

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120721\  
 Data File : VX025596.D  
 Acq On : 07 Dec 2021 23:07  
 Operator : JC/MD  
 Sample : M4886-14ME  
 Misc : 4.06g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 33 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX893ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

Signal : TIC: VX025596.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         | 1.239       | 22            | 25          | 32           | rBV2     | 4190           | 7686          | 1.47%           | 0.168%        |
| 2         | 1.367       | 43            | 46          | 55           | rVB      | 64981          | 74367         | 14.26%          | 1.623%        |
| 3         | 1.648       | 88            | 92          | 98           | rBV      | 38046          | 44774         | 8.58%           | 0.977%        |
| 4         | 2.282       | 189           | 196         | 206          | rBV      | 114733         | 190976        | 36.62%          | 4.167%        |
| 5         | 2.794       | 272           | 280         | 285          | rBV5     | 1154           | 2347          | 0.45%           | 0.051%        |
| 6         | 2.946       | 298           | 305         | 315          | rBV      | 4744           | 12428         | 2.38%           | 0.271%        |
| 7         | 3.410       | 379           | 381         | 384          | rBV2     | 127            | 135           | 0.03%           | 0.003%        |
| 8         | 3.459       | 388           | 389         | 391          | rVV      | 176            | 81            | 0.02%           | 0.002%        |
| 9         | 3.611       | 412           | 414         | 416          | rVB2     | 136            | 87            | 0.02%           | 0.002%        |
| 10        | 4.172       | 504           | 506         | 507          | rBV      | 148            | 82            | 0.02%           | 0.002%        |
| 11        | 4.263       | 519           | 521         | 523          | rBV2     | 101            | 93            | 0.02%           | 0.002%        |
| 12        | 4.367       | 536           | 538         | 541          | rBV2     | 119            | 132           | 0.03%           | 0.003%        |
| 13        | 4.489       | 548           | 558         | 587          | rVV2     | 21704          | 100455        | 19.26%          | 2.192%        |
| 14        | 5.068       | 639           | 653         | 670          | rBV      | 62836          | 198841        | 38.13%          | 4.338%        |
| 15        | 5.257       | 683           | 684         | 685          | rBV      | 157            | 104           | 0.02%           | 0.002%        |
| 16        | 5.312       | 691           | 693         | 695          | rVB      | 138            | 89            | 0.02%           | 0.002%        |
| 17        | 5.446       | 713           | 715         | 716          | rBV2     | 279            | 220           | 0.04%           | 0.005%        |
| 18        | 5.543       | 729           | 731         | 734          | rBV      | 188            | 151           | 0.03%           | 0.003%        |
| 19        | 5.617       | 741           | 743         | 744          | rBV      | 137            | 86            | 0.02%           | 0.002%        |
| 20        | 5.678       | 750           | 753         | 754          | rBV      | 115            | 108           | 0.02%           | 0.002%        |
| 21        | 5.726       | 759           | 761         | 762          | rBV      | 136            | 96            | 0.02%           | 0.002%        |
| 22        | 5.806       | 773           | 774         | 776          | rBV      | 103            | 82            | 0.02%           | 0.002%        |
| 23        | 5.970       | 789           | 801         | 815          | rBV2     | 181682         | 521540        | 100.00%         | 11.379%       |
| 24        | 6.190       | 836           | 837         | 842          | rVB2     | 200            | 198           | 0.04%           | 0.004%        |
| 25        | 6.232       | 842           | 844         | 845          | rVB2     | 129            | 90            | 0.02%           | 0.002%        |
| 26        | 6.251       | 845           | 847         | 848          | rBV      | 183            | 124           | 0.02%           | 0.003%        |
| 27        | 6.367       | 858           | 866         | 878          | rBV4     | 2010           | 6680          | 1.28%           | 0.146%        |
| 28        | 6.568       | 897           | 899         | 900          | rVB2     | 149            | 92            | 0.02%           | 0.002%        |
| 29        | 6.702       | 919           | 921         | 922          | rBV      | 122            | 90            | 0.02%           | 0.002%        |
| 30        | 6.763       | 922           | 931         | 946          | rVV      | 122061         | 309554        | 59.35%          | 6.754%        |
| 31        | 7.129       | 981           | 991         | 1001         | rBV      | 88966          | 199600        | 38.27%          | 4.355%        |
| 32        | 7.311       | 1013          | 1021        | 1038         | rVB2     | 96761          | 232488        | 44.58%          | 5.073%        |
| 33        | 7.458       | 1044          | 1045        | 1047         | rBV      | 125            | 97            | 0.02%           | 0.002%        |
| 34        | 7.488       | 1047          | 1050        | 1051         | rVB      | 191            | 177           | 0.03%           | 0.004%        |
| 35        | 7.549       | 1058          | 1060        | 1061         | rBV2     | 112            | 83            | 0.02%           | 0.002%        |
| 36        | 7.714       | 1086          | 1087        | 1090         | rVB      | 98             | 81            | 0.02%           | 0.002%        |

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 ALS Vial : 33 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX893ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMXLM112221WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 7.775  | 1095 | 1097 | 1102 | rVB3 | 250    | 286    | 0.05%  | 0.006% |
| 38 | 7.824  | 1102 | 1105 | 1108 | rBV3 | 216    | 287    | 0.06%  | 0.006% |
| 39 | 7.848  | 1108 | 1109 | 1111 | rBV  | 190    | 122    | 0.02%  | 0.003% |
| 40 | 7.958  | 1124 | 1127 | 1128 | rBV2 | 423    | 378    | 0.07%  | 0.008% |
| 41 | 8.080  | 1146 | 1147 | 1150 | rVB  | 156    | 128    | 0.02%  | 0.003% |
| 42 | 8.147  | 1156 | 1158 | 1162 | rVB  | 133    | 147    | 0.03%  | 0.003% |
| 43 | 8.177  | 1162 | 1163 | 1165 | rBV  | 115    | 83     | 0.02%  | 0.002% |
| 44 | 8.195  | 1165 | 1166 | 1169 | rBV2 | 80     | 87     | 0.02%  | 0.002% |
| 45 | 8.275  | 1176 | 1179 | 1181 | rBV  | 227    | 263    | 0.05%  | 0.006% |
| 46 | 8.330  | 1181 | 1188 | 1201 | rVB  | 57041  | 105389 | 20.21% | 2.299% |
| 47 | 8.604  | 1229 | 1233 | 1234 | rBV2 | 410    | 538    | 0.10%  | 0.012% |
| 48 | 8.653  | 1234 | 1241 | 1249 | rVV  | 263623 | 439551 | 84.28% | 9.590% |
| 49 | 8.720  | 1249 | 1252 | 1258 | rVB  | 3789   | 5789   | 1.11%  | 0.126% |
| 50 | 8.909  | 1282 | 1283 | 1285 | rBV  | 158    | 104    | 0.02%  | 0.002% |
| 51 | 8.958  | 1285 | 1291 | 1301 | rVV  | 36785  | 66071  | 12.67% | 1.442% |
| 52 | 9.055  | 1305 | 1307 | 1311 | rBV  | 127    | 167    | 0.03%  | 0.004% |
| 53 | 9.275  | 1337 | 1343 | 1357 | rBV  | 276294 | 404473 | 77.55% | 8.825% |
| 54 | 9.396  | 1357 | 1363 | 1376 | rBV  | 135180 | 223830 | 42.92% | 4.884% |
| 55 | 9.561  | 1388 | 1390 | 1393 | rVB3 | 566    | 659    | 0.13%  | 0.014% |
| 56 | 9.616  | 1396 | 1399 | 1404 | rVB  | 765    | 1034   | 0.20%  | 0.023% |
| 57 | 9.713  | 1410 | 1415 | 1418 | rBV3 | 663    | 1008   | 0.19%  | 0.022% |
| 58 | 9.768  | 1422 | 1424 | 1427 | rBV2 | 109    | 81     | 0.02%  | 0.002% |
| 59 | 10.061 | 1466 | 1472 | 1481 | rBV  | 251964 | 363904 | 69.77% | 7.940% |
| 60 | 10.201 | 1492 | 1495 | 1499 | rVB2 | 403    | 483    | 0.09%  | 0.011% |
| 61 | 10.274 | 1505 | 1507 | 1509 | rBV  | 92     | 95     | 0.02%  | 0.002% |
| 62 | 10.311 | 1509 | 1513 | 1518 | rVB2 | 1283   | 2036   | 0.39%  | 0.044% |
| 63 | 10.360 | 1518 | 1521 | 1524 | rBV2 | 480    | 594    | 0.11%  | 0.013% |
| 64 | 10.402 | 1527 | 1528 | 1531 | rBV2 | 119    | 98     | 0.02%  | 0.002% |
| 65 | 10.591 | 1555 | 1559 | 1560 | rBV2 | 185    | 191    | 0.04%  | 0.004% |
| 66 | 10.646 | 1564 | 1568 | 1576 | rVV  | 822    | 1111   | 0.21%  | 0.024% |
| 67 | 10.780 | 1583 | 1590 | 1593 | rVB3 | 585    | 872    | 0.17%  | 0.019% |
| 68 | 10.860 | 1599 | 1603 | 1605 | rBV4 | 359    | 364    | 0.07%  | 0.008% |
| 69 | 10.896 | 1605 | 1609 | 1614 | rVB3 | 553    | 741    | 0.14%  | 0.016% |
| 70 | 10.963 | 1617 | 1620 | 1624 | rVV2 | 202    | 294    | 0.06%  | 0.006% |
| 71 | 11.030 | 1628 | 1631 | 1635 | rVB2 | 286    | 385    | 0.07%  | 0.008% |
| 72 | 11.122 | 1642 | 1646 | 1651 | rVB  | 4050   | 5202   | 1.00%  | 0.113% |
| 73 | 11.195 | 1653 | 1658 | 1666 | rBV  | 176485 | 235240 | 45.10% | 5.133% |
| 74 | 11.280 | 1670 | 1672 | 1673 | rVV2 | 531    | 550    | 0.11%  | 0.012% |
| 75 | 11.311 | 1674 | 1677 | 1683 | rVB3 | 2691   | 4125   | 0.79%  | 0.090% |
| 76 | 11.384 | 1686 | 1689 | 1697 | rVB2 | 739    | 847    | 0.16%  | 0.018% |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 EX893ME

Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

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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\SFAMXML112221WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |        |
|-----|--------|------|------|------|------|--------|--------|--------|--------|
| 77  | 11.475 | 1701 | 1704 | 1707 | rBV2 | 1317   | 1820   | 0.35%  | 0.040% |
| 78  | 11.549 | 1713 | 1716 | 1720 | rVB3 | 680    | 635    | 0.12%  | 0.014% |
| 79  | 11.585 | 1720 | 1722 | 1725 | rBV2 | 82     | 101    | 0.02%  | 0.002% |
| 80  | 11.622 | 1725 | 1728 | 1733 | rBV2 | 463    | 624    | 0.12%  | 0.014% |
| 81  | 11.719 | 1741 | 1744 | 1746 | rBV  | 913    | 1061   | 0.20%  | 0.023% |
| 82  | 11.750 | 1746 | 1749 | 1753 | rVB2 | 3759   | 4756   | 0.91%  | 0.104% |
| 83  | 11.841 | 1761 | 1764 | 1769 | rVB2 | 724    | 898    | 0.17%  | 0.020% |
| 84  | 11.896 | 1769 | 1773 | 1776 | rVB2 | 351    | 471    | 0.09%  | 0.010% |
| 85  | 11.939 | 1776 | 1780 | 1783 | rBV2 | 2044   | 2981   | 0.57%  | 0.065% |
| 86  | 11.969 | 1783 | 1785 | 1789 | rVB4 | 389    | 315    | 0.06%  | 0.007% |
| 87  | 12.024 | 1789 | 1794 | 1800 | rBV  | 301143 | 372966 | 71.51% | 8.138% |
| 88  | 12.128 | 1808 | 1811 | 1812 | rBV2 | 1285   | 1208   | 0.23%  | 0.026% |
| 89  | 12.152 | 1812 | 1815 | 1821 | rVB2 | 3016   | 3965   | 0.76%  | 0.087% |
| 90  | 12.262 | 1826 | 1833 | 1834 | rBV3 | 531    | 854    | 0.16%  | 0.019% |
| 91  | 12.323 | 1836 | 1843 | 1850 | rBV  | 321255 | 398996 | 76.50% | 8.705% |
| 92  | 12.426 | 1856 | 1860 | 1864 | rBV2 | 2391   | 3136   | 0.60%  | 0.068% |
| 93  | 12.475 | 1864 | 1868 | 1873 | rVB5 | 1154   | 2359   | 0.45%  | 0.051% |
| 94  | 12.554 | 1880 | 1881 | 1883 | rBV  | 351    | 354    | 0.07%  | 0.008% |
| 95  | 12.762 | 1912 | 1915 | 1920 | rVB4 | 779    | 1162   | 0.22%  | 0.025% |
| 96  | 12.823 | 1922 | 1925 | 1930 | rVB2 | 1595   | 1826   | 0.35%  | 0.040% |
| 97  | 12.987 | 1949 | 1952 | 1957 | rVB4 | 3098   | 3850   | 0.74%  | 0.084% |
| 98  | 13.048 | 1959 | 1962 | 1964 | rBV4 | 1133   | 1246   | 0.24%  | 0.027% |
| 99  | 13.091 | 1967 | 1969 | 1971 | rBV3 | 567    | 620    | 0.12%  | 0.014% |
| 100 | 13.414 | 2019 | 2022 | 2025 | rBV3 | 3716   | 5160   | 0.99%  | 0.113% |

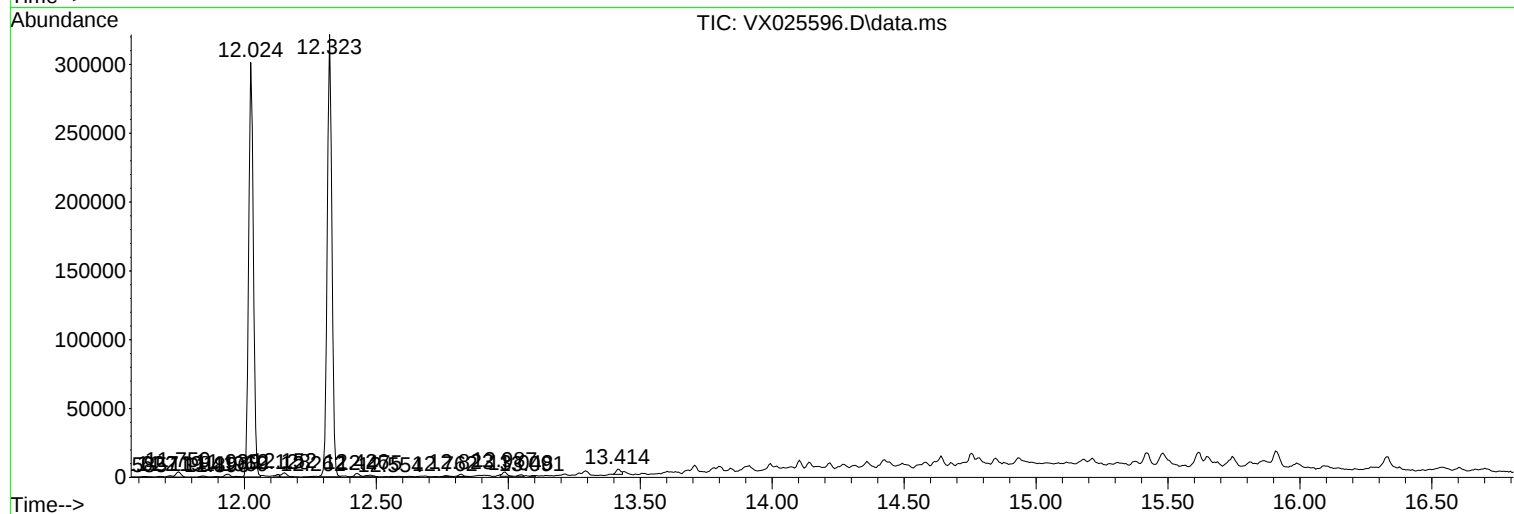
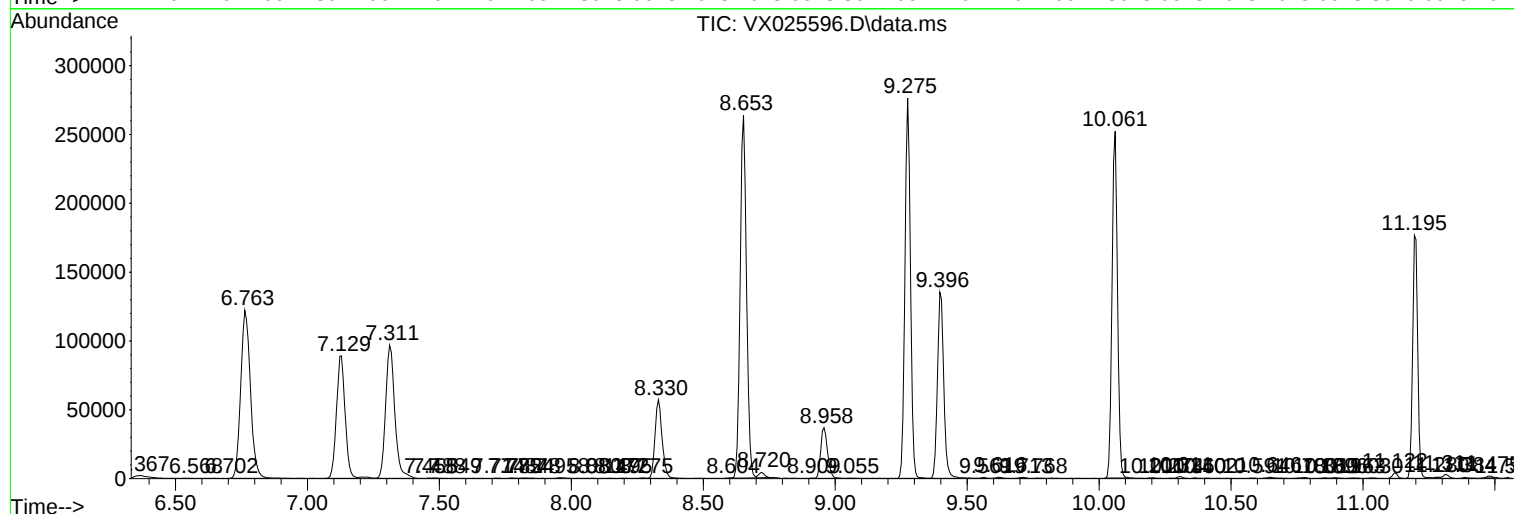
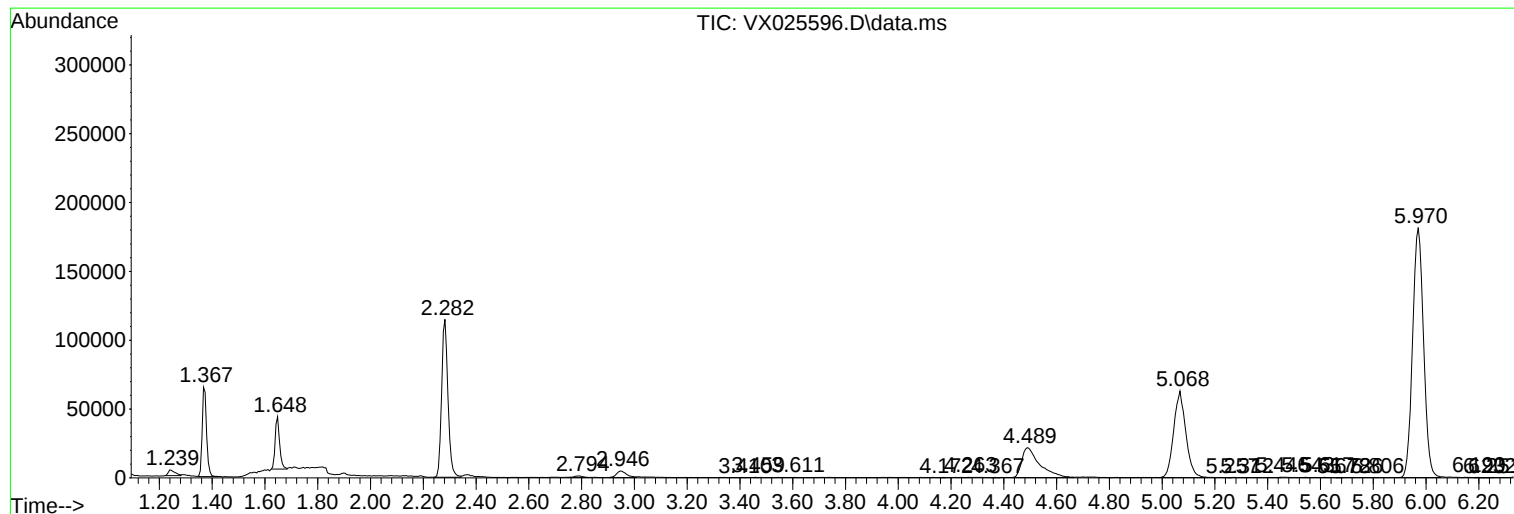
Sum of corrected areas: 4583285

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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
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EX893ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM112221WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120721\  
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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML112221WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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| TIC Top Hit name | RT | EstConc | Units | Response | --Internal Standard-- |    |      |      |
|------------------|----|---------|-------|----------|-----------------------|----|------|------|
|                  |    |         |       |          | #                     | RT | Resp | Conc |