

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010422\  
 Data File : VX026271.D  
 Acq On : 04 Jan 2022 15:04  
 Operator : JC/MD  
 Sample : M5328-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 20938

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\82X123021W.M  
 Title : SW846 8260

Signal : TIC: VX026271.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         | 2.380       | 203           | 212         | 222          | rBV      | 24043          | 40699         | 4.90%           | 0.744%        |
| 2         | 2.532       | 230           | 237         | 247          | rBV      | 10931          | 22349         | 2.69%           | 0.409%        |
| 3         | 2.953       | 299           | 306         | 317          | rBV      | 5757           | 13835         | 1.66%           | 0.253%        |
| 4         | 4.233       | 508           | 516         | 529          | rBV2     | 17291          | 47071         | 5.66%           | 0.860%        |
| 5         | 4.556       | 558           | 569         | 584          | rBV2     | 14160          | 42387         | 5.10%           | 0.775%        |
| 6         | 5.391       | 694           | 706         | 721          | rBV2     | 97807          | 285922        | 34.39%          | 5.227%        |
| 7         | 5.556       | 721           | 733         | 748          | rVB      | 168337         | 472256        | 56.80%          | 8.633%        |
| 8         | 5.958       | 789           | 799         | 809          | rBV      | 115326         | 309504        | 37.23%          | 5.658%        |
| 9         | 6.037       | 809           | 812         | 824          | rVB2     | 10117          | 25225         | 3.03%           | 0.461%        |
| 10        | 6.763       | 920           | 931         | 945          | rBV      | 267527         | 633489        | 76.20%          | 11.580%       |
| 11        | 8.653       | 1234          | 1241        | 1248         | rVV      | 515721         | 831384        | 100.00%         | 15.198%       |
| 12        | 8.720       | 1248          | 1252        | 1259         | rVB      | 25398          | 39718         | 4.78%           | 0.726%        |
| 13        | 10.055      | 1465          | 1471        | 1483         | rBV      | 535142         | 717343        | 86.28%          | 13.113%       |
| 14        | 10.195      | 1491          | 1494        | 1500         | rVB      | 6369           | 8466          | 1.02%           | 0.155%        |
| 15        | 10.299      | 1503          | 1511        | 1517         | rVB      | 25791          | 35644         | 4.29%           | 0.652%        |
| 16        | 10.506      | 1541          | 1545        | 1553         | rBV      | 13115          | 16889         | 2.03%           | 0.309%        |
| 17        | 10.646      | 1563          | 1568        | 1572         | rBV2     | 13101          | 20187         | 2.43%           | 0.369%        |
| 18        | 10.756      | 1581          | 1586        | 1601         | rBV      | 22341          | 35915         | 4.32%           | 0.657%        |
| 19        | 11.079      | 1634          | 1639        | 1645         | rBV      | 413198         | 536633        | 64.55%          | 9.810%        |
| 20        | 11.134      | 1645          | 1648        | 1654         | rVB      | 13062          | 17714         | 2.13%           | 0.324%        |
| 21        | 11.427      | 1691          | 1696        | 1699         | rBV      | 12797          | 16941         | 2.04%           | 0.310%        |
| 22        | 11.573      | 1715          | 1720        | 1723         | rBV      | 14883          | 21633         | 2.60%           | 0.395%        |
| 23        | 11.610      | 1723          | 1726        | 1734         | rVB3     | 13150          | 21166         | 2.55%           | 0.387%        |
| 24        | 11.750      | 1745          | 1749        | 1754         | rVB      | 8487           | 10567         | 1.27%           | 0.193%        |
| 25        | 11.829      | 1756          | 1762        | 1765         | rBV3     | 7740           | 12971         | 1.56%           | 0.237%        |
| 26        | 11.872      | 1765          | 1769        | 1778         | rVV      | 39319          | 64699         | 7.78%           | 1.183%        |
| 27        | 11.957      | 1778          | 1783        | 1787         | rVV      | 13633          | 21470         | 2.58%           | 0.392%        |
| 28        | 12.024      | 1788          | 1794        | 1801         | rVV      | 521864         | 653978        | 78.66%          | 11.955%       |
| 29        | 12.219      | 1821          | 1826        | 1837         | rBV2     | 142673         | 234310        | 28.18%          | 4.283%        |
| 30        | 12.311      | 1838          | 1841        | 1852         | rVV7     | 6349           | 15939         | 1.92%           | 0.291%        |
| 31        | 12.414      | 1854          | 1858        | 1863         | rVB2     | 9359           | 12644         | 1.52%           | 0.231%        |
| 32        | 13.292      | 1998          | 2002        | 2008         | rVB3     | 9505           | 12774         | 1.54%           | 0.234%        |
| 33        | 13.774      | 2074          | 2081        | 2088         | rVB      | 29821          | 39687         | 4.77%           | 0.725%        |
| 34        | 13.847      | 2088          | 2093        | 2100         | rBV      | 35911          | 58726         | 7.06%           | 1.074%        |
| 35        | 13.914      | 2100          | 2104        | 2121         | rVB      | 38432          | 70460         | 8.48%           | 1.288%        |
| 36        | 14.640      | 2218          | 2223        | 2231         | rVB      | 18567          | 24862         | 2.99%           | 0.454%        |

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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
20938

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\82X123021W.M  
Title : SW846 8260

|    |        |      |      |      |     |       |       |       |        |
|----|--------|------|------|------|-----|-------|-------|-------|--------|
| 37 | 14.780 | 2241 | 2246 | 2252 | rBV | 19463 | 24921 | 3.00% | 0.456% |
|----|--------|------|------|------|-----|-------|-------|-------|--------|

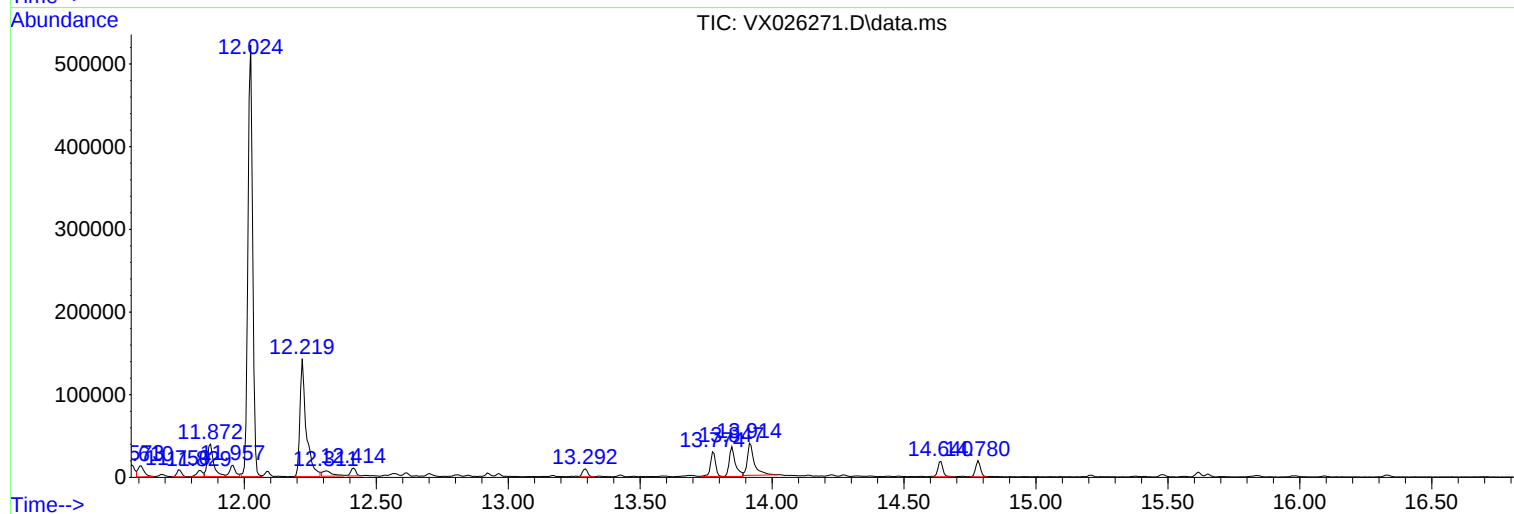
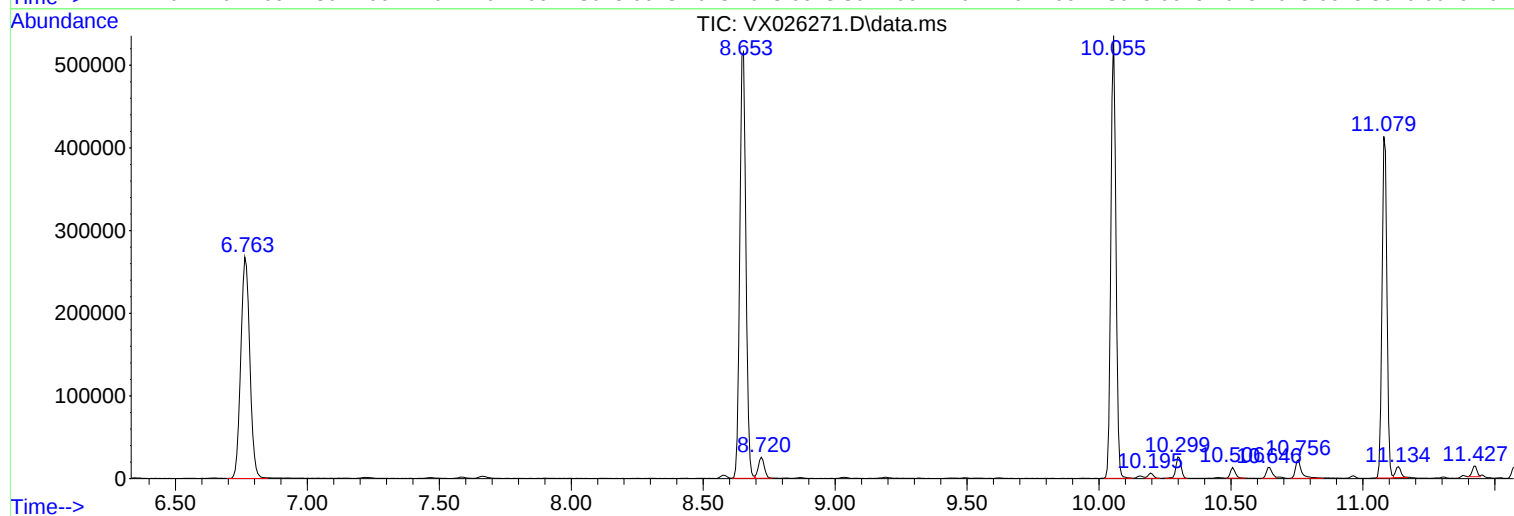
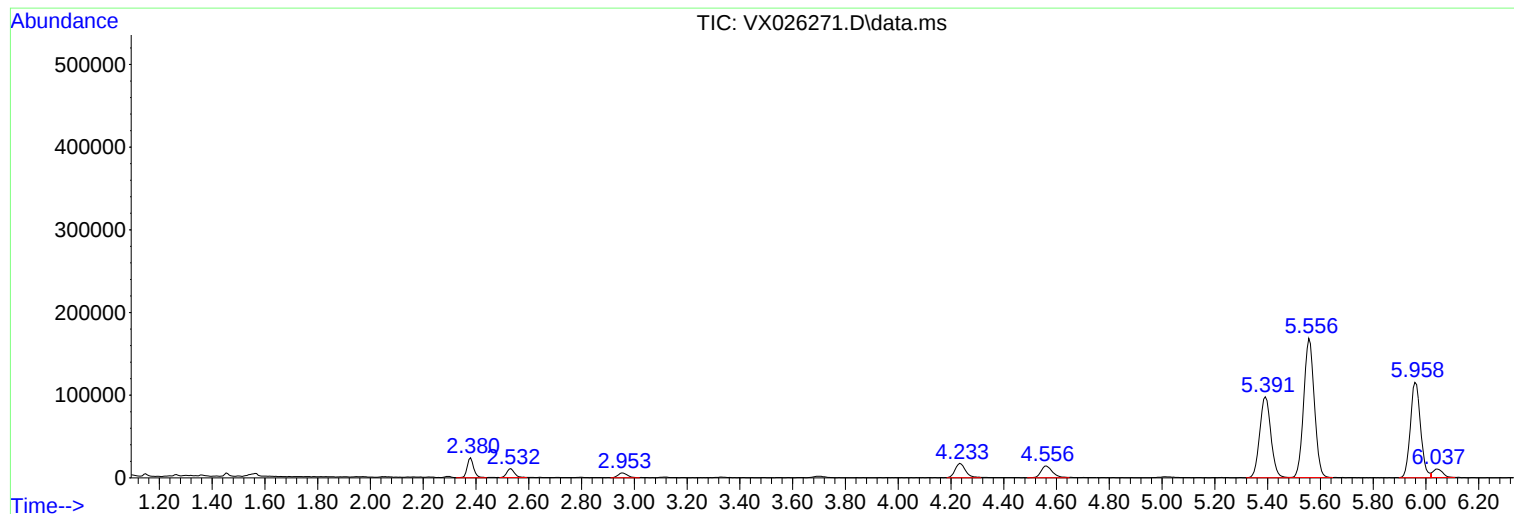
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X123021W.M  
Quant Title : SW846 8260

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X123021W.M  
Quant Title : SW846 8260

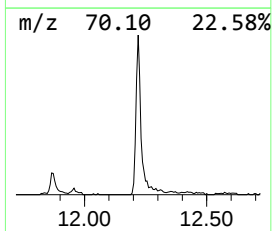
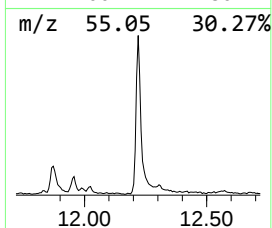
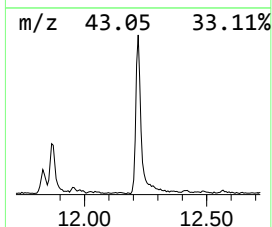
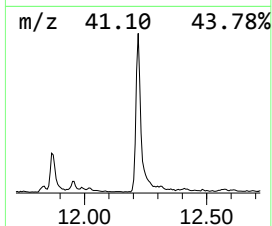
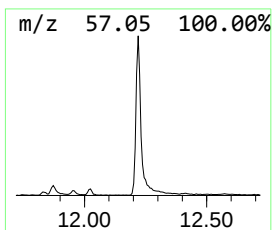
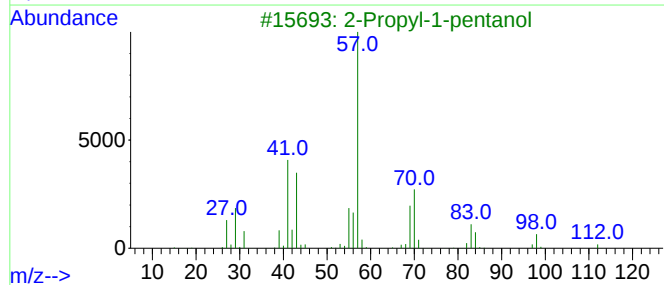
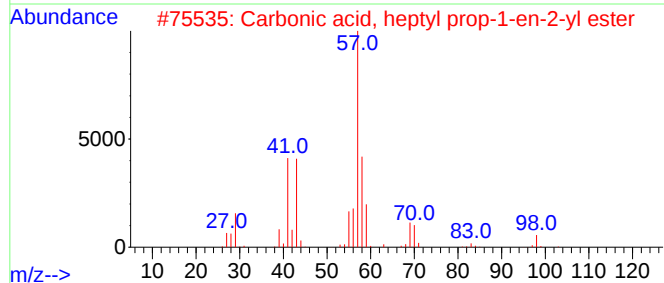
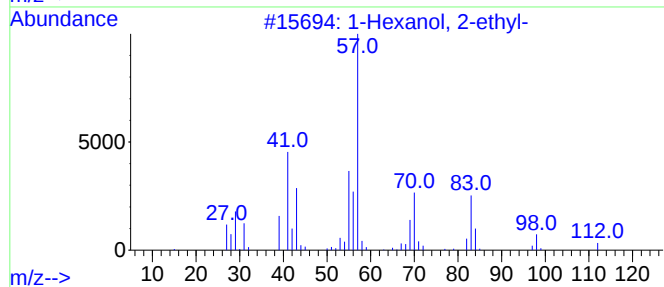
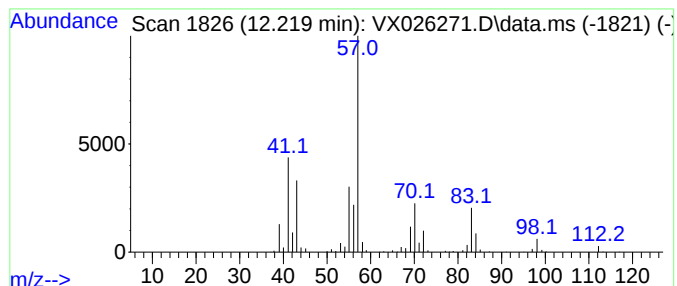
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 12.219 | 17.91 ug/l | 234310 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O   | 000104-76-7  | 72   |
| 2    |    |   | Carbonic acid, heptyl prop-1-en-... | 200 | C11H20O3 | 1000382-54-1 | 47   |
| 3    |    |   | 2-Propyl-1-pentanol                 | 130 | C8H18O   | 058175-57-8  | 47   |
| 4    |    |   | Carbonic acid, heptyl vinyl ester   | 186 | C10H18O3 | 1010383-25-4 | 43   |
| 5    |    |   | Octane, 2,3-dimethyl-               | 142 | C10H22   | 007146-60-3  | 42   |



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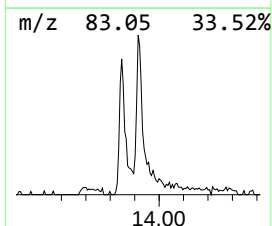
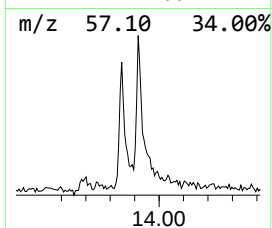
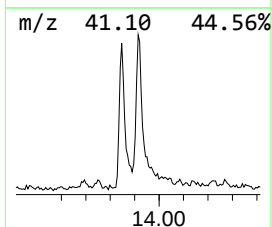
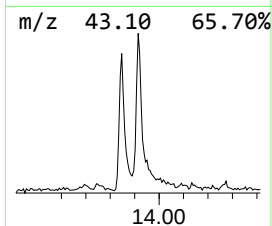
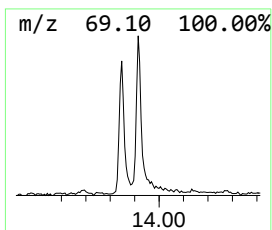
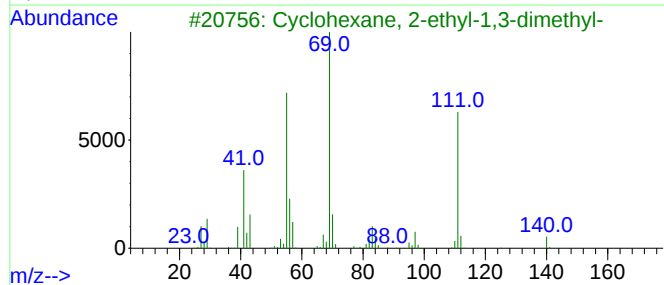
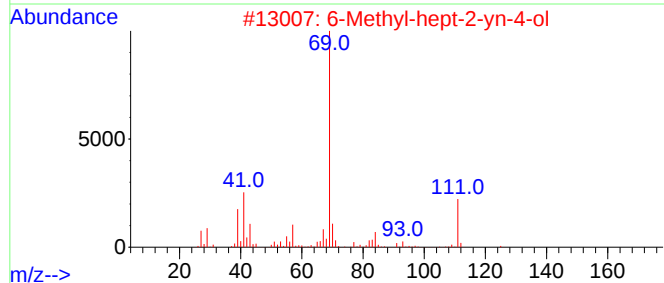
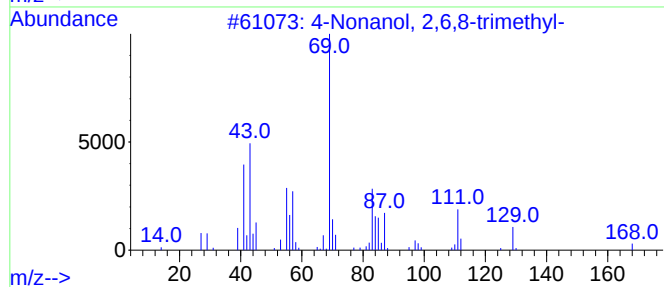
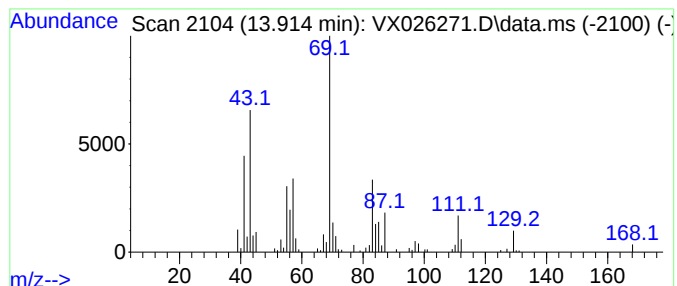
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X123021W.M  
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TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 4-Nonanol, 2,6,8-trimethyl- Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.914 | 5.39 ug/l | 70460 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Nonanol, 2,6,8-trimethyl-          | 186 | C12H26O | 000123-17-1 | 90   |
| 2    |    |   | 6-Methyl-hept-2-yn-4-ol              | 126 | C8H14O  | 060018-69-1 | 47   |
| 3    |    |   | Cyclohexane, 2-ethyl-1,3-dimethyl-   | 140 | C10H20  | 007045-67-2 | 47   |
| 4    |    |   | Cyclopropanecarboxylic acid, buty... | 142 | C8H14O2 | 054947-39-6 | 47   |
| 5    |    |   | 3-Ethyl-4-octene                     | 140 | C10H20  | 019781-32-9 | 47   |



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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 |
| 1-Hexanol, 2-et... | 12.219 | 17.9    | ug/l  | 234310   | 4                     | 12.024 | 653978 | 50.0 |
| 4-Nonanol, 2,6,... | 13.914 | 5.4     | ug/l  | 70460    | 4                     | 12.024 | 653978 | 50.0 |