

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX062222\  
 Data File : VX029728.D  
 Acq On : 23 Jun 2022 07:40  
 Operator : JC/MD  
 Sample : N3422-11 40X  
 Misc : 5.76g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 48 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WC-14A-1A-13-GR

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\82X061822W.M  
 Title : SW846 8260

Signal : TIC: VX029728.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         | 2.947       | 296           | 305         | 316          | rBV      | 23878          | 55941         | 4.05%           | 0.660%        |
| 2         | 5.391       | 692           | 706         | 719          | rBV      | 154007         | 451674        | 32.69%          | 5.327%        |
| 3         | 5.556       | 722           | 733         | 751          | rVB      | 292065         | 838296        | 60.68%          | 9.888%        |
| 4         | 5.958       | 788           | 799         | 815          | rBV      | 165635         | 438830        | 31.76%          | 5.176%        |
| 5         | 6.763       | 921           | 931         | 945          | rBV      | 447677         | 1055025       | 76.37%          | 12.444%       |
| 6         | 7.385       | 1024          | 1033        | 1042         | rBV3     | 17501          | 41150         | 2.98%           | 0.485%        |
| 7         | 8.653       | 1234          | 1241        | 1250         | rVB      | 861556         | 1381514       | 100.00%         | 16.295%       |
| 8         | 10.055      | 1465          | 1471        | 1487         | rVB      | 903040         | 1197948       | 86.71%          | 14.130%       |
| 9         | 10.305      | 1500          | 1512        | 1517         | rBV2     | 14691          | 29775         | 2.16%           | 0.351%        |
| 10        | 11.079      | 1634          | 1639        | 1650         | rBV      | 694974         | 909067        | 65.80%          | 10.722%       |
| 11        | 11.195      | 1650          | 1658        | 1660         | rBV7     | 6614           | 14717         | 1.07%           | 0.174%        |
| 12        | 11.384      | 1685          | 1689        | 1693         | rBV      | 8171           | 13945         | 1.01%           | 0.164%        |
| 13        | 11.476      | 1702          | 1704        | 1711         | rVB      | 23388          | 27224         | 1.97%           | 0.321%        |
| 14        | 11.756      | 1746          | 1750        | 1758         | rVB      | 22273          | 36990         | 2.68%           | 0.436%        |
| 15        | 12.024      | 1788          | 1794        | 1800         | rBV      | 914989         | 1170723       | 84.74%          | 13.808%       |
| 16        | 12.085      | 1800          | 1804        | 1811         | rVB3     | 11980          | 27252         | 1.97%           | 0.321%        |
| 17        | 12.268      | 1826          | 1834        | 1837         | rBV3     | 7768           | 18198         | 1.32%           | 0.215%        |
| 18        | 12.317      | 1837          | 1842        | 1848         | rBV5     | 15956          | 28138         | 2.04%           | 0.332%        |
| 19        | 12.427      | 1851          | 1860        | 1863         | rBV      | 38735          | 55013         | 3.98%           | 0.649%        |
| 20        | 12.463      | 1863          | 1866        | 1873         | rVB5     | 9267           | 17218         | 1.25%           | 0.203%        |
| 21        | 12.555      | 1875          | 1881        | 1883         | rBV5     | 10683          | 17597         | 1.27%           | 0.208%        |
| 22        | 12.683      | 1900          | 1902        | 1913         | rVB10    | 11764          | 33521         | 2.43%           | 0.395%        |
| 23        | 12.890      | 1933          | 1936        | 1944         | rVB9     | 10325          | 21835         | 1.58%           | 0.258%        |
| 24        | 12.969      | 1945          | 1949        | 1954         | rVB3     | 14737          | 27765         | 2.01%           | 0.327%        |
| 25        | 13.042      | 1955          | 1961        | 1964         | rBV6     | 9664           | 15054         | 1.09%           | 0.178%        |
| 26        | 13.164      | 1974          | 1981        | 1984         | rBV8     | 8555           | 18134         | 1.31%           | 0.214%        |
| 27        | 13.268      | 1993          | 1998        | 2000         | rBV      | 38095          | 56997         | 4.13%           | 0.672%        |
| 28        | 13.384      | 2014          | 2017        | 2021         | rVB      | 14505          | 17642         | 1.28%           | 0.208%        |
| 29        | 13.579      | 2047          | 2049        | 2057         | rVB6     | 7780           | 13835         | 1.00%           | 0.163%        |
| 30        | 13.676      | 2061          | 2065        | 2068         | rBV4     | 10448          | 17723         | 1.28%           | 0.209%        |
| 31        | 13.841      | 2089          | 2092        | 2099         | rVB5     | 12147          | 18368         | 1.33%           | 0.217%        |
| 32        | 14.042      | 2121          | 2125        | 2127         | rBV      | 15200          | 17983         | 1.30%           | 0.212%        |
| 33        | 14.213      | 2150          | 2153        | 2159         | rVB5     | 17780          | 28884         | 2.09%           | 0.341%        |
| 34        | 14.481      | 2194          | 2197        | 2206         | rVB10    | 10507          | 27348         | 1.98%           | 0.323%        |
| 35        | 14.640      | 2216          | 2223        | 2226         | rBV5     | 35696          | 71380         | 5.17%           | 0.842%        |
| 36        | 14.756      | 2239          | 2242        | 2244         | rVV2     | 14939          | 19850         | 1.44%           | 0.234%        |

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MSVOA\_X  
ClientSampleId :  
WC-14A-1A-13-GR

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\82X061822W.M  
Title : SW846 8260

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 37 | 14.780 | 2244 | 2246 | 2250 | rVV2 | 19335 | 24501 | 1.77% | 0.289% |
| 38 | 14.914 | 2264 | 2268 | 2274 | rVB9 | 12024 | 28617 | 2.07% | 0.338% |
| 39 | 15.377 | 2341 | 2344 | 2348 | rBV6 | 13219 | 18406 | 1.33% | 0.217% |
| 40 | 15.481 | 2356 | 2361 | 2366 | rBV3 | 20658 | 34086 | 2.47% | 0.402% |
| 41 | 15.615 | 2378 | 2383 | 2386 | rBV  | 23377 | 36147 | 2.62% | 0.426% |
| 42 | 15.652 | 2386 | 2389 | 2396 | rVB3 | 26553 | 45234 | 3.27% | 0.534% |
| 43 | 16.347 | 2501 | 2503 | 2513 | rVB6 | 7669  | 15067 | 1.09% | 0.178% |
| 44 | 16.591 | 2540 | 2543 | 2550 | rVB4 | 13544 | 25333 | 1.83% | 0.299% |
| 45 | 16.652 | 2550 | 2553 | 2560 | rVB2 | 9843  | 18393 | 1.33% | 0.217% |

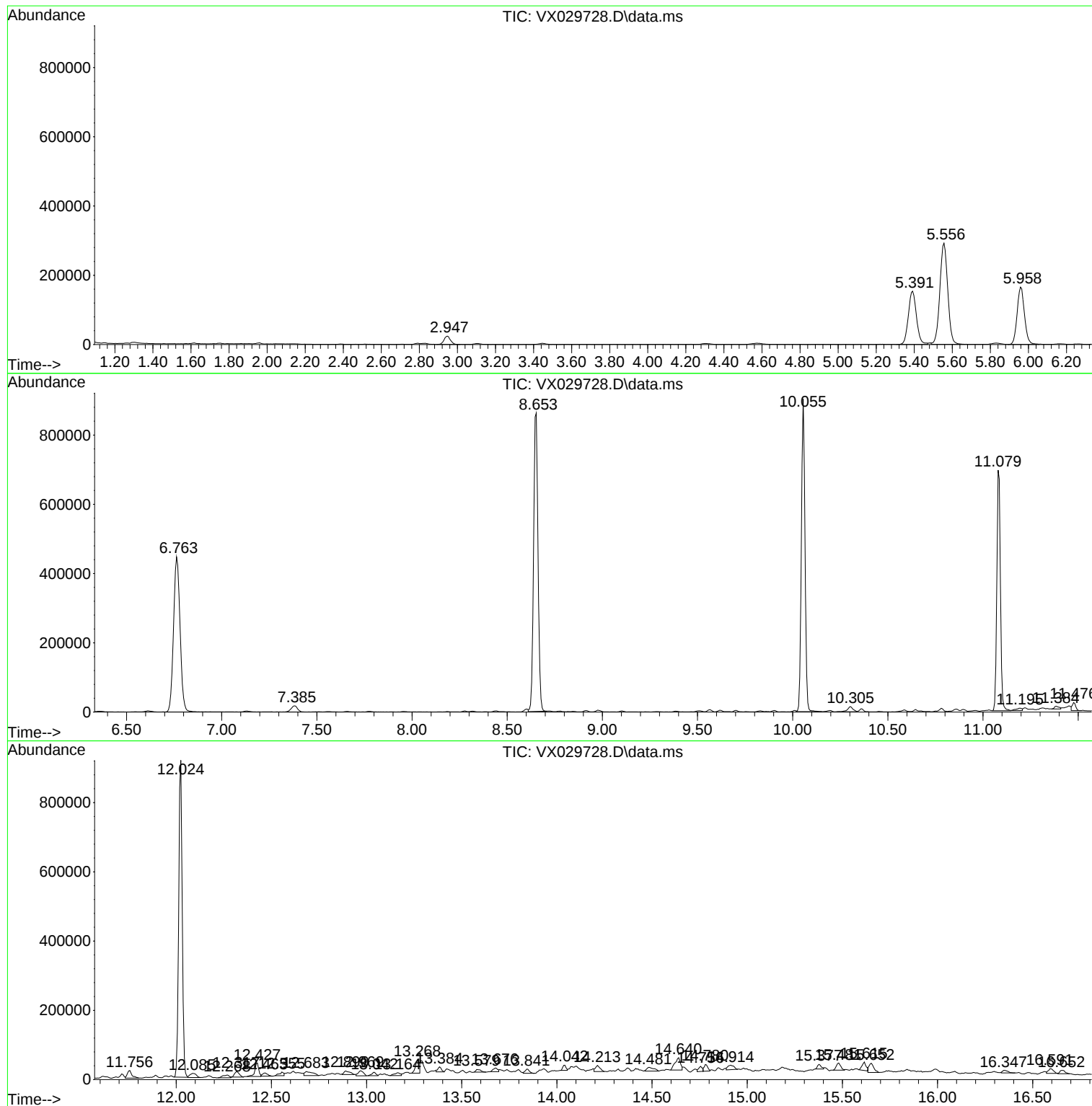
Sum of corrected areas: 8478338

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WC-14A-1A-13-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

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



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Instrument :  
MSVOA\_X  
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WC-14A-1A-13-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

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

No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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