

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_X\DATA\VX103018\  
 Data File : VX005695.D  
 Acq On : 30 Oct 2018 16:47  
 Operator : JC/MD  
 Sample : J5194-10  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 HR-05-102618-B

## 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\_X\METHOD\82X102418W.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         | 1.489       | 51            | 55          | 61           | rBV      | 8278           | 10184         | 1.03%           | 0.144%        |
| 2         | 1.611       | 67            | 75          | 79           | rVB8     | 5580           | 11098         | 1.13%           | 0.157%        |
| 3         | 2.190       | 164           | 170         | 176          | rBV2     | 13005          | 19529         | 1.98%           | 0.275%        |
| 4         | 2.446       | 206           | 212         | 223          | rBV      | 28118          | 45479         | 4.61%           | 0.642%        |
| 5         | 2.776       | 262           | 266         | 272          | rBV      | 8027           | 13500         | 1.37%           | 0.190%        |
| 6         | 2.861       | 274           | 280         | 288          | rVB      | 11211          | 22273         | 2.26%           | 0.314%        |
| 7         | 5.501       | 702           | 713         | 728          | rBV      | 127166         | 361777        | 36.68%          | 5.103%        |
| 8         | 5.665       | 728           | 740         | 760          | rVV2     | 223046         | 627293        | 63.61%          | 8.849%        |
| 9         | 6.068       | 793           | 806         | 816          | rBV      | 142049         | 370736        | 37.59%          | 5.230%        |
| 10        | 6.464       | 859           | 871         | 882          | rBV      | 118742         | 286906        | 29.09%          | 4.047%        |
| 11        | 6.860       | 925           | 936         | 956          | rBV2     | 313655         | 767596        | 77.83%          | 10.828%       |
| 12        | 7.677       | 1062          | 1070        | 1075         | rBV4     | 9081           | 22544         | 2.29%           | 0.318%        |
| 13        | 7.884       | 1097          | 1104        | 1119         | rBV      | 118352         | 209956        | 21.29%          | 2.962%        |
| 14        | 8.622       | 1218          | 1225        | 1229         | rBV      | 5902           | 10769         | 1.09%           | 0.152%        |
| 15        | 8.714       | 1233          | 1240        | 1249         | rVV      | 609245         | 986216        | 100.00%         | 13.911%       |
| 16        | 8.781       | 1249          | 1251        | 1262         | rVB      | 11996          | 22946         | 2.33%           | 0.324%        |
| 17        | 9.409       | 1350          | 1354        | 1359         | rVB      | 11770          | 14938         | 1.51%           | 0.211%        |
| 18        | 9.543       | 1372          | 1376        | 1380         | rBV      | 60290          | 83372         | 8.45%           | 1.176%        |
| 19        | 9.585       | 1380          | 1383        | 1388         | rVV2     | 27785          | 41343         | 4.19%           | 0.583%        |
| 20        | 9.640       | 1388          | 1392        | 1400         | rVB      | 17147          | 24810         | 2.52%           | 0.350%        |
| 21        | 9.976       | 1441          | 1447        | 1459         | rBV      | 71615          | 98759         | 10.01%          | 1.393%        |
| 22        | 10.116      | 1463          | 1470        | 1489         | rVV      | 623337         | 872476        | 88.47%          | 12.307%       |
| 23        | 10.360      | 1505          | 1510        | 1517         | rVB      | 6739           | 10338         | 1.05%           | 0.146%        |
| 24        | 10.701      | 1561          | 1566        | 1570         | rBV2     | 7725           | 10714         | 1.09%           | 0.151%        |
| 25        | 11.140      | 1632          | 1638        | 1652         | rBV      | 514113         | 659052        | 66.83%          | 9.297%        |
| 26        | 11.433      | 1681          | 1686        | 1694         | rBV      | 10270          | 22948         | 2.33%           | 0.324%        |
| 27        | 11.670      | 1714          | 1725        | 1733         | rBV      | 13804          | 20853         | 2.11%           | 0.294%        |
| 28        | 11.811      | 1744          | 1748        | 1755         | rVB      | 28231          | 39594         | 4.01%           | 0.559%        |
| 29        | 12.079      | 1786          | 1792        | 1799         | rBV      | 679302         | 827959        | 83.95%          | 11.679%       |
| 30        | 12.146      | 1799          | 1803        | 1810         | rVB      | 23004          | 31916         | 3.24%           | 0.450%        |
| 31        | 12.298      | 1820          | 1828        | 1831         | rBV3     | 15171          | 26357         | 2.67%           | 0.372%        |
| 32        | 12.371      | 1836          | 1840        | 1849         | rVB3     | 10640          | 18208         | 1.85%           | 0.257%        |
| 33        | 12.518      | 1859          | 1864        | 1869         | rVB      | 8457           | 11308         | 1.15%           | 0.160%        |
| 34        | 12.585      | 1869          | 1875        | 1877         | rBV      | 8520           | 12073         | 1.22%           | 0.170%        |

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 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\_X\METHOD\82X102418W.M  
 Title : SW846 8260

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 35 | 12.609 | 1877 | 1879 | 1882 | rVV  | 9890  | 10835 | 1.10% | 0.153% |
| 36 | 12.670 | 1882 | 1889 | 1892 | rVB2 | 9485  | 16132 | 1.64% | 0.228% |
| 37 | 12.756 | 1898 | 1903 | 1911 | rBV3 | 11182 | 19325 | 1.96% | 0.273% |
| 38 | 12.908 | 1923 | 1928 | 1934 | rVB3 | 9468  | 14134 | 1.43% | 0.199% |
| 39 | 13.018 | 1943 | 1946 | 1952 | rVB  | 12429 | 15763 | 1.60% | 0.222% |
| 40 | 13.225 | 1971 | 1980 | 1985 | rBV  | 13386 | 21273 | 2.16% | 0.300% |
| 41 | 13.347 | 1996 | 2000 | 2006 | rBV2 | 34470 | 48236 | 4.89% | 0.680% |
| 42 | 13.481 | 2016 | 2022 | 2027 | rBV  | 34058 | 41395 | 4.20% | 0.584% |
| 43 | 13.646 | 2044 | 2049 | 2054 | rVV5 | 7261  | 12387 | 1.26% | 0.175% |
| 44 | 13.719 | 2054 | 2061 | 2068 | rVB2 | 8816  | 19029 | 1.93% | 0.268% |
| 45 | 13.835 | 2074 | 2080 | 2086 | rVB  | 20516 | 28820 | 2.92% | 0.407% |
| 46 | 13.914 | 2088 | 2093 | 2098 | rVB2 | 10820 | 15380 | 1.56% | 0.217% |
| 47 | 13.981 | 2099 | 2104 | 2109 | rBV2 | 12603 | 18839 | 1.91% | 0.266% |
| 48 | 14.133 | 2124 | 2129 | 2132 | rBV  | 8709  | 10921 | 1.11% | 0.154% |
| 49 | 14.286 | 2147 | 2154 | 2163 | rVB  | 32467 | 52431 | 5.32% | 0.740% |
| 50 | 14.432 | 2174 | 2178 | 2182 | rVB  | 9833  | 13862 | 1.41% | 0.196% |
| 51 | 14.536 | 2191 | 2195 | 2202 | rVB2 | 23173 | 32446 | 3.29% | 0.458% |
| 52 | 14.694 | 2212 | 2221 | 2225 | rBV2 | 23452 | 40815 | 4.14% | 0.576% |
| 53 | 14.841 | 2240 | 2245 | 2248 | rBV  | 18384 | 24709 | 2.51% | 0.349% |
| 54 | 15.249 | 2309 | 2312 | 2320 | rBV5 | 7513  | 16664 | 1.69% | 0.235% |

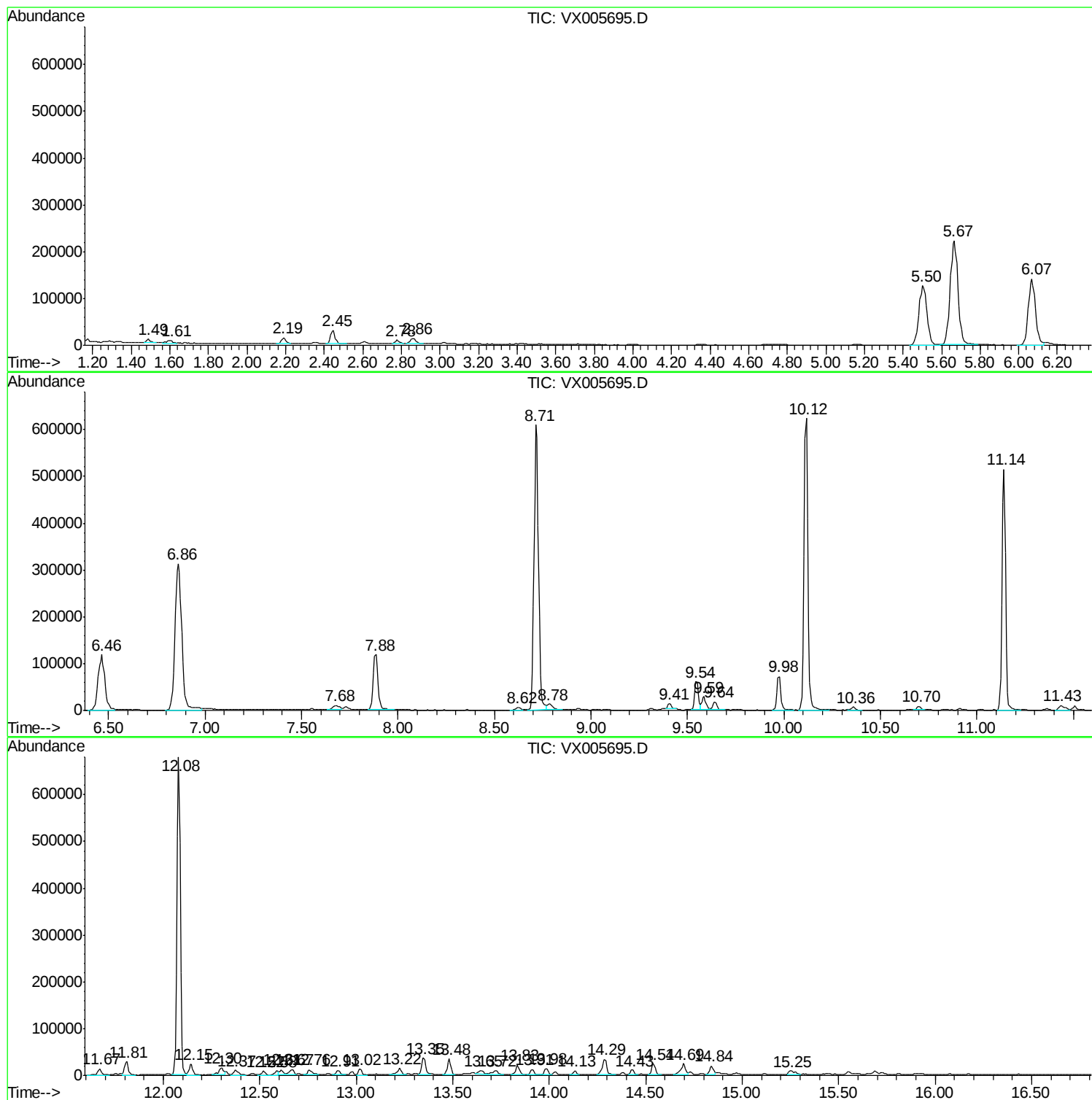
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X102418W.M  
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX103018\  
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Instrument :  
MSVOA\_X  
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HR-05-102618-B

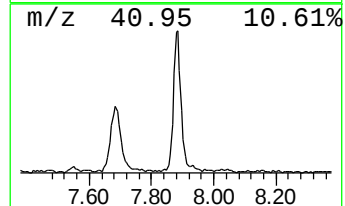
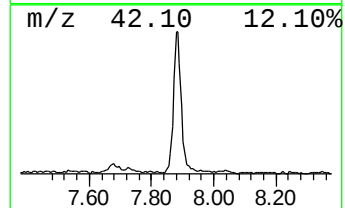
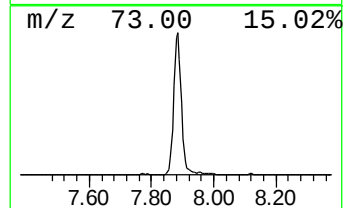
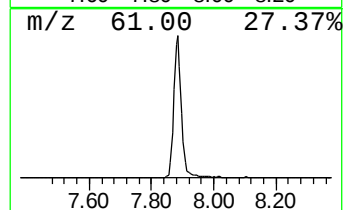
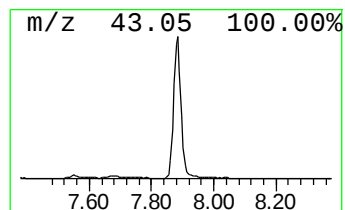
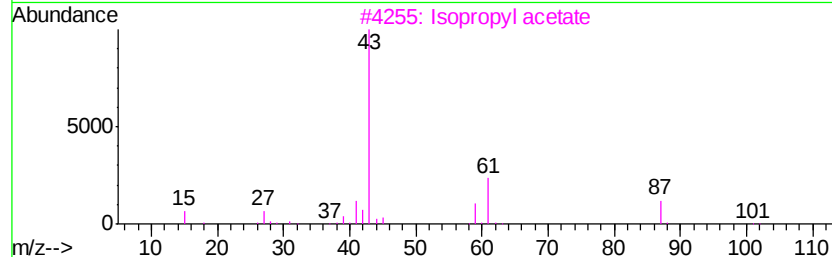
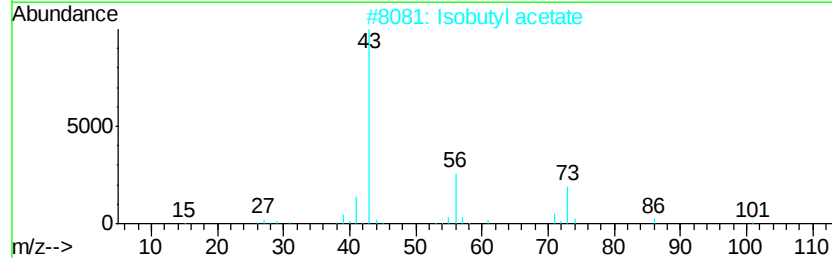
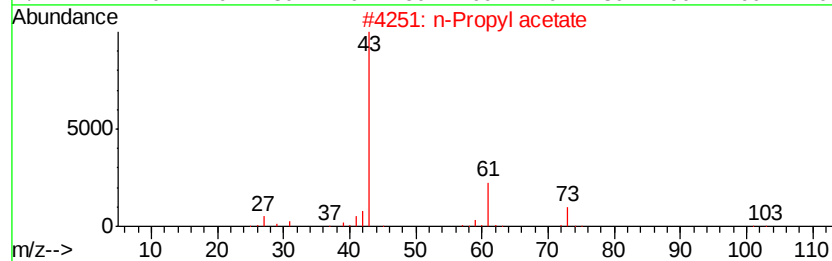
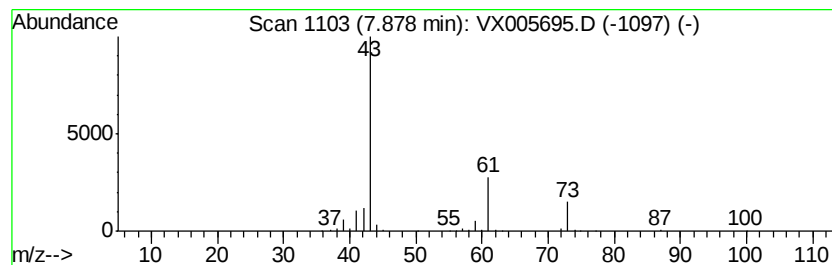
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X102418W.M  
Quant Title : SW846 8260

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

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Peak Number 1 n-Propyl acetate Concentration Rank 1

| R.T. | EstConc    | Area   | Relative to ISTD    | R.T. |
|------|------------|--------|---------------------|------|
| 7.88 | 13.68 ug/l | 209956 | 1,4-Difluorobenzene | 6.86 |

| Hit# | of | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------|-----|---------|-------------|------|
| 1    | 5  | n-Propyl acetate  | 102 | C5H10O2 | 000109-60-4 | 83   |
| 2    |    | Isobutyl acetate  | 116 | C6H12O2 | 000110-19-0 | 9    |
| 3    |    | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 9    |
| 4    |    | Isobutylamine     | 73  | C4H11N  | 000078-81-9 | 7    |
| 5    |    | Isobutane         | 58  | C4H10   | 000075-28-5 | 7    |



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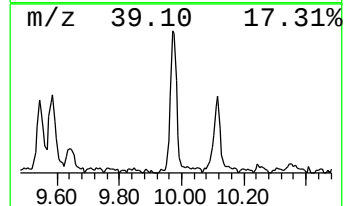
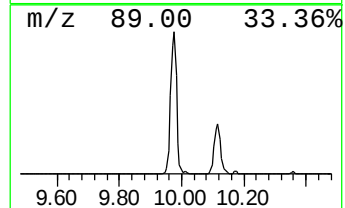
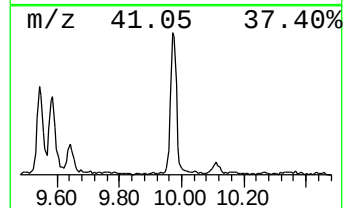
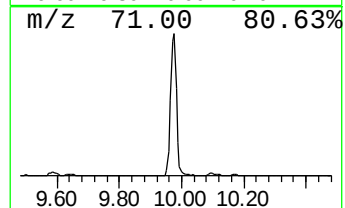
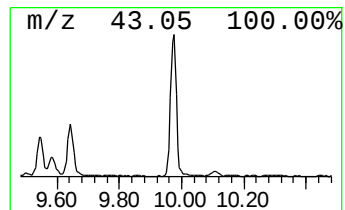
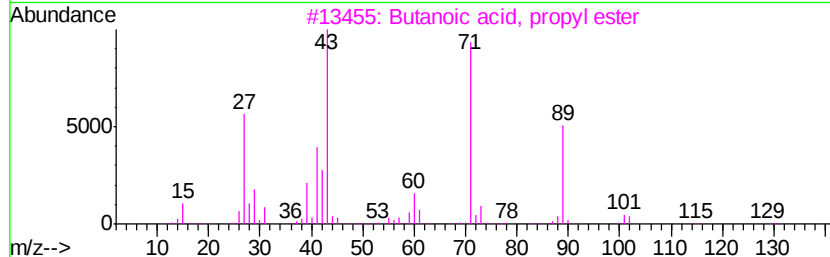
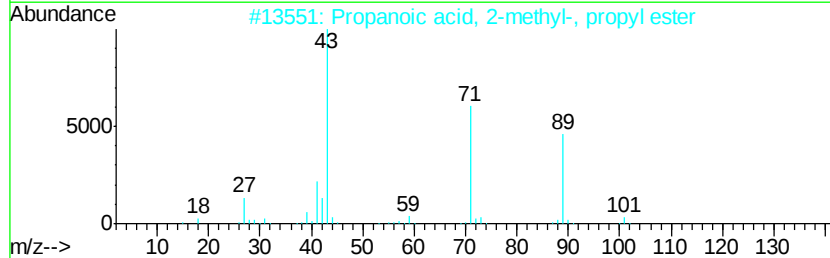
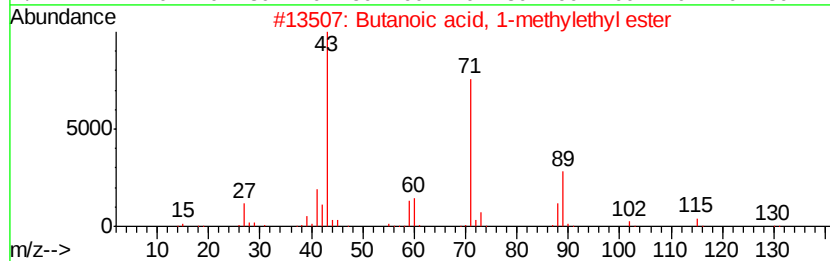
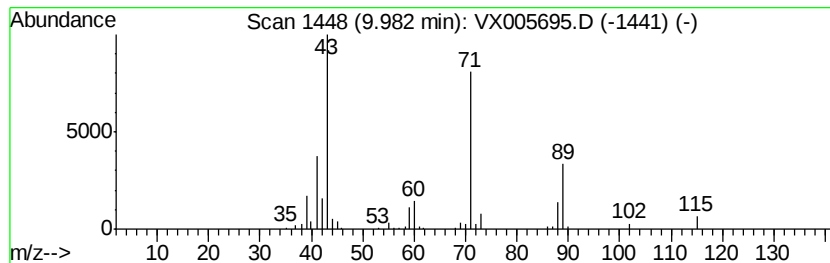
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Peak Number 2 Butanoic acid, 1-methylethy... Concentration Rank 2

| R.T. | EstConc   | Area  | Relative to ISTD | R.T.  |
|------|-----------|-------|------------------|-------|
| 9.98 | 5.66 ug/l | 98759 | Chlorobenzene-d5 | 10.12 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Butanoic acid, 1-methylethyl ester  | 130 | C7H14O2 | 000638-11-9 | 90   |
| 2    |    | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 72   |
| 3    |    | Butanoic acid, propyl ester         | 130 | C7H14O2 | 000105-66-8 | 59   |
| 4    |    | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 56   |
| 5    |    | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2 | 000097-85-8 | 53   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |      |         |       |          | #                     | RT    | Resp   | Conc |
| n-Propyl acetate     | 7.88 | 13.7    | ug/l  | 209956   | 2                     | 6.86  | 767596 | 50.0 |
| Butanoic acid, 1-... | 9.98 | 5.7     | ug/l  | 98759    | 3                     | 10.12 | 872476 | 50.0 |