | 045378-62-9 | 23   |
| 3    |    |   | 2-[(2-Aminoethyl)sulfanyl]acetic... | 149 | C5H11NO2S | 366446-58-4 | 9    |
| 4    |    |   | Propanoic acid, 2-(ethylthio)-, ... | 162 | C7H14O2S  | 020461-97-6 | 9    |
| 5    |    |   | Propanoic acid, 3-(methylthio)-     | 120 | C4H8O2S   | 000646-01-5 | 9    |



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_D\Method\82D061623S.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 |
| unknown7.057     | 7.057 | 15.4    | ug/l  | 2629     | 1                     | 7.875 | 8548 | 50.0 |