

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD081319\  
 Data File : VD063564.D  
 Acq On : 14 Aug 2019 9:49  
 Operator : JC/SY  
 Sample : K4294-07  
 Misc : 5.08g/5ml/MSVOA D/SOIL  
 ALS Vial : 56 Sample Multiplier: 1

Instrument :  
 MSVOA\_D  
 ClientSampleId :  
 RBR-200052RE

## Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_D\METHOD\82D080919S.M  
 Title : SW846 8260

Signal : TIC

| 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         | 1.651       | 22            | 23          | 26           | rVB      | 4959           | 5702          | 2.01%           | 0.259%        |
| 2         | 1.691       | 26            | 27          | 28           | rBV      | 4219           | 3606          | 1.27%           | 0.164%        |
| 3         | 1.740       | 28            | 32          | 33           | rVV      | 7769           | 11795         | 4.16%           | 0.536%        |
| 4         | 1.770       | 33            | 35          | 36           | rVV      | 6180           | 7430          | 2.62%           | 0.338%        |
| 5         | 1.819       | 39            | 40          | 41           | rVB      | 6933           | 4366          | 1.54%           | 0.198%        |
| 6         | 1.966       | 53            | 55          | 56           | rBV      | 4418           | 3914          | 1.38%           | 0.178%        |
| 7         | 2.075       | 62            | 66          | 70           | rBV4     | 6052           | 20394         | 7.20%           | 0.927%        |
| 8         | 2.153       | 73            | 74          | 75           | rVV      | 3500           | 3779          | 1.33%           | 0.172%        |
| 9         | 2.203       | 77            | 79          | 87           | rVB2     | 12882          | 29428         | 10.38%          | 1.337%        |
| 10        | 2.291       | 87            | 88          | 91           | rVB2     | 2599           | 2983          | 1.05%           | 0.136%        |
| 11        | 2.380       | 94            | 97          | 99           | rVB3     | 4147           | 8982          | 3.17%           | 0.408%        |
| 12        | 2.419       | 99            | 101         | 103          | rBV      | 6330           | 9531          | 3.36%           | 0.433%        |
| 13        | 2.459       | 103           | 105         | 107          | rVB      | 6855           | 10170         | 3.59%           | 0.462%        |
| 14        | 2.498       | 107           | 109         | 111          | rBV2     | 5847           | 10638         | 3.75%           | 0.483%        |
| 15        | 2.528       | 111           | 112         | 115          | rVB      | 7071           | 9091          | 3.21%           | 0.413%        |
| 16        | 2.587       | 115           | 118         | 120          | rBV2     | 7982           | 14791         | 5.22%           | 0.672%        |
| 17        | 2.616       | 120           | 121         | 125          | rVB4     | 3735           | 5532          | 1.95%           | 0.251%        |
| 18        | 2.665       | 125           | 126         | 127          | rBV      | 5698           | 4993          | 1.76%           | 0.227%        |
| 19        | 2.823       | 140           | 142         | 144          | rVB2     | 3707           | 5085          | 1.79%           | 0.231%        |
| 20        | 3.000       | 158           | 160         | 163          | rVV2     | 5133           | 10418         | 3.68%           | 0.473%        |
| 21        | 3.069       | 165           | 167         | 170          | rVV3     | 7685           | 15048         | 5.31%           | 0.684%        |
| 22        | 3.108       | 170           | 171         | 177          | rVB2     | 11690          | 26306         | 9.28%           | 1.195%        |
| 23        | 3.226       | 177           | 183         | 187          | rBV      | 26764          | 60842         | 21.47%          | 2.764%        |
| 24        | 3.276       | 187           | 188         | 194          | rVB2     | 4816           | 9695          | 3.42%           | 0.440%        |
| 25        | 3.374       | 194           | 198         | 205          | rVB2     | 11825          | 30763         | 10.86%          | 1.398%        |
| 26        | 3.463       | 205           | 207         | 208          | rBV      | 2064           | 2916          | 1.03%           | 0.132%        |
| 27        | 3.532       | 212           | 214         | 216          | rVB      | 2001           | 3035          | 1.07%           | 0.138%        |
| 28        | 3.817       | 238           | 243         | 247          | rBV3     | 13919          | 34887         | 12.31%          | 1.585%        |
| 29        | 3.925       | 251           | 254         | 256          | rVB      | 1609           | 2850          | 1.01%           | 0.129%        |
| 30        | 4.211       | 281           | 283         | 285          | rBV      | 2183           | 3330          | 1.18%           | 0.151%        |
| 31        | 4.555       | 317           | 318         | 322          | rVB      | 2253           | 3110          | 1.10%           | 0.141%        |
| 32        | 4.841       | 342           | 347         | 348          | rBV      | 2248           | 4356          | 1.54%           | 0.198%        |
| 33        | 6.170       | 479           | 482         | 489          | rBV      | 2516           | 8858          | 3.13%           | 0.402%        |
| 34        | 6.465       | 508           | 512         | 517          | rBV      | 4372           | 11894         | 4.20%           | 0.540%        |

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Method : Z:\VOASRV\HPCHEM1\MSVOA\_D\METHOD\82D080919S.M  
 Title : SW846 8260

|    |        |      |      |      |      |        |        |         |         |
|----|--------|------|------|------|------|--------|--------|---------|---------|
| 35 | 6.928  | 551  | 559  | 565  | rBV3 | 58665  | 166028 | 58.59%  | 7.543%  |
| 36 | 7.046  | 565  | 571  | 580  | rVV  | 63295  | 197286 | 69.62%  | 8.963%  |
| 37 | 7.154  | 580  | 582  | 585  | rVB  | 2771   | 5058   | 1.78%   | 0.230%  |
| 38 | 7.450  | 606  | 612  | 620  | rBV3 | 46573  | 134633 | 47.51%  | 6.117%  |
| 39 | 8.218  | 685  | 690  | 700  | rVB  | 111082 | 283392 | 100.00% | 12.875% |
| 40 | 8.877  | 755  | 757  | 760  | rVB  | 1829   | 3141   | 1.11%   | 0.143%  |
| 41 | 10.413 | 908  | 913  | 919  | rBV  | 103856 | 233033 | 82.23%  | 10.587% |
| 42 | 11.289 | 1001 | 1002 | 1006 | rBV  | 1801   | 3779   | 1.33%   | 0.172%  |
| 43 | 11.466 | 1018 | 1020 | 1024 | rBB  | 1531   | 3665   | 1.29%   | 0.167%  |
| 44 | 11.683 | 1040 | 1042 | 1047 | rBV  | 2010   | 3792   | 1.34%   | 0.172%  |
| 45 | 12.037 | 1076 | 1078 | 1081 | rVB  | 1843   | 2995   | 1.06%   | 0.136%  |
| 46 | 12.372 | 1108 | 1112 | 1117 | rBV  | 182973 | 281730 | 99.41%  | 12.800% |
| 47 | 13.563 | 1229 | 1233 | 1238 | rVB  | 133908 | 181564 | 64.07%  | 8.249%  |
| 48 | 13.721 | 1245 | 1249 | 1250 | rVB  | 3341   | 5881   | 2.08%   | 0.267%  |
| 49 | 14.095 | 1284 | 1287 | 1289 | rBV  | 1611   | 2848   | 1.00%   | 0.129%  |
| 50 | 14.518 | 1327 | 1330 | 1336 | rVB  | 168860 | 223569 | 78.89%  | 10.157% |
| 51 | 14.803 | 1356 | 1359 | 1362 | rVB  | 2183   | 3576   | 1.26%   | 0.162%  |
| 52 | 14.862 | 1362 | 1365 | 1370 | rBV  | 2351   | 5651   | 1.99%   | 0.257%  |
| 53 | 14.951 | 1370 | 1374 | 1375 | rBV  | 2043   | 2949   | 1.04%   | 0.134%  |
| 54 | 15.030 | 1378 | 1382 | 1383 | rBV  | 2005   | 4349   | 1.53%   | 0.198%  |
| 55 | 15.118 | 1388 | 1391 | 1395 | rBV2 | 2592   | 4075   | 1.44%   | 0.185%  |
| 56 | 15.325 | 1408 | 1412 | 1415 | rBV  | 1316   | 3055   | 1.08%   | 0.139%  |
| 57 | 15.522 | 1430 | 1432 | 1436 | rVB2 | 2277   | 3772   | 1.33%   | 0.171%  |
| 58 | 15.945 | 1474 | 1475 | 1479 | rVB  | 2230   | 3606   | 1.27%   | 0.164%  |
| 59 | 16.073 | 1487 | 1488 | 1491 | rBV  | 1684   | 3068   | 1.08%   | 0.139%  |
| 60 | 16.132 | 1491 | 1494 | 1495 | rVB  | 2236   | 3236   | 1.14%   | 0.147%  |
| 61 | 16.369 | 1513 | 1518 | 1520 | rBV  | 1679   | 3465   | 1.22%   | 0.157%  |
| 62 | 16.428 | 1522 | 1524 | 1526 | rBV  | 2331   | 3063   | 1.08%   | 0.139%  |
| 63 | 16.674 | 1546 | 1549 | 1552 | rVV  | 2125   | 3242   | 1.14%   | 0.147%  |
| 64 | 16.733 | 1552 | 1555 | 1558 | rVB  | 2439   | 3386   | 1.19%   | 0.154%  |
| 65 | 16.910 | 1569 | 1573 | 1575 | rVB  | 1961   | 3763   | 1.33%   | 0.171%  |
| 66 | 16.959 | 1575 | 1578 | 1579 | rBV  | 2452   | 4140   | 1.46%   | 0.188%  |
| 67 | 17.137 | 1593 | 1596 | 1600 | rBV3 | 1808   | 3426   | 1.21%   | 0.156%  |
| 68 | 17.284 | 1609 | 1611 | 1613 | rBV  | 2295   | 3456   | 1.22%   | 0.157%  |
| 69 | 17.471 | 1627 | 1630 | 1631 | rBV  | 1948   | 2834   | 1.00%   | 0.129%  |

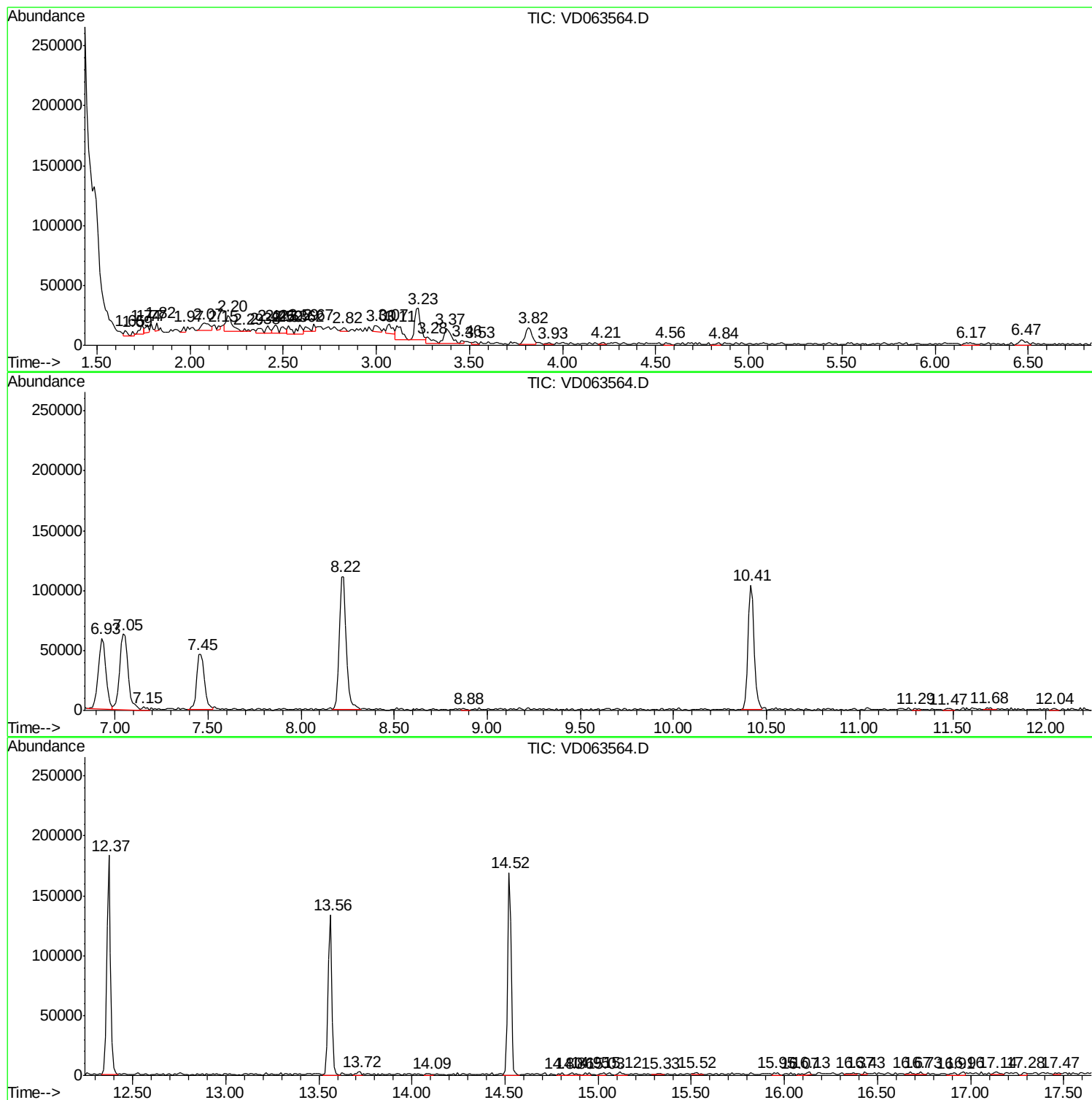
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ALS Vial : 56 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
RBR-200052RE

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_D\METHOD\82D080919S.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Instrument :  
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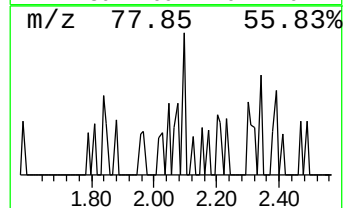
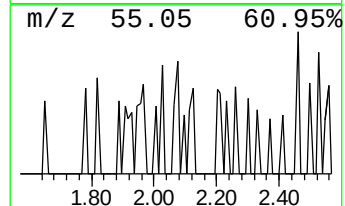
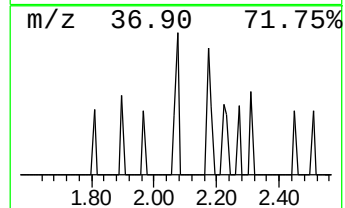
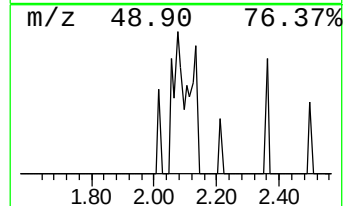
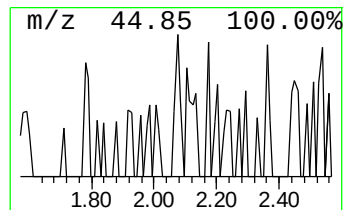
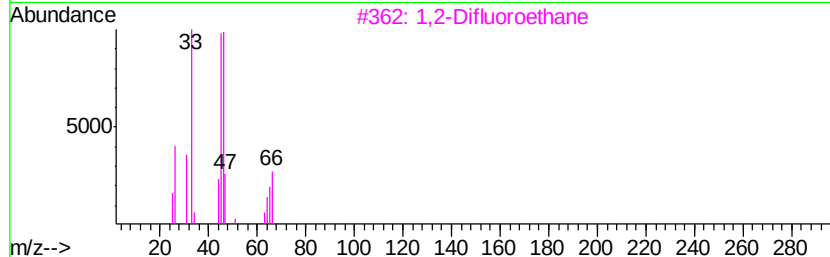
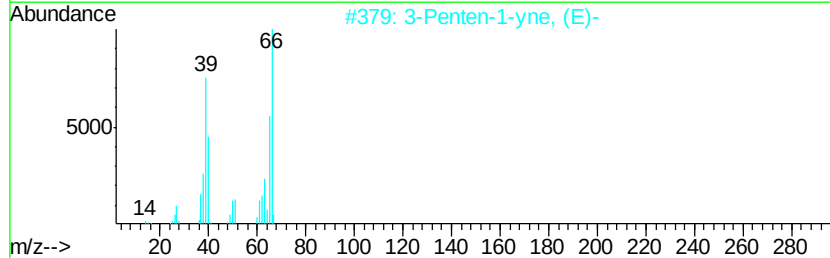
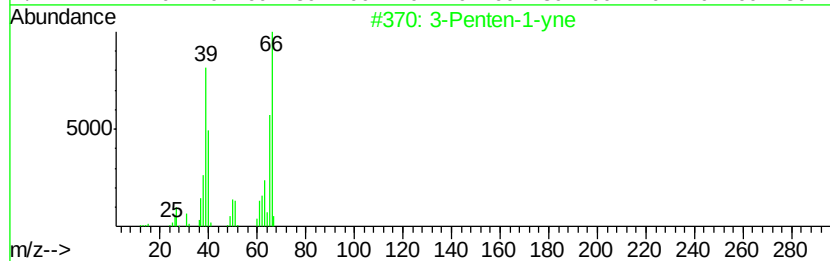
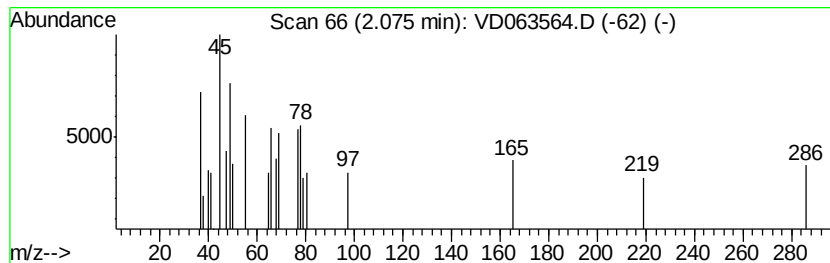
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_D\METHOD\82D080919S.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.07 Concentration Rank 3

| R.T. | EstConc   | Area  | Relative to ISTD   | R.T. |
|------|-----------|-------|--------------------|------|
| 2.07 | 5.17 ug/l | 20394 | Pentafluorobenzene | 7.05 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Penten-1-yne                      | 66  | C5H6    | 002206-23-7 | 10   |
| 2    |    |   | 3-Penten-1-yne, (E)-                | 66  | C5H6    | 002004-69-5 | 10   |
| 3    |    |   | 1,2-Difluoroethane                  | 66  | C2H4F2  | 000624-72-6 | 9    |
| 4    |    |   | Tetrazolo[1,5-a]pyrimidine, 5,7-... | 149 | C6H7N5  | 003210-44-4 | 9    |
| 5    |    |   | 1,1,2,2-Cyclopropane-tetracarbon... | 142 | C7H2N4  | 002424-32-0 | 9    |



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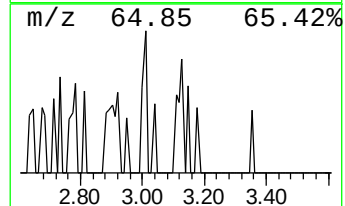
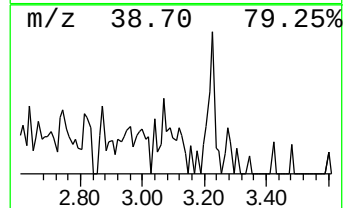
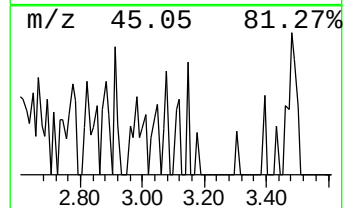
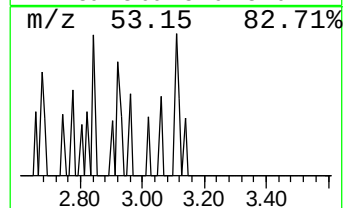
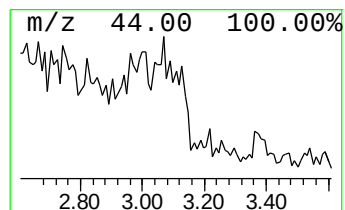
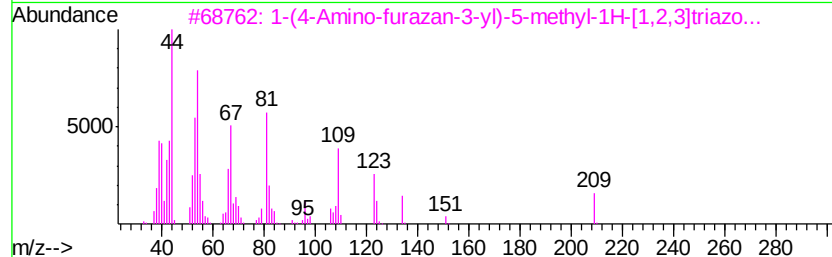
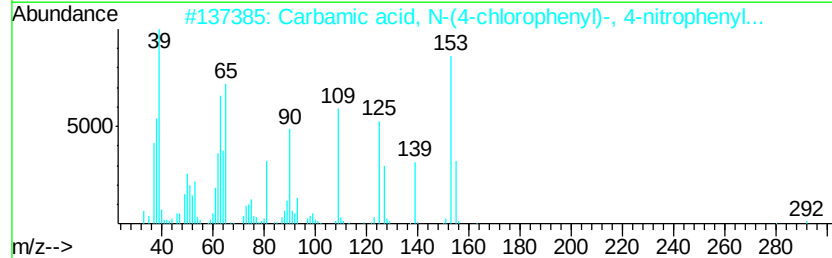
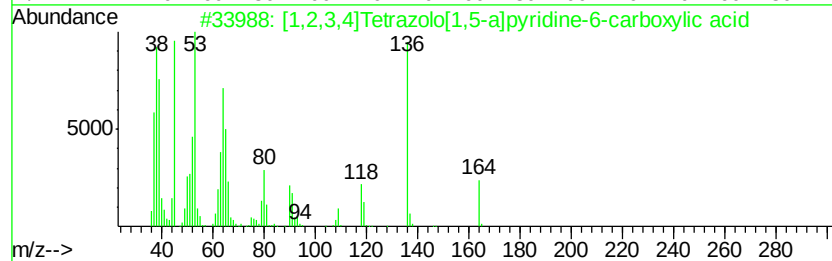
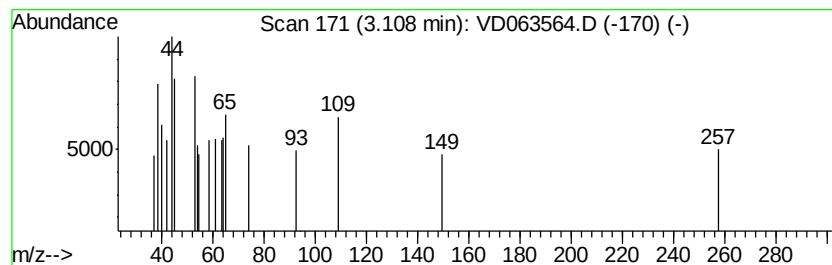
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown3.11 Concentration Rank 2

| R.T.    | EstConc                             | Area         | Relative to ISTD   | R.T.         |      |      |
|---------|-------------------------------------|--------------|--------------------|--------------|------|------|
| 3.11    | 6.67 ug/l                           | 26306        | Pentafluorobenzene | 7.05         |      |      |
| Hit# of | 5                                   | Tentative ID | MW                 | MolForm      | CAS# | Qual |
| 1       | [1,2,3,4]Tetrazolo[1,5-a]pyridin... | 164          | C6H4N4O2           | 1000362-60-7 | 40   |      |
| 2       | Carbamic acid, N-(4-chlorophenyl... | 292          | C13H9ClN2O4        | 003848-41-7  | 25   |      |
| 3       | 1-(4-Amino-furazan-3-yl)-5-methv... | 209          | C6H7N7O2           | 1000300-80-6 | 25   |      |
| 4       | 1,2,5-Oxadiazole-3-carbohydroxym... | 144          | C3H4N4O3           | 302796-65-2  | 10   |      |
| 5       | 3-Butynoic acid                     | 84           | C4H4O2             | 002345-51-9  | 9    |      |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown2.07      | 2.07 | 5.2     | ug/l  | 20394    | 1                     | 7.05 | 197286 | 50.0 |
| unknown3.11      | 3.11 | 6.7     | ug/l  | 26306    | 1                     | 7.05 | 197286 | 50.0 |