# **Library Search Results - NonTarget Hits with Details**



D:\MassHunter\GCMS\1\data\RBEL\240501 scan **Batch Path** 

240502 data.uaf **Analysis File Name** 

**Analyst Name** admin **Analysis Time** 5/2/2024 11:31:09 AM

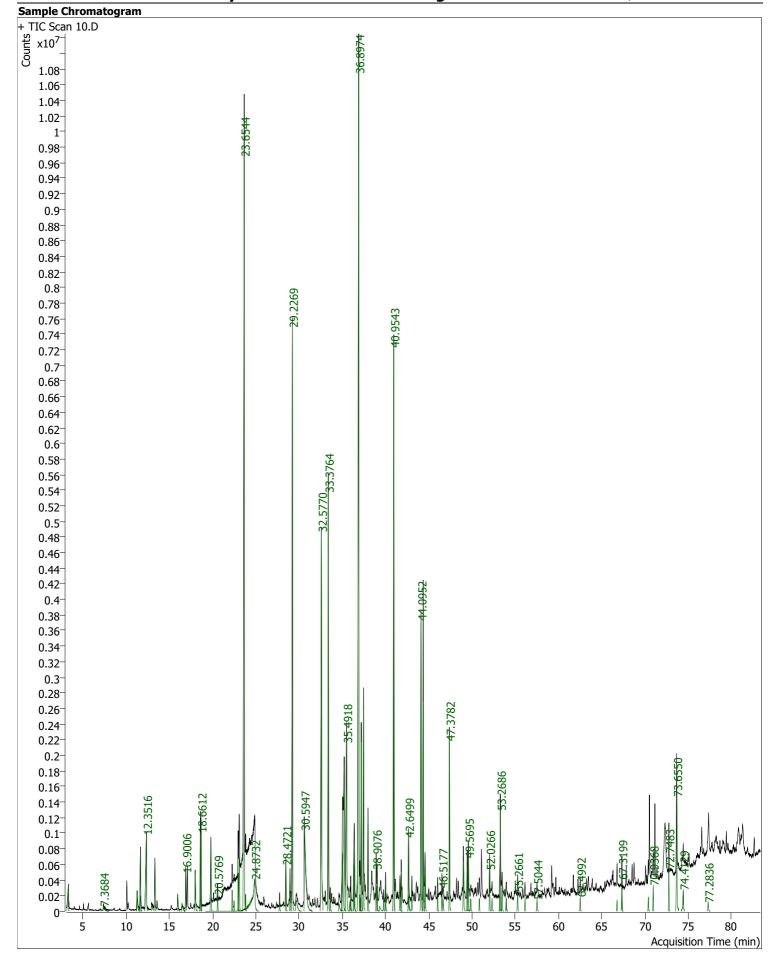
D:\MassHunter\GCMS\1\data\RBEL\240501 scan **File Name** 10.D **Path Name Sample Name** 10 **Sample Type** Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

Acq. Date-Time 5/2/2024 1:43:25 AM **Instrument Name** GCMSD Dil. 1

| Component R1       | Compound Name  | CAS#                       | Formula           | Component<br>Area      | Match Factor | Estimated<br>Conc. |
|--------------------|--|----------------------------|-------------------|------------------------|--------------|--------------------|
| 3.3277             | Propanoic acid   | 79-09-4                    | C3H6O2            | 1876986.6              | 98.8         |                    |
| 7.3684             | 1,3-Propanediol  | 504-63-2                   | C3H8O2            | 638257.5               | 92.2         |                    |
| 11.2838            | Ethanol, 2,2'-oxybis-  | 111-46-6                   | C4H10O3           | 1225358.3              | 84.1         |                    |
| 11.2850            | 1,2-Propanediol, 3-methoxy-  | 623-39-2                   | C4H10O3           | 1566273.2              | 87.9         |                    |
| 11.6559            | Propane, 1,1-diethoxy-   | 4744-08-5                  | C7H16O2           | 3635474.5              | 78.6         |                    |
| 11.6572            | Oxazolidin-2-one   | 497-25-6                   | C3H5NO2           | 965736.2               | 77.1         |                    |
| 12.3516            | Butyrolactone  | 96-48-0                    | C4H6O2            | 7168594.3              | 97.6         |                    |
| 12.9337            | Propanoic acid, 2-hydroxy-, ethyl ester  | 97-64-3                    | C5H10O3           | 680886.6               | 75.0         |                    |
| 13.3285            | Propane, 1,1-diethoxy-   | 4744-08-5                  | C7H16O2           | 2900302.0              | 79.9         |                    |
| 15.9672            | 2-Cyclopenten-1-one, 3-methyl-   | 2758-18-1                  | C6H8O             | 936447.1               | 96.6         |                    |
| 16.4652            | Glycerol triethyl ether  | 162614-45-1                | C9H20O3           | 783260.3               | 76.1         |                    |
| 16.9006            | 1,3-Dioxolane-4-methanol, 2-ethyl-   | 53951-44-3                 | C6H12O3           | 2038169.3              | 85.3         |                    |
| 17.9862            | Phenol   | 108-95-2                   | C6H6O             | 2231714.0              | 98.1         |                    |
| 18.5959            | 1,3-Dioxolane-4-methanol, 2-ethyl-   | 53951-44-3                 | C6H12O3           | 4191906.0              | 78.0         |                    |
| 18.6597            | Hydrogen isocyanate  | 75-13-8                    | CHNO              | 1824018.7              | 83.3         |                    |
| 18.6612            | Diisoamyl ether  | 544-01-4                   | C10H22O           | 3829017.6              | 93.7         |                    |
| 19.8045            | 1,3-Dioxolane-4-methanol, 2-ethyl-   | 53951-44-3                 | C6H12O3           | 3513208.8              | 94.6         |                    |
| 20.5769<br>22.2583 | 2-Cyclopenten-1-one, 2,3-dimethyl-   | 1121-05-7                  | C7H10O            | 910291.4               | 93.1         |                    |
|                    | Phenol, 2-methyl-  | 95-48-7                    | C7H8O             | 1099911.1              | 92.8         |                    |
| 22.4821            | Pentanoic acid, 4-oxo-, ethyl ester  | 539-88-8                   | C7H12O3           | 752274.2               | 84.4         |                    |
| 22.9536<br>23.0790 | 1-Propanol, 2-(2-hydroxypropoxy)-  1-Octanol   | 106-62-7<br>111-87-5       | C6H14O3<br>C8H18O | 1925931.2<br>3801554.6 | 78.5<br>97.0 |                    |
| 23.6544            | Phenol, 2-methoxy-   | 90-05-1                    | C7H8O2            | 50811022.5             | 98.7         |                    |
| 23.8234            | Ethanone, 1-(2-thienyl)-   | 88-15-3                    | C6H6OS            | 759996.2               | 95.0         |                    |
| 24.8732            | 1,2,3-Propanetriol, 1-acetate  | 106-61-6                   | C5H10O4           | 10507411.6             | 82.9         |                    |
| 27.7392            | Propanal ethyl isopentyl acetal  | 1000431-61-6               | C10H22O2          | 636176.4               | 77.5         |                    |
| 28.4721            | 2-Methoxy-5-methylphenol   | 1195-09-1                  | C8H10O2           | 2247290.6              | 95.4         |                    |
| 28.9479            | 2-Methoxy-5-methylphenol   | 1195-09-1                  | C8H10O2           | 1674696.1              | 97.7         |                    |
| 29.2269            | 2-Methoxy-5-methylphenol   | 1195-09-1                  | C8H10O2           | 32479725.7             | 99.1         |                    |
| 29.6703            | Alpha-monopropionin  | 624-47-5                   | C6H12O4           | 1842333.7              | 84.2         |                    |
| 30.5947            | Catechol   | 120-80-9                   | C6H6O2            | 12897459.7             | 89.1         |                    |
| 32.5770            | 1,2-Benzenediol, 3-methoxy-  | 934-00-9                   | C7H8O3            | 27470676.7             | 97.0         |                    |
| 33.3764            | Phenol, 4-ethyl-2-methoxy-   | 2785-89-9                  | C9H12O2           | 21501433.2             | 96.8         |                    |
| 33.6112            | Phenol, 4-ethyl-2-methoxy-   | 2785-89-9                  | C9H12O2           | 677129.8               | 78.4         |                    |
| 34.6294            | Hydroquinone   | 123-31-9                   | C6H6O2            | 768580.4               | 81.3         |                    |
| 35.0235            | 1,2-Benzenediol, 4-methyl-   | 452-86-8                   | C7H8O2            | 6420675.4              | 94.2         |                    |
| 35.2112            | Butanoic acid, anhydride   | 106-31-0                   | C8H14O3           | 15434879.8             | 80.8         |                    |
| 35.4918            | 2,3-dihydroxypropyl isobutyrate  | 1010458-45-6               | C7H14O4           | 15454879.6             | 78.2         |                    |
| 35.8779            | Phenol, 3,4-dimethoxy-   | 2033-89-8                  | C8H10O3           | 719484.9               | 75.2         |                    |
| 35.8780            | 3,4-Dimethoxyphenol, 2-methylpropionate  | 1000447-30-5               | C12H16O4          | 707517.6               | 75.2         |                    |
| 35.9724            | 3-Methoxy-5-methylphenol   | 3209-13-0                  | C8H10O2           | 997402.7               | 89.8         |                    |
| 36.3314            | Furan, tetrahydro-2-(methoxymethyl)-   | 19354-27-9                 | C6H12O2           | 3058832.1              | 78.5         |                    |
| 36.3867            | Phenol, 3,4-dimethoxy-   | 2033-89-8                  | C8H10O3           | 3375660.1              | 86.6         |                    |
| 36.8974            | Phenol, 2,6-dimethoxy-   | 91-10-1                    | C8H10O3           | 60161738.7             | 98.5         |                    |
| 37.0221            | 1,4-Benzenedicarboxaldehyde, 2-methyl-   | 27587-17-3                 | C9H8O2            | 700859.6               | 85.8         |                    |
| 37.1194            | Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-   | 703-23-1                   | C9H10O3           | 648510.7               | 81.5         |                    |
| 37.1860            | Phenol, 3,4-dimethoxy-   | 2033-89-8                  | C8H10O3           | 8811160.7              | 88.9         |                    |
| 37.4484            | Phenol, 2-methoxy-4-propyl-  | 2785-87-7                  | C10H14O2          | 9722226.6              | 94.4         |                    |
| 37.9646            | 1,2,3-Trimethoxybenzene  | 634-36-6                   | C9H12O3           | 4471208.3              | 91.5         |                    |
| 38.9076            | 4-Ethylcatechol  | 1124-39-6                  | C8H10O2           | 2559552.6              | 95.7         |                    |
| 39.0272            | Benzaldehyde, 3-hydroxy-4-methoxy-   | 621-59-0                   | C8H8O3            | 1402918.8              | 88.8         |                    |
| 39.3333            | 1,2-Benzenediol, 3-methoxy-  | 934-00-9                   | C7H8O3            | 528091.7               | 79.7         |                    |
| 39.7589            | 1,4-Benzenediol, 2,3,5-trimethyl-  | 700-13-0                   | C9H12O2           | 610052.8               | 76.0         |                    |
| 39.9992<br>40.0002 | Ethanone, 1-(2,3,4-trihydroxyphenyl)-  | 528-21-2                   | C8H8O4<br>C9H12OS | 1109384.9<br>1543577.6 | 83.0<br>83.0 |                    |
| 40.9515            | 4-Methoxy-2-methyl-1-(methylthio)benzene<br>2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]- | 22583-04-6<br>1000131-52-4 | C8H11NO2          | 13629249.6             | 81.5         |                    |
| 40.9513            | 3,5-Dimethoxy-4-hydroxytoluene   | 6638-05-7                  | C9H12O3           | 32754775.5             | 94.3         |                    |
| 41.6638            | Ethanone, 1-(2,3,4-trihydroxyphenyl)-  | 528-21-2                   | C8H8O4            | 1032440.7              | 94.3<br>83.9 |                    |
| 41.8018            | 3-Allyl-6-methoxyphenol  | 526-21-2<br>501-19-9       | C10H12O2          | 1891872.6              | 86.1         |                    |
| 42.6499            | Apocynin   | 498-02-2                   | C9H10O3           | 4363657.7              | 98.4         |                    |
| 42.6633            | Glycine, N-(2-fluorobenzoyl)-, propyl ester  | 1000314-47-6               | C12H14FNO3        | 1007147.9              | 78.8         |                    |
| 43.0431            | Benzene, 1,2,3-trimethoxy-5-methyl-  | 6443-69-2                  | C10H14O3          | 1115287.8              | 88.4         |                    |
| 44.0952            | 4-Ethyl-2,6-dimethoxyphenol  | 14059-92-8                 | C10H14O3          | 14416889.7             | 99.2         |                    |
| 44.3392            | 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-  | 2503-46-0                  | C10H12O3          | 12973649.2             | 91.1         |                    |
| ··                 |  |                            |                   |                        |              |                    |



| 6887321.2<br>2165010.4<br>909150.9<br>1286737.8<br>652460.7<br>8188459.8<br>3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4<br>711080.8 | 94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
|--|--|--|
| 909150.9<br>1286737.8<br>652460.7<br>8188459.8<br>3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4                                       | 84.1<br>89.2<br>75.4<br>95.8<br>89.4<br>94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6 |  |
| 1286737.8<br>652460.7<br>8188459.8<br>3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4   | 89.2<br>75.4<br>95.8<br>89.4<br>94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6         |  |
| 652460.7<br>8188459.8<br>3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 75.4<br>95.8<br>89.4<br>94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6                 |  |
| 8188459.8<br>3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 95.8<br>89.4<br>94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6                         |  |
| 3282726.2<br>2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4   | 89.4<br>94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6                                 |  |
| 2417524.6<br>2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 94.6<br>88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
| 2781323.1<br>641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4   | 88.0<br>75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
| 641414.1<br>622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 75.0<br>78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
| 622274.9<br>2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 78.4<br>96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
| 2209689.5<br>804704.1<br>788564.9<br>5155337.9<br>1477406.4  | 96.4<br>92.7<br>78.9<br>96.4<br>85.6   |  |
| 804704.1<br>788564.9<br>5155337.9<br>1477406.4   | 92.7<br>78.9<br>96.4<br>85.6   |  |
| 788564.9<br>5155337.9<br>1477406.4   | 78.9<br>96.4<br>85.6   |  |
| 5155337.9<br>1477406.4   | 96.4<br>85.6   |  |
| 1477406.4  | 85.6   |  |
|  |  |  |
| 711000 0   |  |  |
| /11000.0   | 80.9   |  |
| 703073.0   | 79.7   |  |
| 1148453.6  | 89.0   |  |
| 653464.3   | 78.5   |  |
| 701213.7   | 92.0   |  |
| 797803.7   | 77.0   |  |
| 593046.3   | 75.7   |  |
| 1663560.7  | 95.2   |  |
| 1624290.9  | 94.7   |  |
| 746944.6   | 77.4   |  |
| 1229401.8  | 92.7   |  |
| 2105981.8  | 84.4   |  |
| 7511105.7  | 94.5   |  |
| 1532604.3  | 80.6   |  |
| 1559037.2  |  |  |
|  | 89 3   |  |
|  | 2105981.8<br>7511105.7<br>1532604.3<br>1559037.2   | 2105981.8       84.4         7511105.7       94.5         1532604.3       80.6 |



#### Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1876986.6 79-09-4 C3H6O2 3.3277 Propanoic acid 98.8 Component RT: 3.3277 y x10<sup>2</sup> 0.9 74.0 0.8 29.0 0.7 45.0 0.6 0.5 0.4 57.0 0.3 55.0 0.2 0.1 42.1 55 15 20 25 35 70 10 40 45 50 65 80 Mass-to-Charge (m/z) Propanoic acid (NIST20.L) Square x10<sup>2</sup> 0.9 28.0 0.8 74.0 0.7 0.6 45.0 0.5 0.4 0.3 57.0 0.2 55.0 0.1 15.0 42.0 53.0 15 30 10 20 25 35 40 45 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.1239-3.3962 min, 46 scans) 10.D st x10<sup>2</sup> 0.9 0.8 0.7 45.0 0.6 29.1 0.5 0.4 57.0 0.3 0.2 0.1 60 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.3277 Counts st x10<sup>5</sup> 2.5 x10<sup>4</sup> 74.0 Component 74.0 29.0 6 2.5 ОН 29.0 45.0 5 2 73.0 73.0 1.5 57.0 45.0

3-

2

1

3.2

3.3

Acquisition Time (min)

57.0

1

0.5

3.2

3.3

Acquisition Time (min)

CH3

#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 504-63-2 7.3684 1,3-Propanediol 638257.5 92.2 C3H8O2 Component RT: 7.3684 v10<sup>2</sup> 0.9 58.0 0.8 31.0 $0.7^{-}$ 0.6 0.5 0.4 0.3 43.0 0.2 0.1 40.0 15 25 30 55 65 70 75 5 10 20 35 40 45 50 80 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 28.0 31.0 0.8 0.7 57.0 0.6 0.5 0.4 0.3 43.0 0.2 15.0 0.1 39.0 55.0 18.0 75.0 55 70 5 10 15 20 25 30 35 40 45 50 65 75 80 Mass-to-Charge (m/z) + Scan (7.3388-8.0104 min, 113 scans) 10.D st x10<sup>2</sup> 0.9 57.0 31.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 0.1 0 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 7.3684 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 58.0 Component 58.0 57.0 5 31.0 31.0 1.2 57.0 43.0



7.4 7.5 7.6 7.7 7.8 7.9

Acquisition Time (min)

45.0

3

2

7.4

7.6

7.8

Acquisition Time (min)

43.0

45.0

0.8

0.6

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 11.2838 Ethanol, 2,2'-oxybis-1225358.3 111-46-6 C4H10O3 Component RT: 11.2838 v10<sup>2</sup> 0.9 45.0 0.8 $0.7^{-}$ 0.6 43.0 75.0 0.5 0.4 0.3 31.0 0.2 60.0 88.0 0.1 63.0 0 25 75 10 15 20 30 35 40 50 55 60 65 70 85 90 95 Mass-to-Charge (m/z) Ethanol, 2,2'-oxybis- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 75.0 0.2 43.0 31.0 27.0 0.1 15.0 19.0 58.061.0 73.0 88.0 75 5 10 15 20 25 30 35 40 50 55 60 65 70 80 85 90 95 Mass-to-Charge (m/z) + Scan (11.1867-11.5188 min, 56 scans) 10.D St x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 75.0 0.3 31.0 61.0 0.2 0.1 88.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.2838 **EIC Peaks** Counts x10<sup>5</sup> 1.4 x10<sup>4</sup>-45.0 Component 45.0 43.0 1.4 5 1.2 43.0 75.0 4 31.0 75.0 1

11.3

11.4

Acquisition Time (min)

0.8

0.6

0.4

0.2

11.3

11.4

Acquisition Time (min)

31.0

76.0

3-

2-

1

76.0

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 623-39-2 11.2850 1,2-Propanediol, 3-methoxy-1566273.2 C4H10O3 Component RT: 11.2850 v10<sup>2</sup> 0.9 45.0 0.8 $0.7^{-}$ 0.6 43.0 75.0 0.5 0.4 61.0 0.3 31.0 0.2 33.0 88.0 0.1 29.0 0 75 85 5 10 15 20 25 30 35 40 45 50 55 60 65 90 95 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 45.0 0.8 0.7 0.6 43.0 0.5 0.4 75.0 0.3 31.0 61.0 0.2 15.0 33.0 0.1 27.0 47.0 88.0 19.0 57.0 63.0 39.0 75 5 10 15 20 25 30 35 40 45 50 55 60 65 70 80 85 90 95 Mass-to-Charge (m/z) + Scan (11.1867-11.5188 min, 56 scans) 10.D St x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 75.0 0.3 31.0 61.0 0.2 0.1 88.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.2850 **EIC Peaks** Counts x10<sup>5</sup> Counts x10<sup>5</sup>-43.0 Component 45.0 45.0 0.9 1.6 0.8



11.3 11.4 11.5 11.6

Acquisition Time (min)

31.0

75.0

43.0

75.0

61.0

31.0

11.6

11.4

Acquisition Time (min)

0.7

 $0.6^{-}$ 

0.5

 $0.4^{-}$ 

0.3

0.2

 $0.1^{\circ}$ 

1.4

1.2

0.8

0.6

0.4

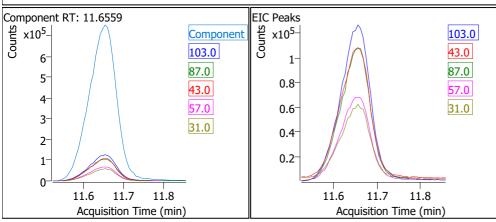
0.2

0-

CH3

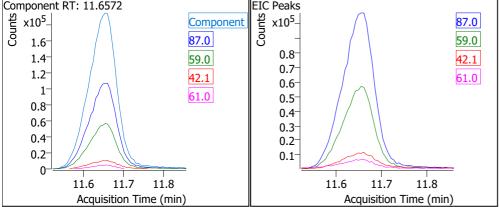
ОН

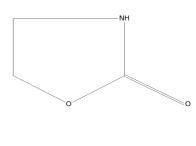
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 11.6559 Propane, 1,1-diethoxy-3635474.5 78.6 C7H16O2 Component RT: 11.6559 v10<sup>2</sup> 0.9 103.0 87.0 43.0 0.8 $0.7^{-}$ 0.6 57.0 0.5 31.0 0.4 0.3 0.2 117.0 0.1 0 30 40 70 130 10 20 50 60 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 131.0 130 0 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.5192-11.8574 min, 57 scans) 10.D St x10<sup>2</sup> 0.9 103.0 87.0 0.8 0.7 0.6 31.0 57.0 0.5 $0.4^{-}$ 0.3 0.2 67.0 0.1 96.1 117.0 53.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.6559 **EIC Peaks** x10<sup>5</sup> 103.0 Component



Н3С <

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 497-25-6 11.6572 Oxazolidin-2-one C3H5NO2 Component RT: 11.6572 v10<sup>2</sup> 0.9 87.0 0.8 0.7 0.6 0.5 0.4 0.3 59.0 0.2 0.1 42.1 61.0 75 90 10 15 20 25 30 35 50 55 60 65 70 80 95 Mass-to-Charge (m/z) Oxazolidin-2-one (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 87.0 0.8 0.7 0.6 59.0 0.5 0.4 28.0 0.3 42.0 0.2 0.1 56.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (11.5192-11.8574 min, 57 scans) 10.D St x10<sup>2</sup> 0.9 103.0 87.0 0.8 0.7 0.6 31.0 57.0 0.5 $0.4^{-}$ 0.3 0.2 67.0 0.1 96.1 117.0 53.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.6572 **EIC Peaks** Counts stuno x10<sup>5</sup> x10<sup>5</sup>-87.0 Component 87.0 59.0 1.6 0.8 1.4 59.0 42.1 $0.7^{-1}$ 1.2





#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 96-48-0 12.3516 Butyrolactone 7168594.3 97.6 C4H6O2 Component RT: 12.3516 v10<sup>2</sup> 0.9 42.0 0.8 $0.7^{-}$ 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 0.1 70 75 10 15 20 25 30 35 40 50 55 60 65 80 85 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 42.0 28.0 0.8 0.7 0.6 0.5 0.4 56.0 86.0 0.3 0.2 39.0 0.1 15.0<sub>18.0</sub> 53.0 67.0 71.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.1615-12.5056 min, 58 scans) 10.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 29.0 0.3 86.0 0.2 56.0 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 12.3516 EIC Peaks Counts Counts x10<sup>5</sup> x10<sup>5</sup>-42.0 Component 42.0 41.0 8 2.25 7 41.0 86.0 2 6 29.0 86.0 1.75



56.0

12.5

12.4

Acquisition Time (min)

1.5

1.25

0.75

0.5

12.2

12.3

1

29.0

56.0

5

4

3

2

1

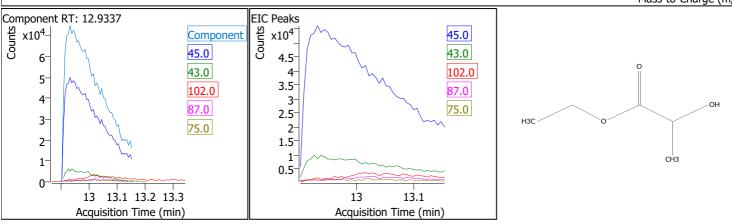
12.2

12.3

12.4

Acquisition Time (min)

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 97-64-3 Propanoic acid, 2-hydroxy-, ethyl ester 680886.6 C5H10O3 Component RT: 12.9337 v10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 0.1 102.0 87.0 29.0 45 60 85 100 105 10 15 20 25 30 35 40 55 95 110 Mass-to-Charge (m/z) Propanoic acid, 2-hydroxy-, ethyl ester (NIST20.L) st x10<sup>2</sup>\_ 0.9-45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 29.0 0.1 43.0 75.0 15.0 31.0 56.0 89.0 103.0 75 10 20 25 30 35 50 55 60 65 70 80 85 95 100 105 110 Mass-to-Charge (m/z) + Scan (12.8981-13.1537 min, 43 scans) 10.D st x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 0.1 29.0 102.0 87.0 100 110 10 20 30 40 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 12.9337 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 45.0 Component 45.0 43.0 6 4.5



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2900302.0 4744-08-5 13.3285 Propane, 1,1-diethoxy-79.9 C7H16O2 Component RT: 13.3285 v10<sup>2</sup> 0.9 103.0 43.0 0.8 87.0 0.7 0.6 57.0 0.5 31.0 0.4 0.3 0.2 0.1 0 40<sup>2</sup> 30 70 130 10 20 50 60 90 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 131.0 130 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (13.2193-13.4731 min, 42 scans) 10.D St x10<sup>2</sup> 0.9 103.0 0.8 43.0 0.7 87.0 0.6 0.5 31.0 $0.4^{-}$ 57.0 0.3 0.2 0.1 117.0 69.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 13.3285 **EIC Peaks** Counts Counts x10<sup>5</sup> 103.0 Component 103.0 43.0 0.9 5 43.0 0.8 87.0 4 Н3С <



13.3

13.4 Acquisition Time (min)

57.0

31.0

 $0.7^{-}$ 

 $0.6^{-}$ 

0.5

0.4

0.3 0.2

87.0

57.0

31.0

3-

2-

1-

13.3

13.4

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2758-18-1 15.9672 2-Cyclopenten-1-one, 3-methyl-936447.1 96.6 C6H8O Component RT: 15.9672 v10<sup>2</sup> 0.9 96.0 0.8 $0.7^{-}$ 67.0 0.6 0.5 53.0 0.4 81.0 39.0 0.3 0.2 65.0 0.1 65 10 15 20 25 30 35 45 50 55 60 75 80 85 90 100 105 110 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3-methyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 96.0 0.8 0.7 0.6 0.5 67.0 0.4 53.0 81.0 0.3 39.0 0.2 27.0 0.1 56.0 51.0 99.0 10 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 105 110 Mass-to-Charge (m/z) + Scan (15.8953-16.2040 min, 52 scans) 10.D st x10<sup>2</sup> 0.9 96.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 53.0 67.0 0.3 81.0 39.0 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 15.9672 **EIC Peaks** Counts Counts x10<sup>4</sup> 96.0 Component 96.0 67.0 3.5 1.4 67.0 53.0 CH3 3 1.2 81.0

16

16.1

Acquisition Time (min)

39.0

53.0

81.0

39.0

1

0.8

0.6 0.4

0.2

16

16.1

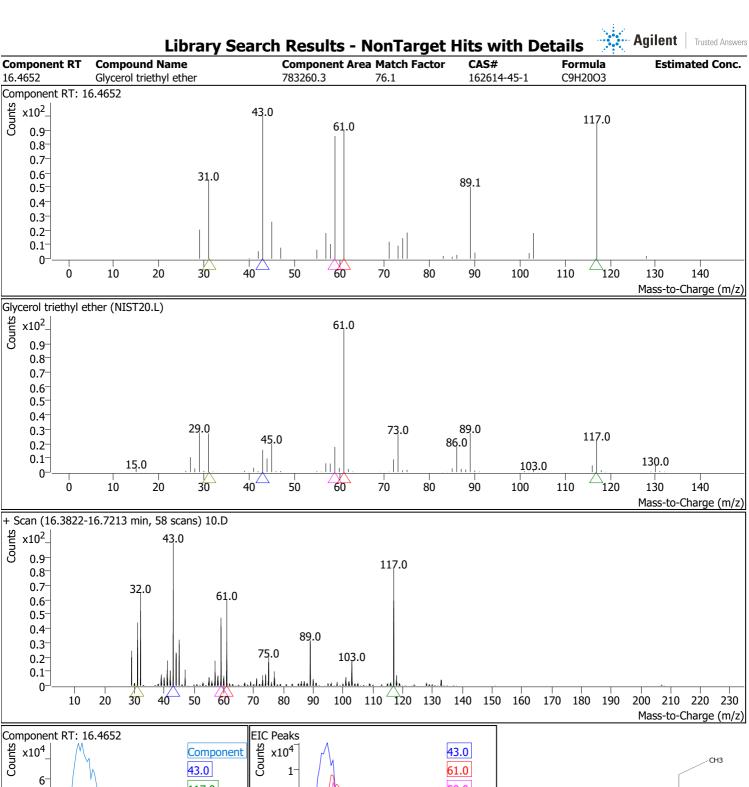
Acquisition Time (min)

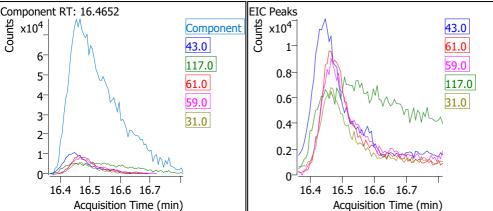
2.5

1.5

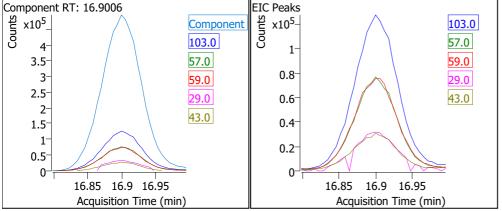
1 0.5

2





#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 16.9006 1,3-Dioxolane-4-methanol, 2-ethyl-2038169.3 85.3 53951-44-3 C6H12O3 Component RT: 16.9006 v10<sup>2</sup> 0.9 103.0 0.8 $0.7^{-}$ 57.0 0.6 0.5 0.4 0.3 29.0 43.0 131.0 0.2 0.1 40 100 Ó 10 20 30 50 60 70 80 90 110 120 130 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (16.8104-17.0007 min, 32 scans) 10.D St x10<sup>2</sup> 0.9 103.0 0.8 57.0 0.7 0.6 0.5 $0.4^{-}$ 44.0 0.3 29.0 131.1 0.2 0.1 117.0 72.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 16.9006 Counts x10<sup>5</sup> x10<sup>5</sup>-103.0 Component 103.0 57.0



#### ... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 108-95-2 17.9862 Phenol 2231714.0 98.1 C6H6O Component RT: 17.9862 v10<sup>2</sup> 0.9 94.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 55.0 63.0 50.0 0 <sup>4</sup>95 25 40 85 10 15 20 30 35 45 50 55 60 65 70 75 90 100 105 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10<sup>2</sup>\_0.9 94.0 0.8 0.7 0.6 0.5 0.4 0.3 66.0 0.2 39.0 0.1 47.0 51.0 55.0 14.0 18.0 63.0 27.0 31.0 42.0 74.0 79.0 40 95 10 15 20 25 30 35 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) + Scan (17.9119-18.2792 min, 62 scans) 10.D St x10<sup>2</sup> 0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 55.0 103.0 117.0 60 Ó 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 17.9862 Counts x10<sup>5</sup> 94.0 Component 94.0 66.0 1.6 3.5 66.0 1.4 65.0 3 1.2 39.0 65.0 2.5 1 39.0 40.0

18.1

Acquisition Time (min)

18.2

0.8

0.6

0.4

0.2

18

40.0

2-

1

18

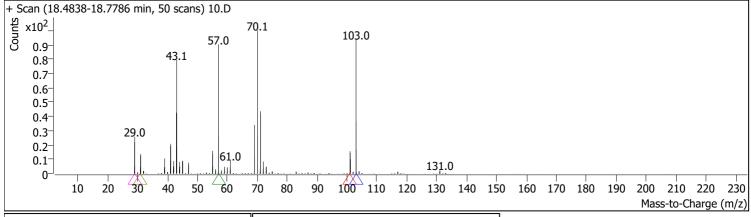
18.1

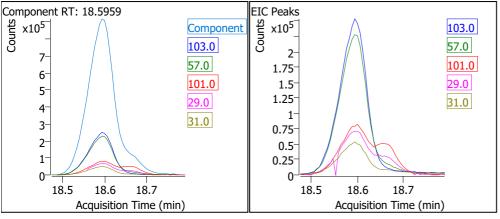
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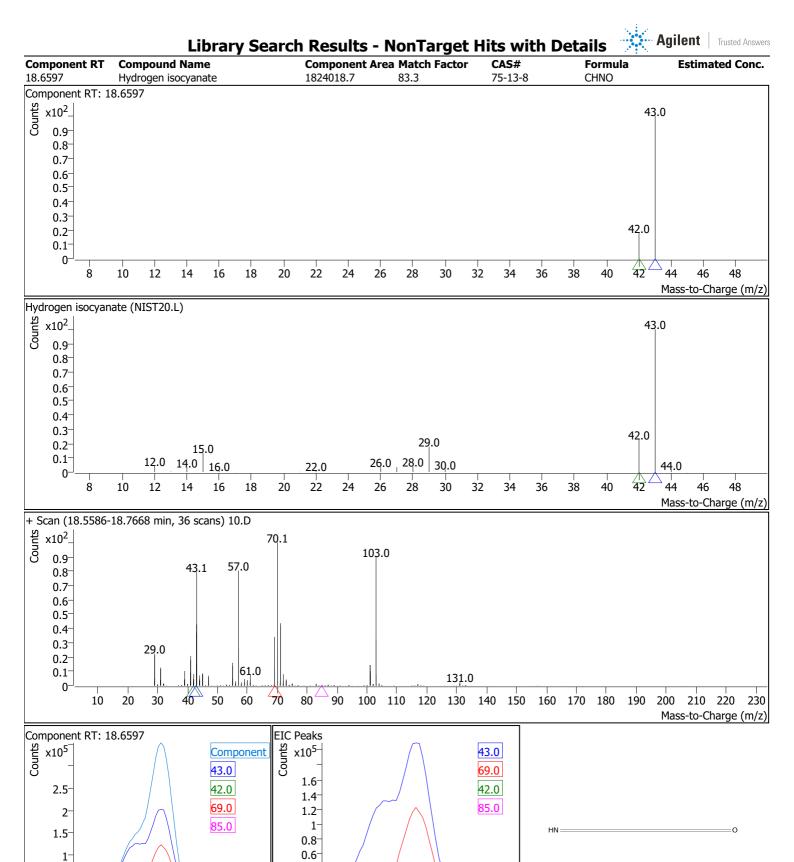
18.2

1.5









18.6

18.7

Acquisition Time (min)

0.4

0.2

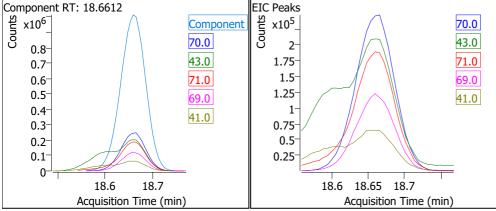
0.5

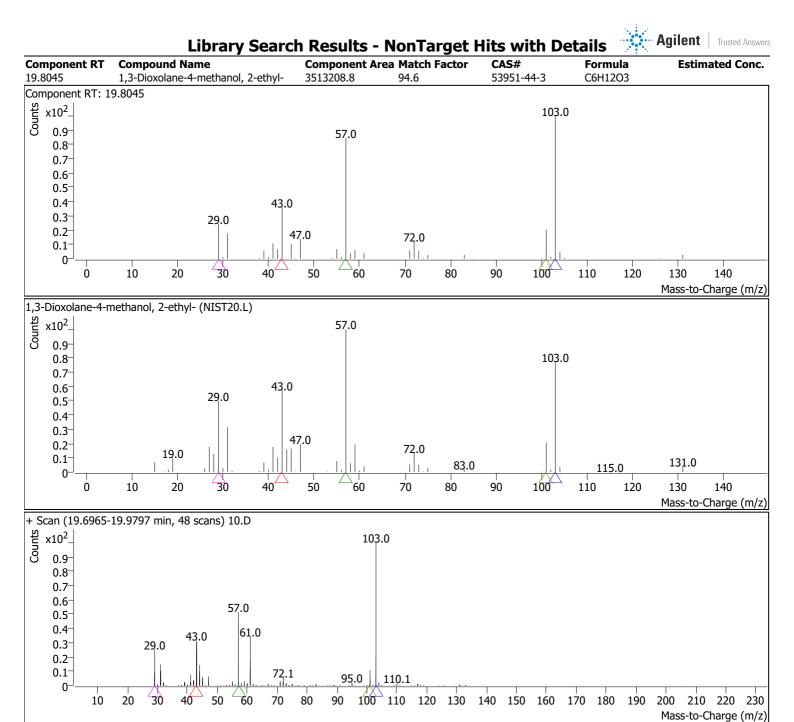
18.5

18.6

Acquisition Time (min)

#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 544-01-4 18.6612 Diisoamyl ether 3829017.6 93.7 C10H22O Component RT: 18.6612 v10<sup>2</sup> 0.9 70.0 43.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 41.0 55.0 101.0 0.2 39.0 0.1 100 20 25 30 35 40 50 55 60 65 75 80 85 90 95 105 110 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 43.0 70.0 0.8 0.7 0.6 0.5 0.4 0.3 41.0 55.0 0.2 101.0 29.0 39.0 45.0 0.1 31.0 53.0 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (18.5586-18.7668 min, 36 scans) 10.D St x10<sup>2</sup> 0.9 70.1 103.0 57.0 43.1 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 29.0 0.2 61.0 0.1 131.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 18.6612 **EIC Peaks** Counts Counts x10<sup>5</sup> 70.0 Component 70.0 43.0 2 8.0 43.0 1.75 71.0 0.7





19.8

19.9

Acquisition Time (min)

103.0

57.0

43.0

29.0

101.0

EIC Peaks

1.6

1.4

1.2

0.6

0.4

0.2

1<sup>-</sup> 0.8<sup>-</sup>

Counts x10<sup>5</sup>

Component 103.0

57.0

43.0

29.0

101.0

Component RT: 19.8045

Counts

6

5

4

3

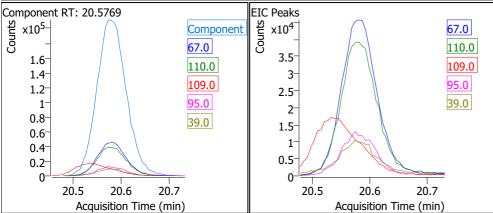
2

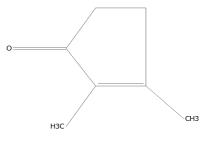
1

19.8

19.9

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.5769 2-Cyclopenten-1-one, 2,3-dimethyl-910291.4 93.1 1121-05-7 C7H10O Component RT: 20.5769 v10<sup>2</sup> 0.9 67.0 110.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 95.0 0.3 39.0 0.2 53.0 0.1 124.0 29.0 40 25 30 35 50 55 65 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 110.0 67.0 0.8 0.7 0.6 0.5 0.4 82.0 95.0 0.3 54.0 39.0 0.2 27.0 0.1 51.0 65.0 79.0 99.0 91.0 10 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (20.4922-20.7289 min, 40 scans) 10.D st x10<sup>2</sup> 0.9 61.0 0.8 43.0 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 67.0 110.1 0.3 31.0 0.2 81.1 95.0 0.1 117.0 53.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 20.5769 **EIC Peaks** Counts Counts x10<sup>4</sup> 67.0 Component 67.0 110.0 3.5 1.6 110.0 109.0 1.4 3





### - Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 95-48-7 22.2583 Phenol, 2-methyl-1099911.1 92.8 C7H8O Component RT: 22.2583 y x10<sup>2</sup> 0.9 108.0 0.8 0.7 0.6 0.5 0.4 0.3 90.0 0.2 103.0 0.1 29.0 75 85 95 100 105 Mass-to-Charge (m/z) Phenol, 2-methyl- (NIST20.L) St x10<sup>2</sup>\_ 0.9 108.0 0.8 0.7 0.6 0.5 0.4 0.3 79.0 90.0 0.2 0.1 17.0 58.0 <sup>63.0</sup> 68.0 74.0 86.0 | 94.0 100.0 90 100 105 110 115 120 10 15 20 30 35 40 50 55 60 65 70 75 80 85 95 Mass-to-Charge (m/z) + Scan (22.1800-22.4057 min, 38 scans) 10.D Sounds x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 43.0 $0.4^{-}$ 0.3 108.0 0.2 31.0 0.1 89.0 117.0 **110** 10 20 30 40 50 60 70 80 100 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 22.2583 stuno 2.25 Counts x10<sup>4</sup> 108.0 Component 108.0 107.0 5 77.0 107.0 1.75 79.0 79.0 1.5



22.3

Acquisition Time (min)

90.0

3-

2

77.0

90.0

1.25

0.75<sup>-</sup> 0.5<sup>-</sup> 0.25<sup>-</sup>

1

0-

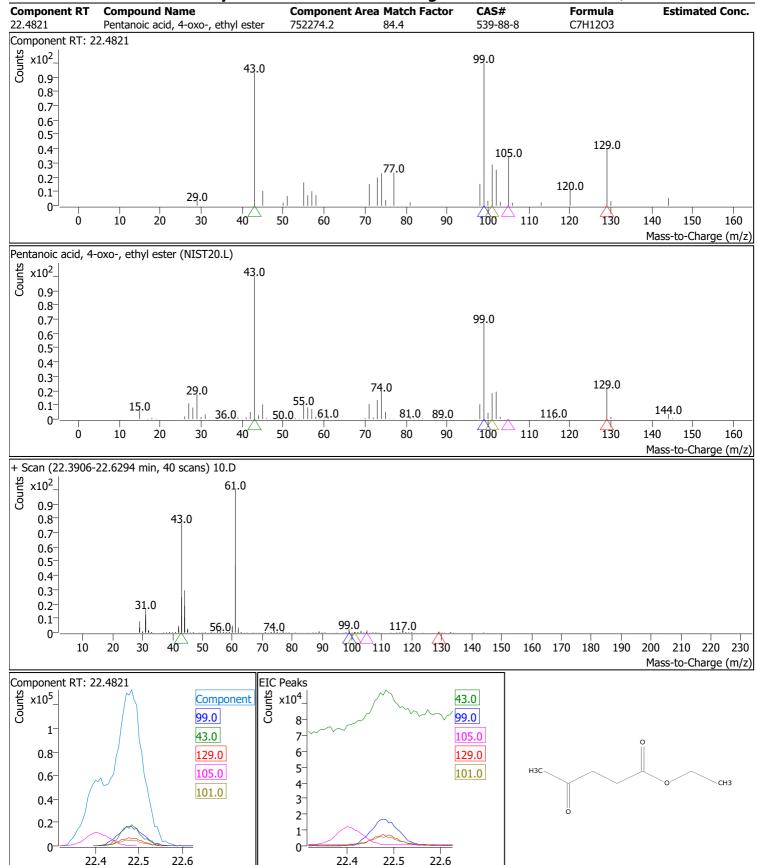
22.3

Acquisition Time (min)

H3C



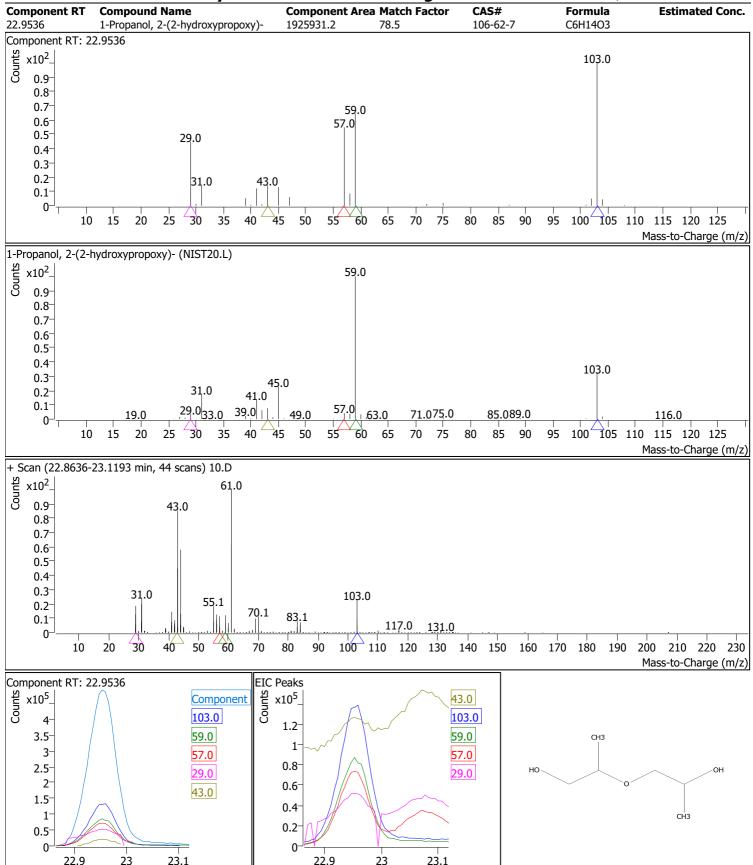




Acquisition Time (min)







Acquisition Time (min)

#### --- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0790 1-Octanol 3801554.6 97.0 111-87-5 C8H18O Component RT: 23.0790 v10<sup>2</sup> 0.9 56.0 41.1 0.8 70.1 $0.7^{-}$ 84.1 0.6 0.5 0.4 0.3 0.2 0.1 55 100 105 110 115 120 125 130 135 140 50 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 55 20 25 35 40 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9587-23.2382 min, 48 scans) 10.D st x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 31.0 55.1 0.2 103.0 70.1 83.1 0.1 117.0 504 10 20 30 40 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 90 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.0790 Counts Counts x10<sup>4</sup>\_ 56.0 Component 56.0 55.0 5 55.0 6 41.1 41.1 5 70.1

70.1

69.1

23.1 23.2 23.3

Acquisition Time (min)

3

2

23

23.1

23.2

Acquisition Time (min)

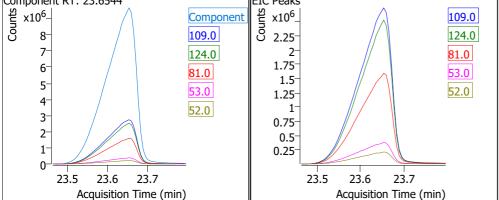
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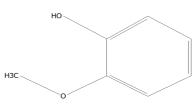
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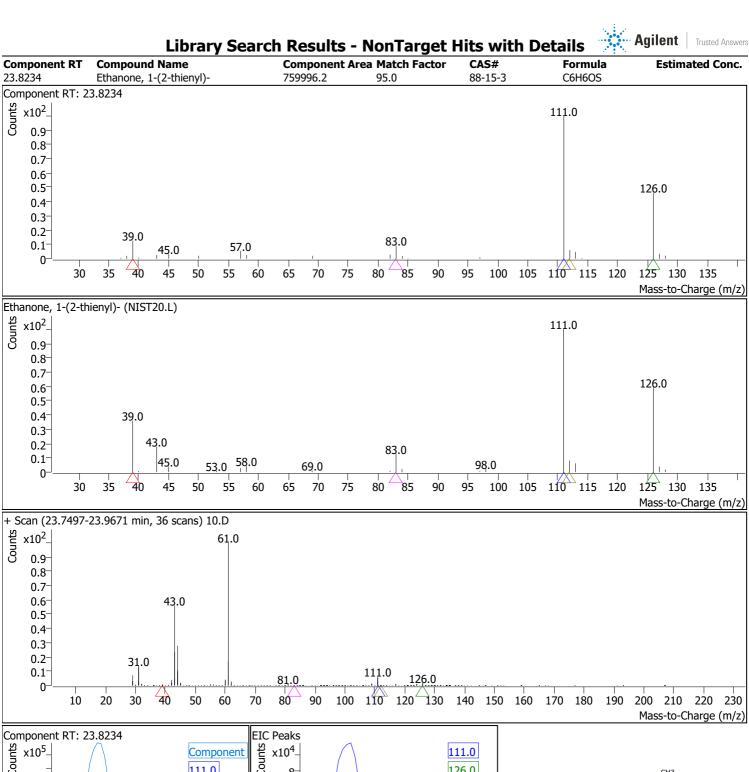
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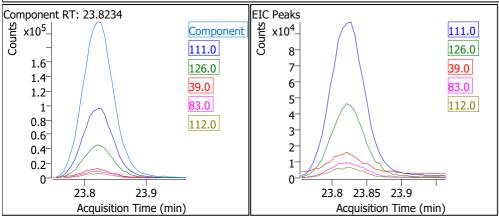
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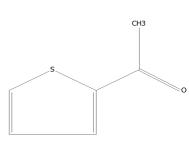
#### --- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6544 Phenol, 2-methoxy-50811022.5 98.7 C7H8O2 Component RT: 23.6544 v10<sup>2</sup> 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 0.1 39.0 65.0 80 110 120 10 20 30 40 90 100 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) St x10<sup>2</sup>\_ 0.9 109.0 124.0 0.8 81.0 0.7 0.6 0.5 0.4 0.3 53.0 0.2 39.0 63.0 0.1 27.0 77.0 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4655-23.7912 min, 55 scans) 10.D 109.0 124.0 st x10<sup>2</sup> 0.9 0.8 81.0 0.7 0.6 0.5 0.4 61.0 0.3 43.0 0.2 0.1 31.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.6544 Counts Counts x10<sup>6</sup> x10<sup>6</sup>\_ 109.0 Component 109.0 124.0 2.25 7 2-124.0 81.0 1.75

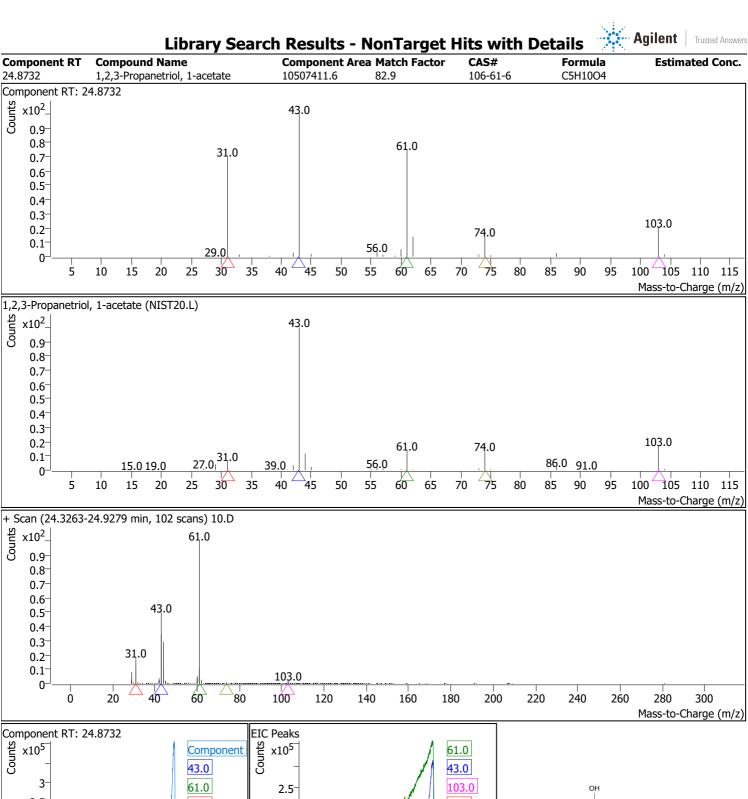


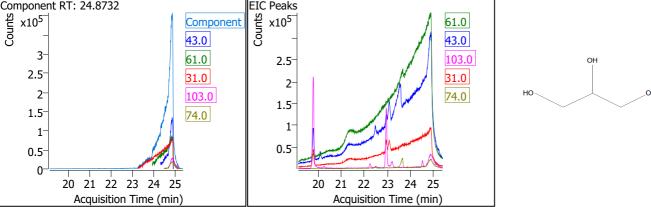








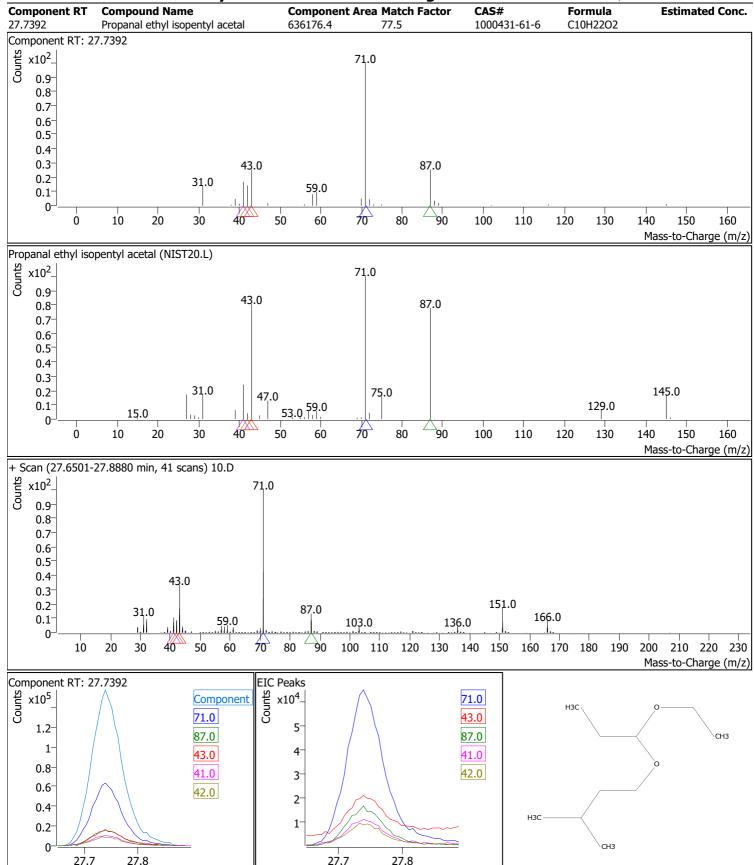




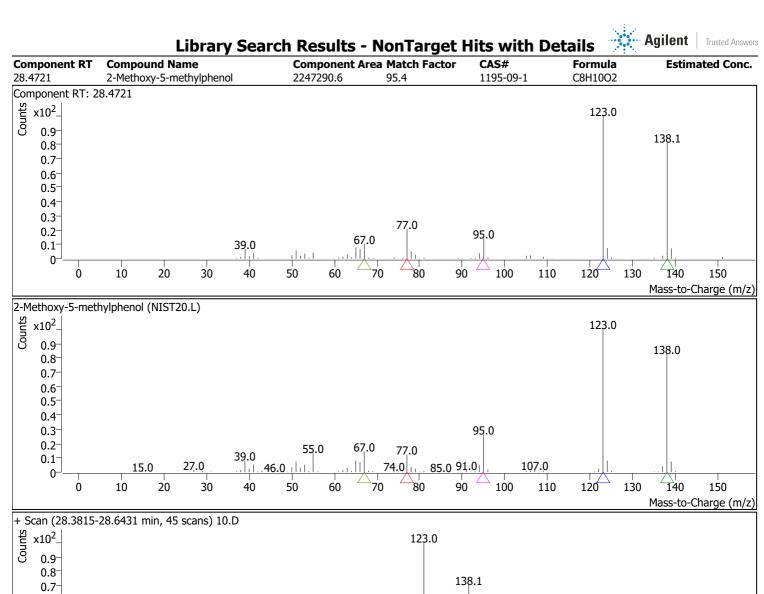
CH3

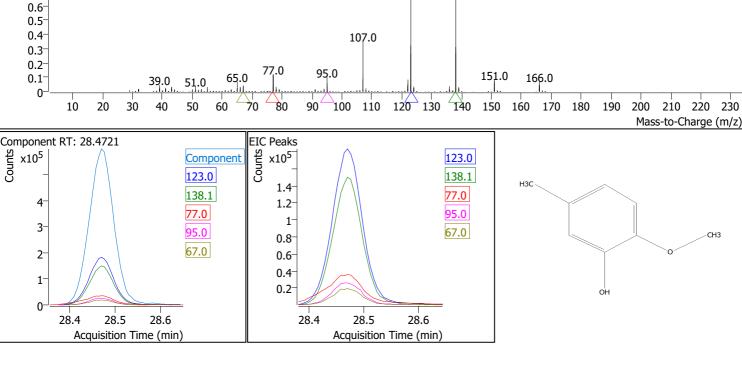
## **Library Search Results - NonTarget Hits with Details**

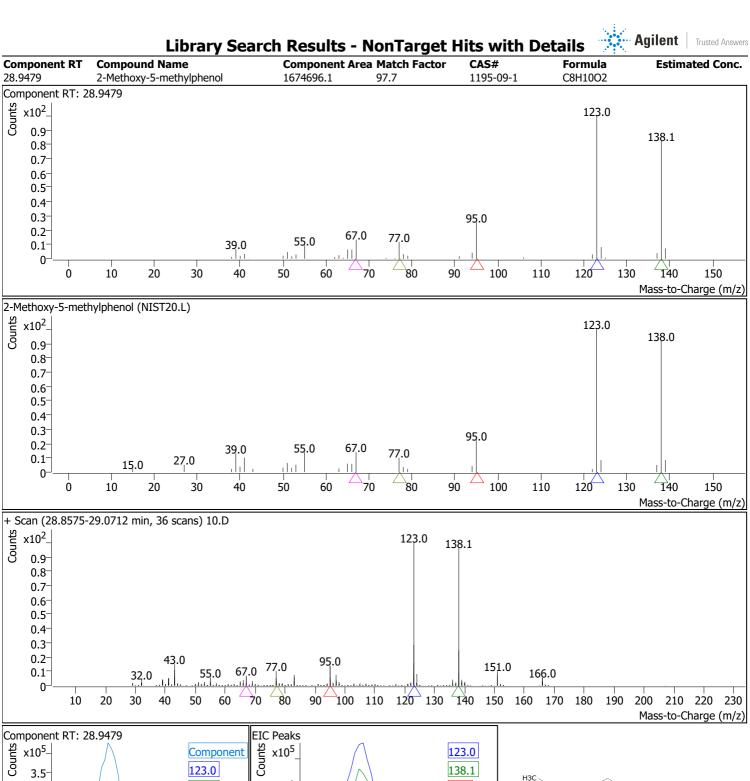


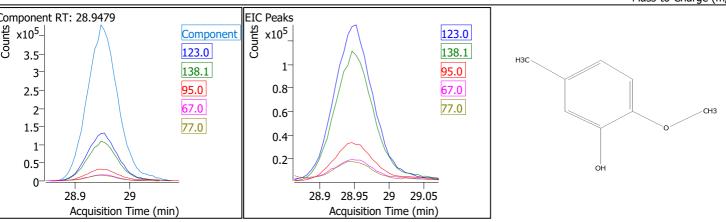


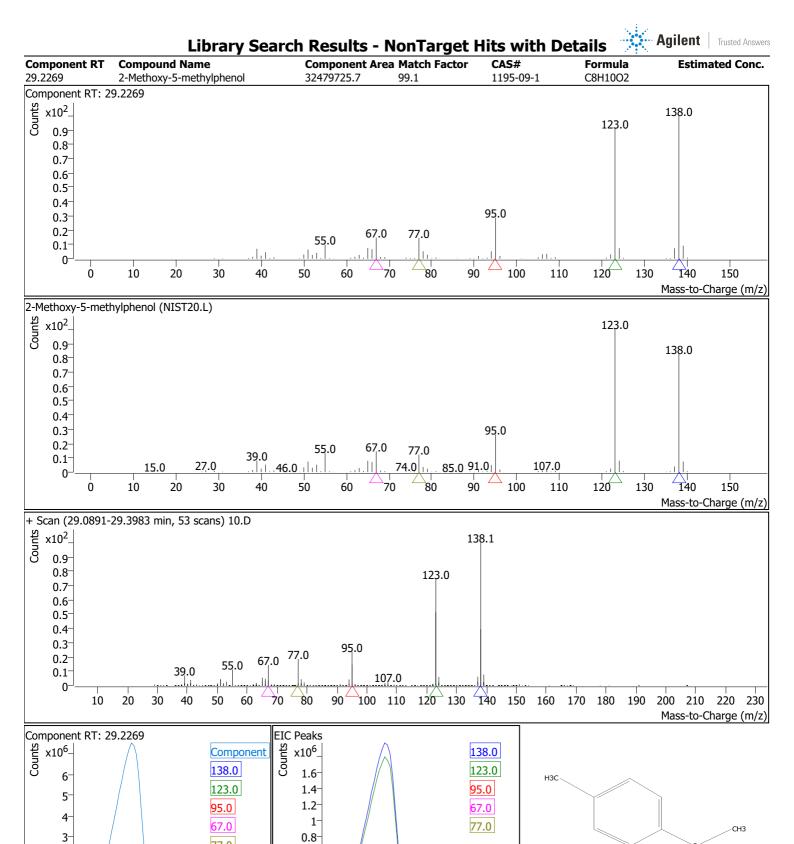
Acquisition Time (min)











29.2

29.3

Acquisition Time (min)

77.0

2

1

29.2

29.3

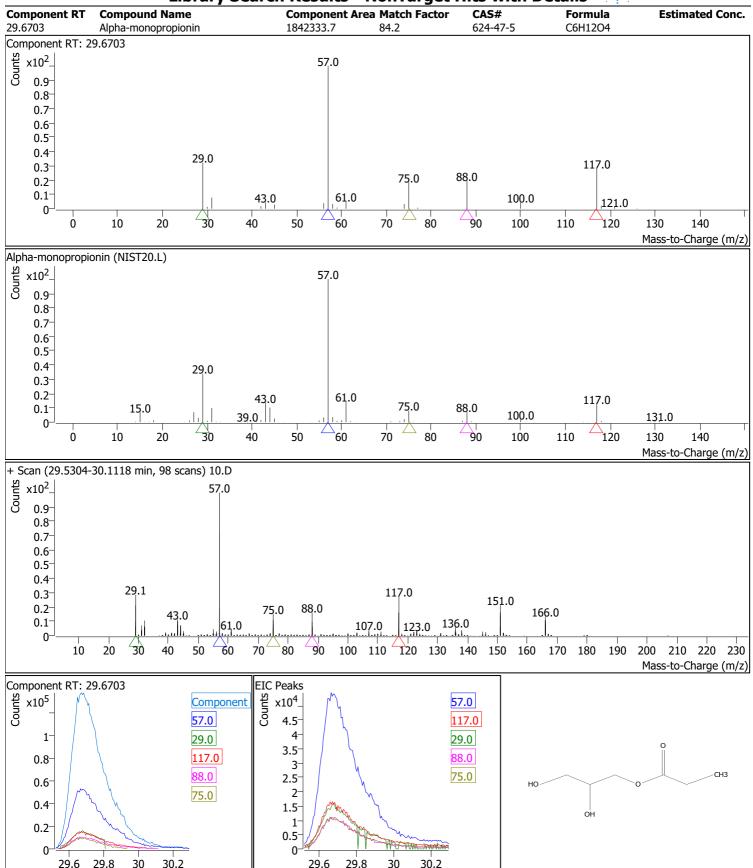
Acquisition Time (min)

0.6

0.4







Acquisition Time (min)

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.5947 Catechol 12897459.7 89.1 C6H6O2 Component RT: 30.5947 v10<sup>2</sup> 0.9 110.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 64.0 0.2 81.0 53.0 0.1 100 105 110 115 120 125 10 15 35 50 60 65 75 80 85 95 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 81.0 92.0 0.1 69.0 74.0 79.0 95.0 65 10 15 20 30 35 40 45 50 55 60 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.5459-31.5626 min, 172 scans) 10.D st x10<sup>2</sup> 0.9 110.0 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 64.0 0.2 81.092.0 0.1 39.0 53.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.5947 **EIC Peaks** Counts Counts x10<sup>5</sup>-110.0 Component 110.0 64.0 4 0.8 64.0 3.5 63.0 0.7 3-63.0 81.0 0.6 2.5

30.8 31 31.2 31.4 Acquisition Time (min)

53.0

 $0.5^{-}$ 

 $0.4^{-}$ 

0.3 0.2

0.1

30.75

31

31.25

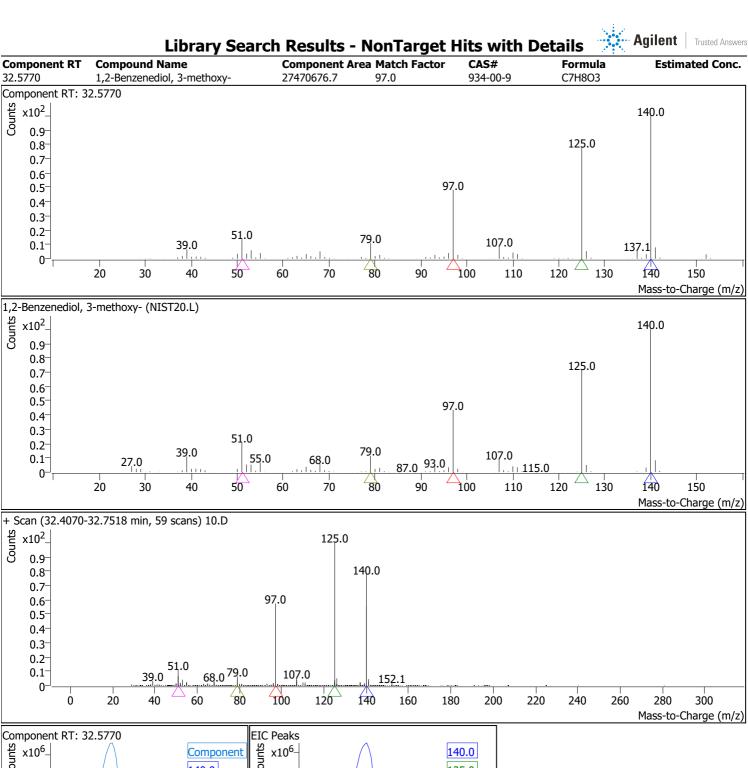
Acquisition Time (min)

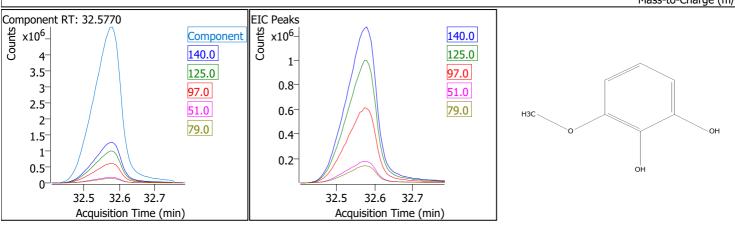
81.0

53.0

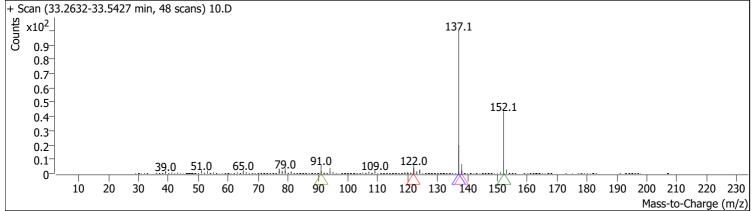
2-

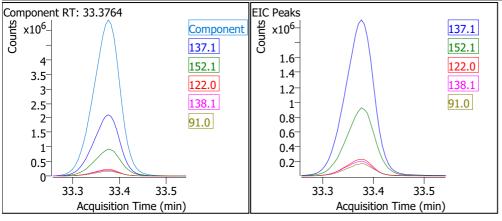
1.5

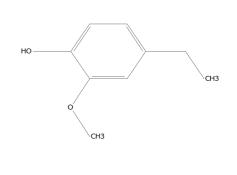




#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 33.3764 Phenol, 4-ethyl-2-methoxy-21501433.2 96.8 2785-89-9 C9H12O2 Component RT: 33.3764 v10<sup>2</sup> 0.9 137.1 0.8 $0.7^{-}$ 0.6 0.5 152.1 0.4 0.3 0.2 122.0 91.0 77.0 0.1 109.0 0 90 150 10 20 30 40 50 60 70 80 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Phenol, 4-ethyl-2-methoxy- (NIST20.L) St x10<sup>2</sup>\_ 0.9 137.0 0.8 152.0 0.7 0.6 0.5 0.4 0.3 0.2 122.0 0.1 91.0 77.0 39.0 109.0 27.0 65.0 140 90 10 20 30 40 50 60 70 80 100 110 120 130 150 160 170



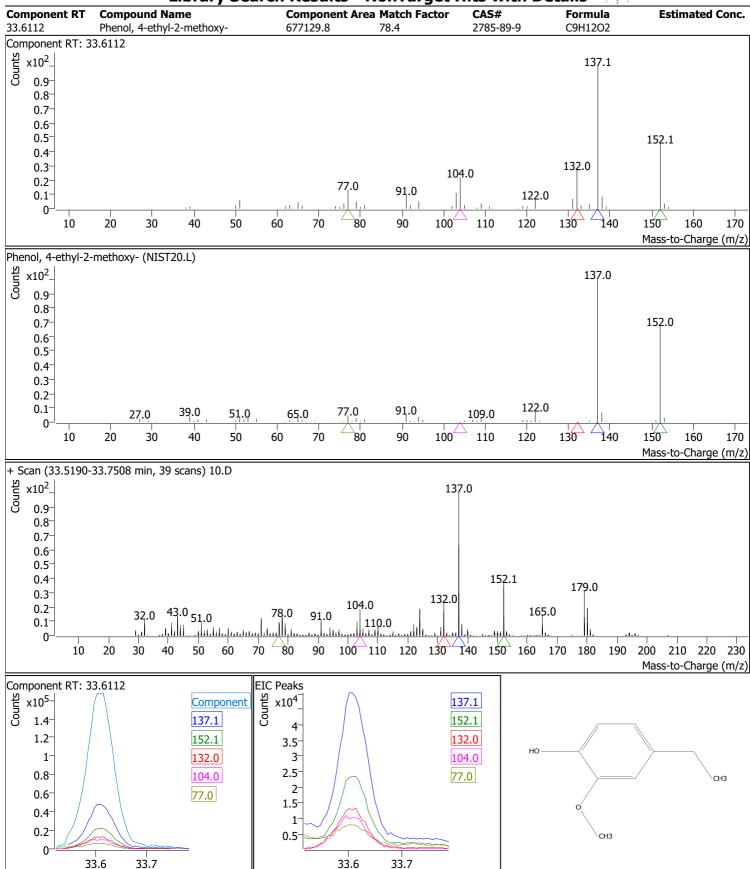




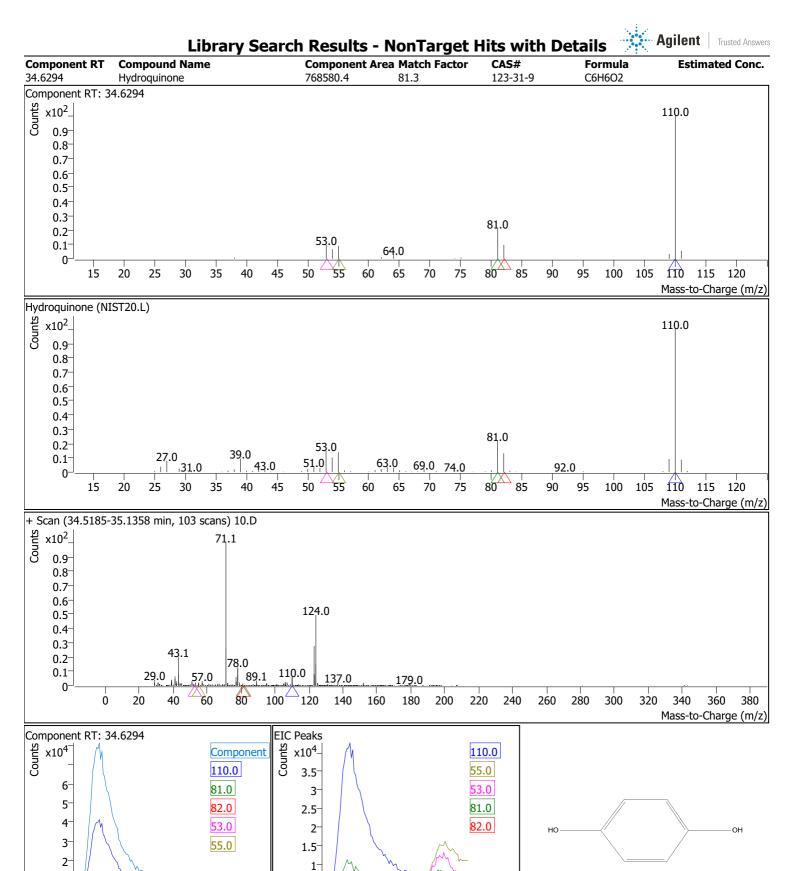
Mass-to-Charge (m/z)







Acquisition Time (min)



34.8

Acquisition Time (min)

35

0.5

34.6

1

34.6

34.8

Acquisition Time (min)

35

### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 452-86-8 35.0235 1,2-Benzenediol, 4-methyl-6420675.4 C7H8O2 Component RT: 35.0235 v10<sup>2</sup> 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 0.2 107.0 51.0 95.0 0.1 110 10 20 30 40 50 60 70 90 100 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 4-methyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 124.0 0.8 0.7 0.6 0.5 78.0 0.4 0.3 0.2 51.0 107.0 39.0 95.0 0.1 62.0 67.0 27.0 47.0 10 20 30 40 50 60 70 80 90 100 110 130 140 Mass-to-Charge (m/z) + Scan (34.8330-35.4513 min, 105 scans) 10.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.1 124.0 0.1 78.089.1<sub>101.1</sub> 29.0 57.0 80 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0235 Counts x10<sup>5</sup> x10<sup>5</sup>\_ 124.0 Component 124.0 123.0 1.8 6 1.6 123.0 78.0 5 1.4 78.0 77.0

35.2

Acquisition Time (min)

107.0

35.4

1.2

0.8

0.6

1

77.0

107.0

35.4

35.2

Acquisition Time (min)

4

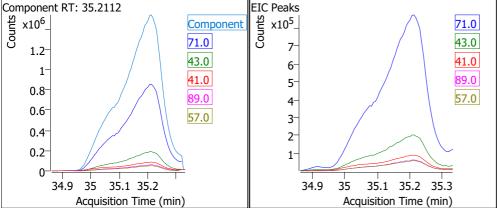
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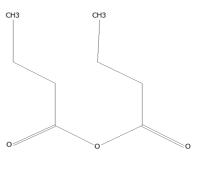
2

1

СНЗ

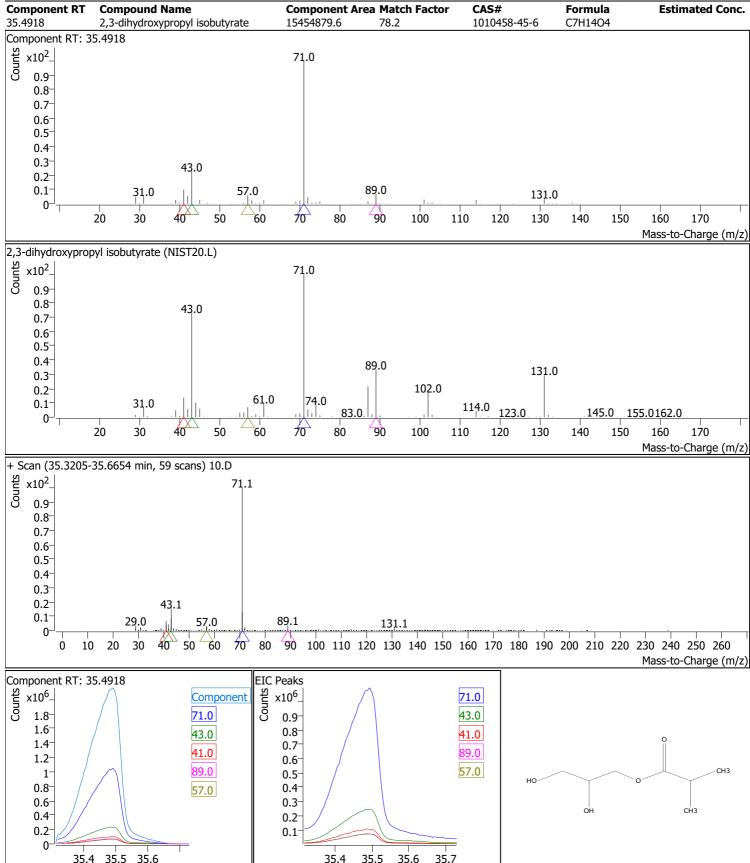
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.2112 Butanoic acid, anhydride 15434879.8 80.8 C8H14O3 Component RT: 35.2112 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 89.0 0.1 57.0 31.0 55 90 10 15 20 25 30 35 40 65 70 75 80 85 95 Mass-to-Charge (m/z) Butanoic acid, anhydride (NIST20.L) st x10<sup>2</sup>\_ 0.9-71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 41.0 0.1 55.0 29.0 15.0 60.0 85.0 89.0 5 10 15 20 25 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (34.9519-35.3205 min, 63 scans) 10.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 0.4 0.3 43.1 0.2 124.0 0.1 78.089.1<sub>101.1114.1</sub> 29.0 57.0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.2112 Counts Counts x10<sup>5</sup>\_ 71.0 Component CH3 CH3 71.0 43.0 1.2 43.0 41.0 6 1





# **Library Search Results - NonTarget Hits with Details**

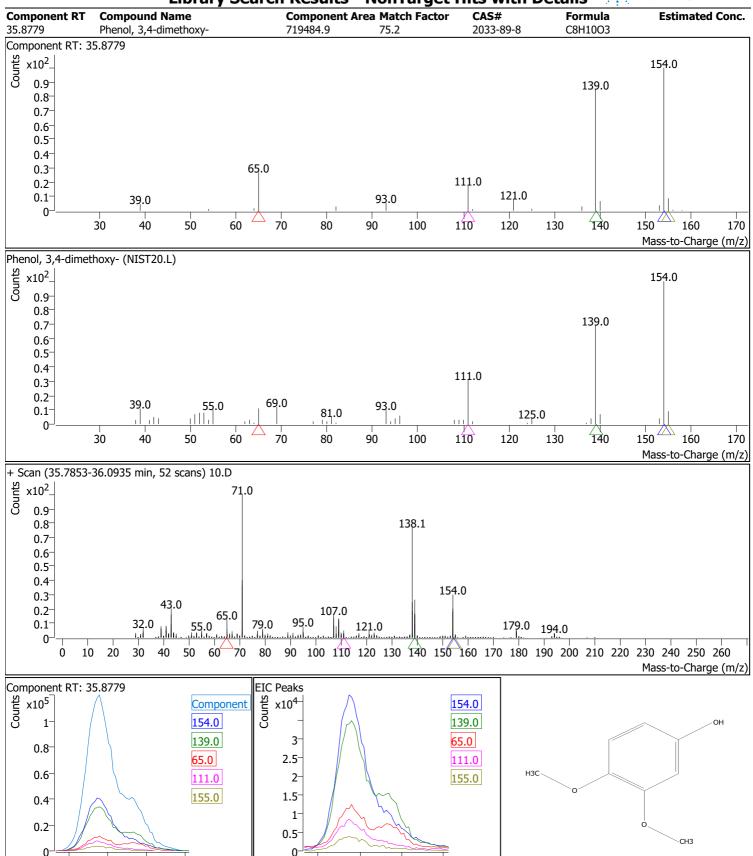




Acquisition Time (min)







35.8

35.9

36

Acquisition Time (min)

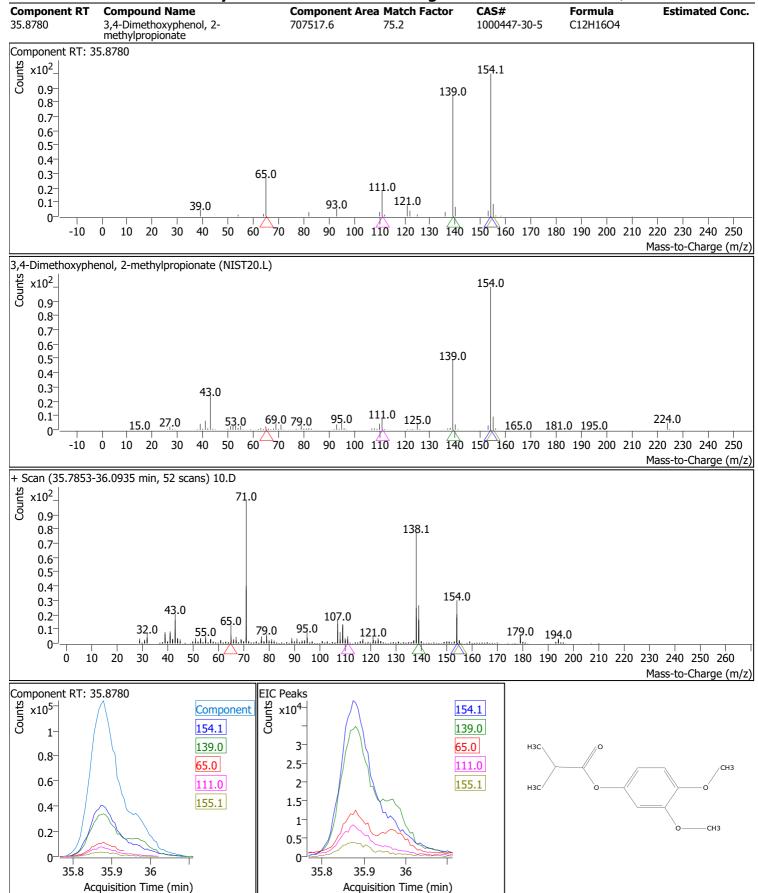
35.8

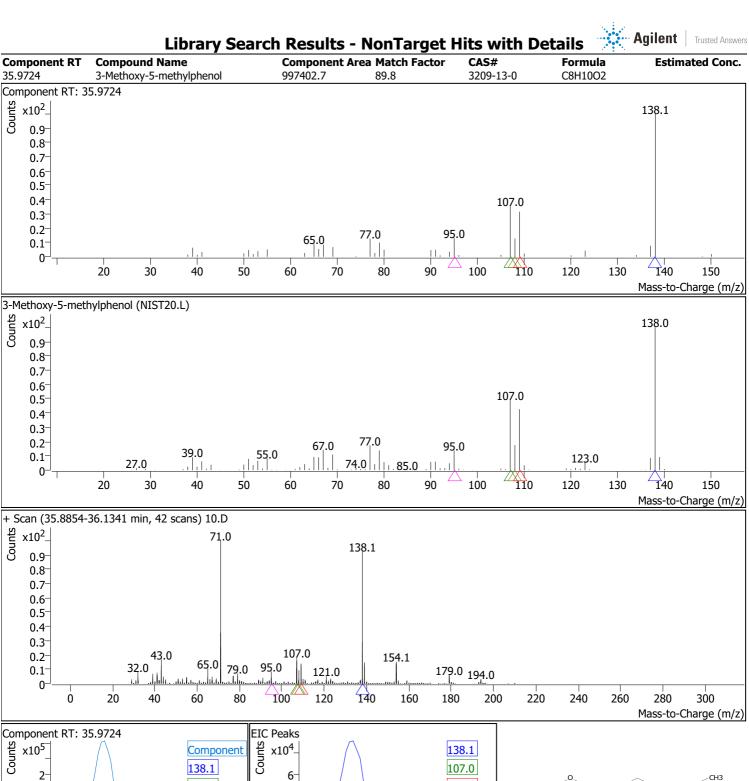
35.9

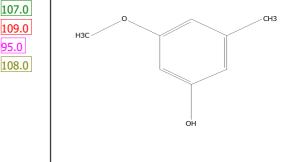
36

# **Library Search Results - NonTarget Hits with Details**









36

Acquisition Time (min)

36.1

107.0

109.0

95.0

108.0

36.1

5

4

3

2-

1.75

1.5

1.25

0.75

0.5 0.25

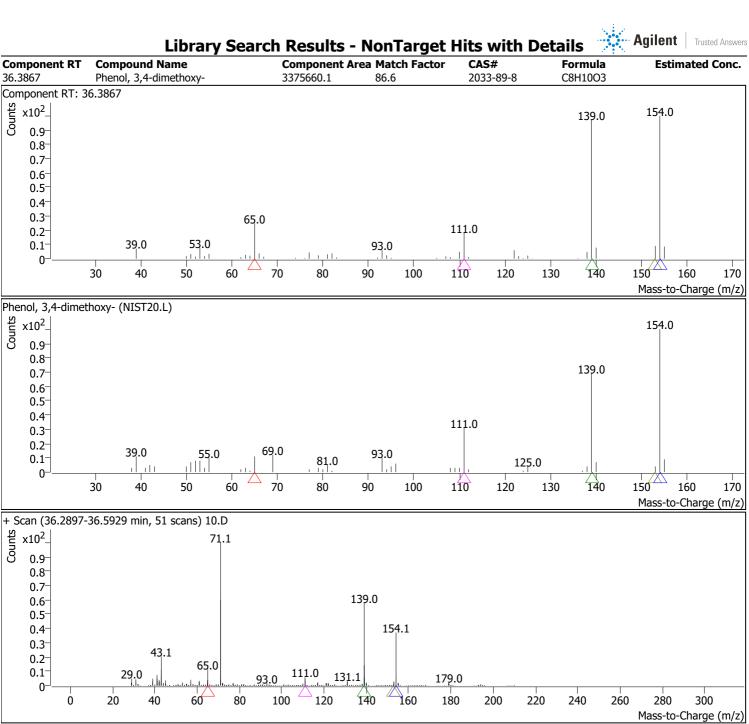
35.9

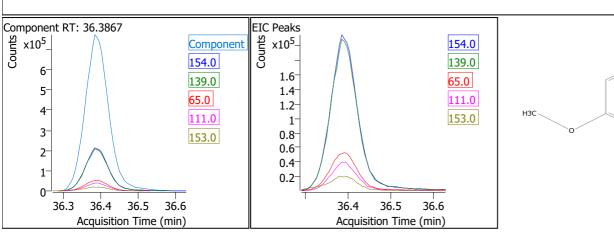
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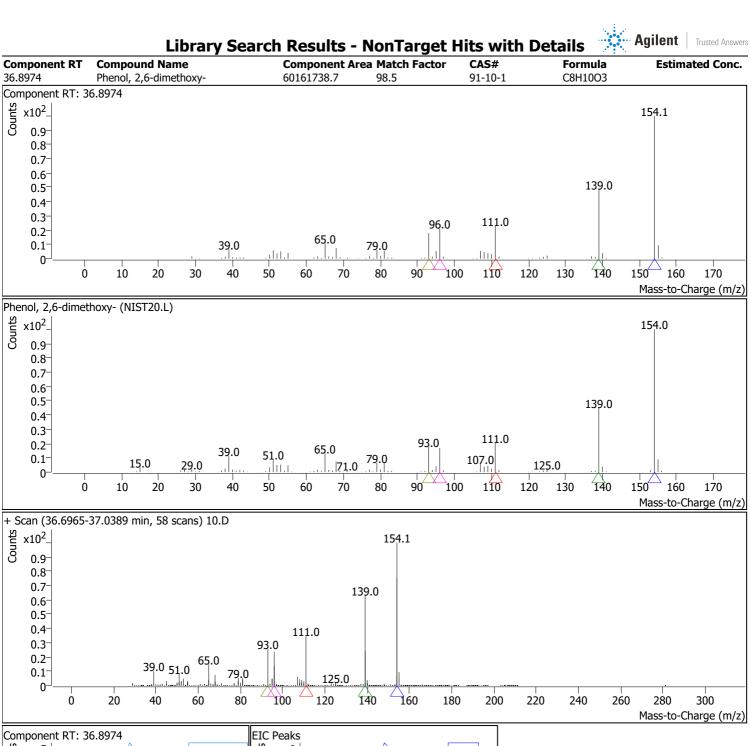
Acquisition Time (min)

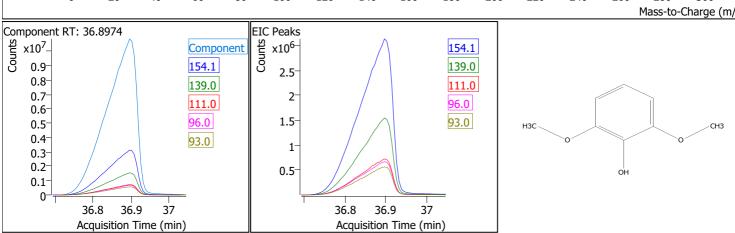
1

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.3314 Furan, tetrahydro-2-(methoxymethyl)- 3058832.1 19354-27-9 C6H12O2 Component RT: 36.3314 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 0.1 31.0 57.0 95 100 105 110 115 120 125 60 65 Mass-to-Charge (m/z) Furan, tetrahydro-2-(methoxymethyl)- (NIST20.L) st x10<sup>2</sup>\_ 0.9-71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 0.1 58.0 15.0 85.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (36.2243-36.5514 min, 56 scans) 10.D st x10<sup>2</sup> 0.9 0.8 $0.7^{-}$ 0.6 139.0 0.5 $0.4^{-}$ 154.1 0.3 43.1 0.2 65.0 0.1 111.0 131.1 179.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 36.3314 Counts Counts x10<sup>5</sup> 71.0 Component 71.0 43.0

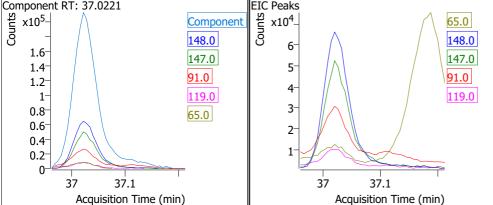


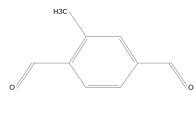






### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 37.0221 1,4-Benzenedicarboxaldehyde, 2-700859.6 85.8 27587-17-3 C9H8O2 methyl-Component RT: 37.0221 x10<sup>2</sup>\_ 148.0 0.9 8.0 0.7 0.6 0.5 91.0 0.4 0.3 $0.2^{-}$ 119.0 0.1 90 10 20 30 40 100 110 120 130 140 160 Mass-to-Charge (m/z) 1,4-Benzenedicarboxaldehyde, 2-methyl- (NIST20.L) Counts $x10^{2}$ 148.0 0.9 0.8 0.7 91.0 0.6 0.5 119.0 0.4 0.3 65.0 39.0 0.2 28.0 51.0 0.1 86.0 97.0 105.0 133.0 0 90 100 150 10 20 30 80 110 120 130 140 160 Mass-to-Charge (m/z) + Scan (36.9616-37.1876 min, 39 scans) 10.D st x10<sup>2</sup> 154.1 139.0 0.8 0.7 0.6 0.5 0.4 0.3 111.0 0.2 0.1 60 40 80 100 120 200 260 280 0 20 160 180 220 240 300 Mass-to-Charge (m/z) Component RT: 37.0221 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>4</sup>\_ 65.0 Component 148.0 148.0 6 1.6 147.0 147.0 НЗС 1.4 5 91.0 91.0 1.2





#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 703-23-1 37.1194 Ethanone, 1-(2-hydroxy-6-648510.7 81.5 C9H10O3 methoxyphenyl)-Component RT: 37.1194 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 166.0 0.4 0.3 $0.2^{-}$ 136.0 0.1 105.0 0-150 170 30 40 50 60 70 80 90 100 110 120 130 140 160 180 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-6-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 166.0 0.5 0.4 0.3 0.2 136.0 108.0 0.1 93.0 43.0 65.0 77.0 121.0 0 150 30 40 50 60 70 80 90 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (37.0211-37.2708 min, 43 scans) 10.D st x10<sup>2</sup> 0.9 154.1 139.0 0.8 0.7 0.6 0.5 0.4 0.3 111.0 0.2 39.0 53.0 65.0 0.1 123.0 166.1179.0 83.0 0 Ó 140 160 180 200 220 260 20 40 60 80 100 120 240 280 300 Mass-to-Charge (m/z) Component RT: 37.1194 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup> 151.0 Component 151.0 166.0 1.4 0.8 СНЗ 166.0 152.0 1.2 0.7 1 152.0 0.6 136.0 0.5 0.8 136.0 167.0 CH3 $0.4^{-}$

37.1

37.2

Acquisition Time (min)

0.6

0.4

0.2

37.1

37.2

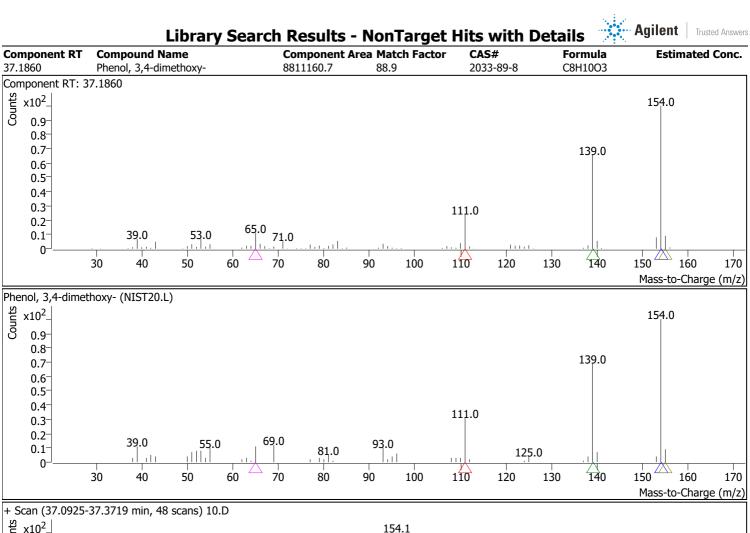
Acquisition Time (min)

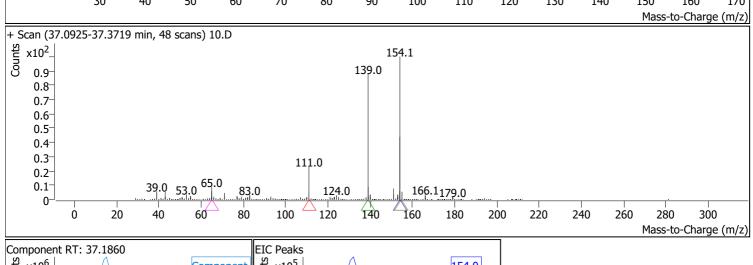
167.0

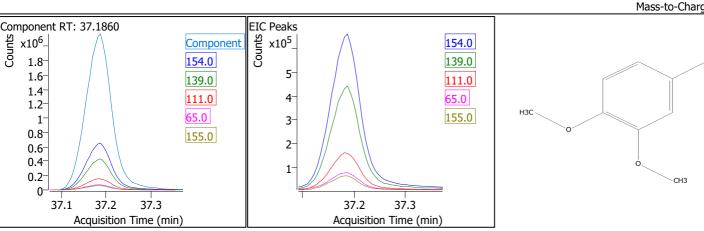
0.3

0.2

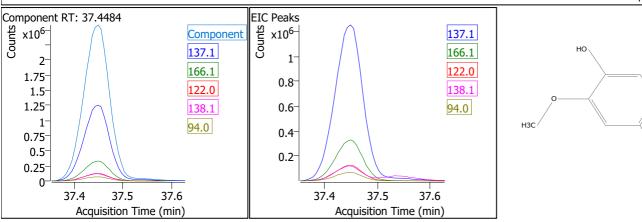
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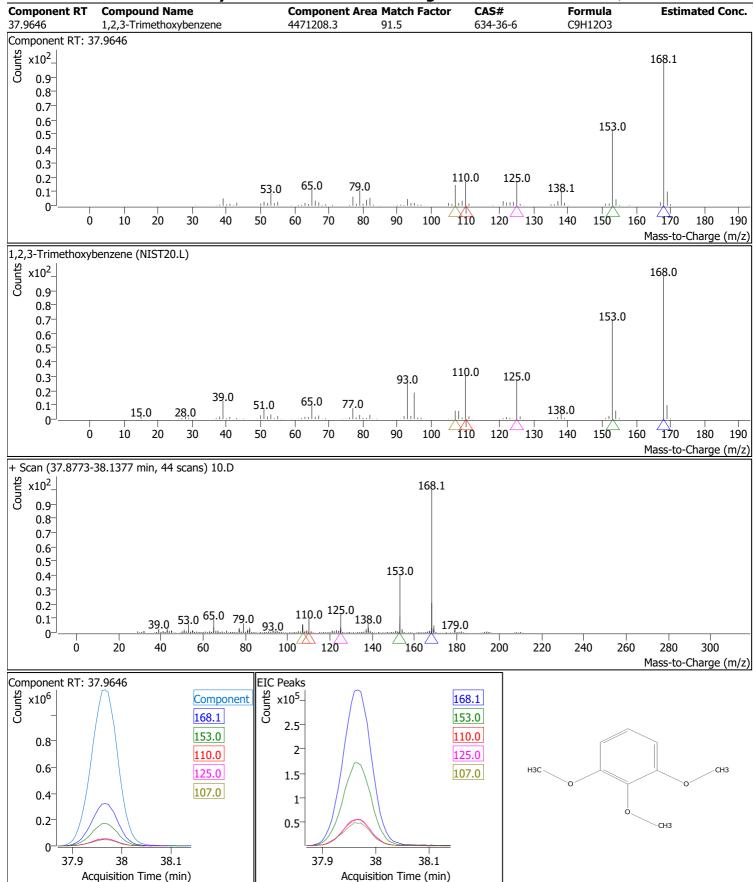


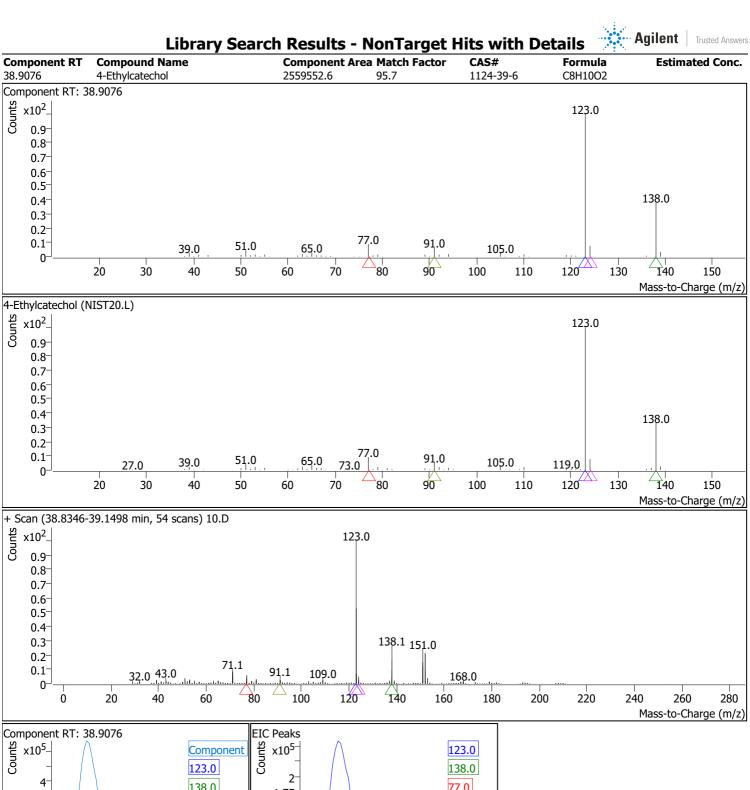
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4484 Phenol, 2-methoxy-4-propyl-9722226.6 C10H14O2 Component RT: 37.4484 v10<sup>2</sup> 0.9 137.1 0.8 0.7 0.6 0.5 0.4 0.3 166.1 0.2 122.0 0.1 94.0 77.0 65,0 105.0 160 170 120 10 20 30 40 50 60 70 80 100 110 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 150 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 180 Mass-to-Charge (m/z) + Scan (37.3541-37.6276 min, 47 scans) 10.D st x10<sup>2</sup> 0.9 137.1 0.8 $0.7^{-}$ 0.6 0.5 0.4 166.1 0.3 0.2 122.0 0.1 94.0 43.0 65.0,77.0 179.0 29.0 154.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 37.4484 Counts Counts x10<sup>6</sup> 137.1 Component 137.1 166.1 2 1

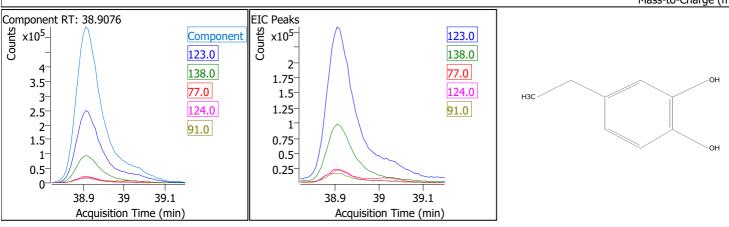


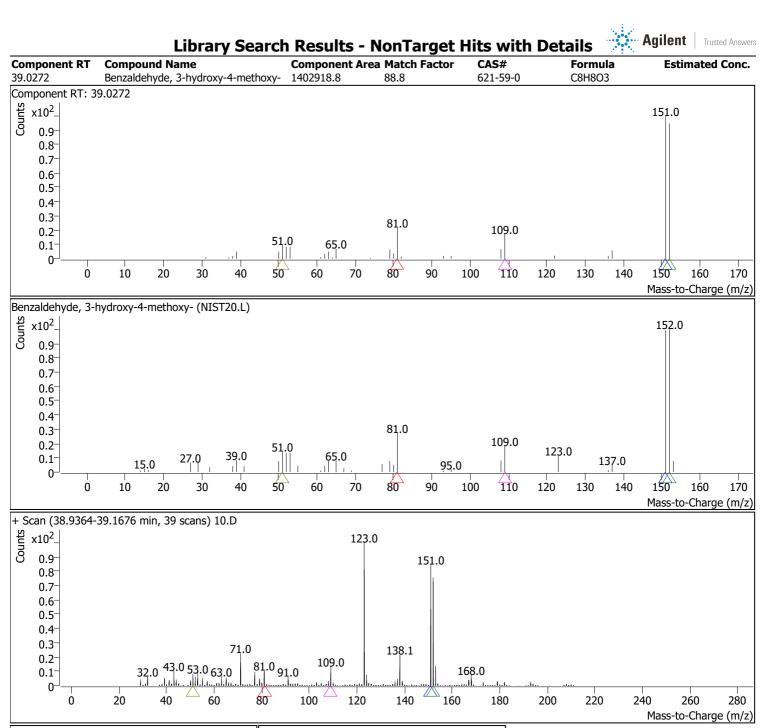


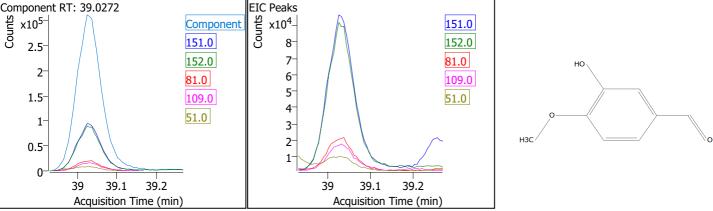


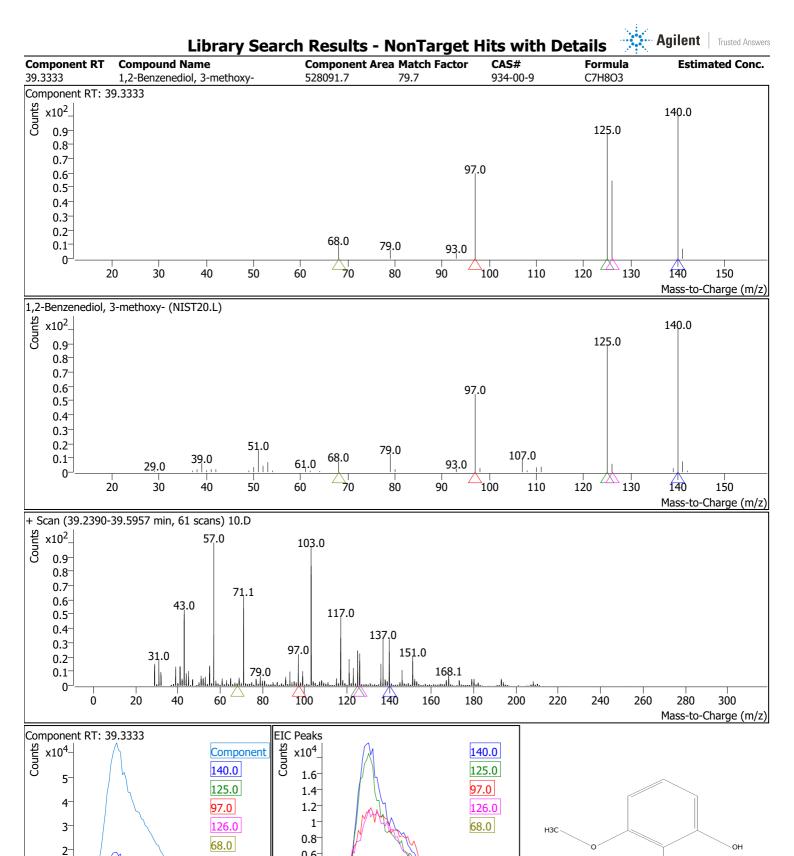


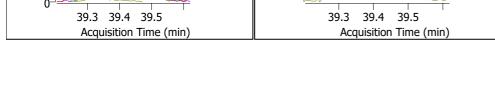








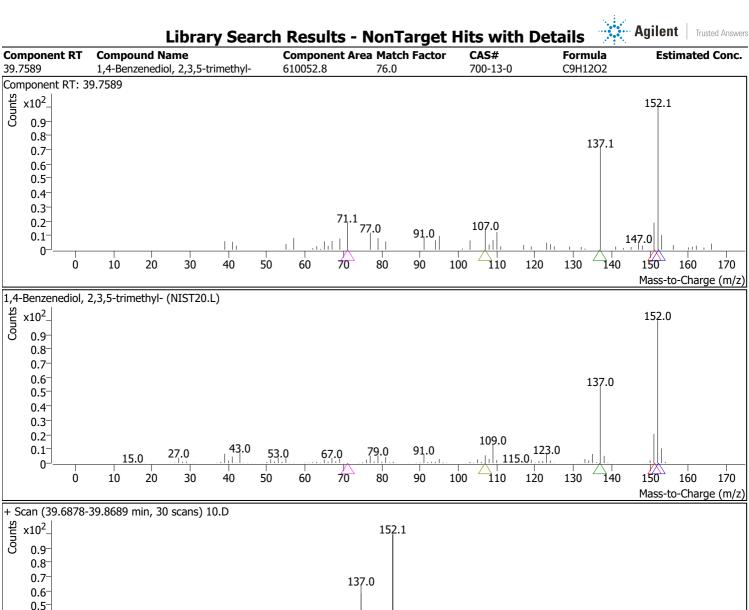


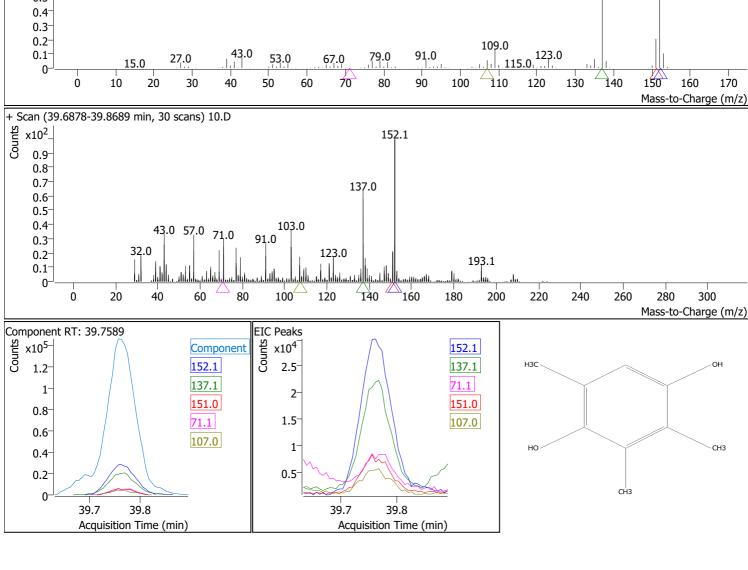


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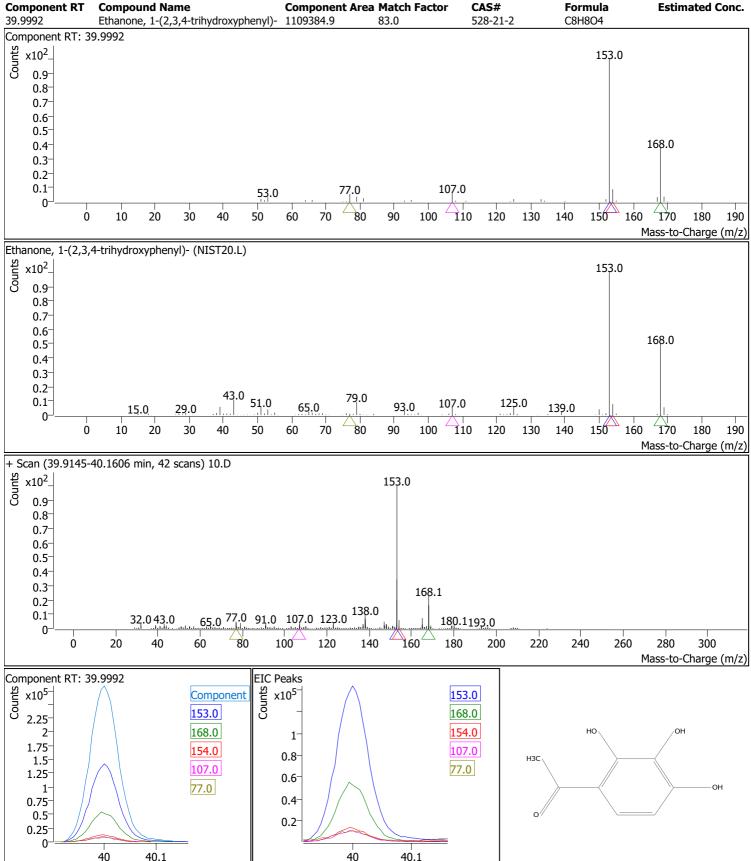
0.6 0.4

ОН



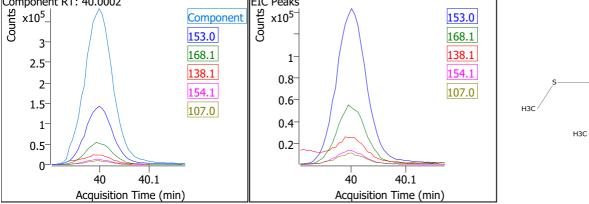




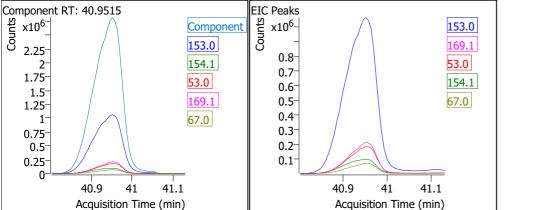


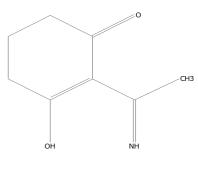
Acquisition Time (min)

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 40.0002 4-Methoxy-2-methyl-1-1543577.6 83.0 22583-04-6 C9H12OS (methylthio)benzene Component RT: 40.0002 x10<sup>2</sup>\_ 153.0 0.9 8.0 0.7 0.6 0.5 168.1 0.4 0.3 138.1 $0.2^{-}$ 107.0 0.1 0-110 170 140 0 10 20 30 40 50 60 70 80 90 100 120 130 150 160 180 190 Mass-to-Charge (m/z) 4-Methoxy-2-methyl-1-(methylthio)benzene (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 153.0 0.6 0.5 0.4 0.3 138.0 0.2 109.0 45.0 0.1 77.0 84.0 91.0 65.0 125.0 28.0 0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 180 190 Mass-to-Charge (m/z) + Scan (39.9049-40.1725 min, 46 scans) 10.D st x10<sup>2</sup> 0.9 153.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 168.1 0.2 77.0 91.0 <sub>107.0</sub> 123.0 <sup>138.0</sup> 0.1 32.043.0 180.1193.1 63.0 0 Ó 40 60 80 100 120 140 20 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 40.0002 **EIC Peaks** Counts Counts x10<sup>5</sup> 153.0 x10<sup>5</sup>. Component 153.0 168.1 3 168.1 138.1 1 2.5 138.1 154.1 0.8 2



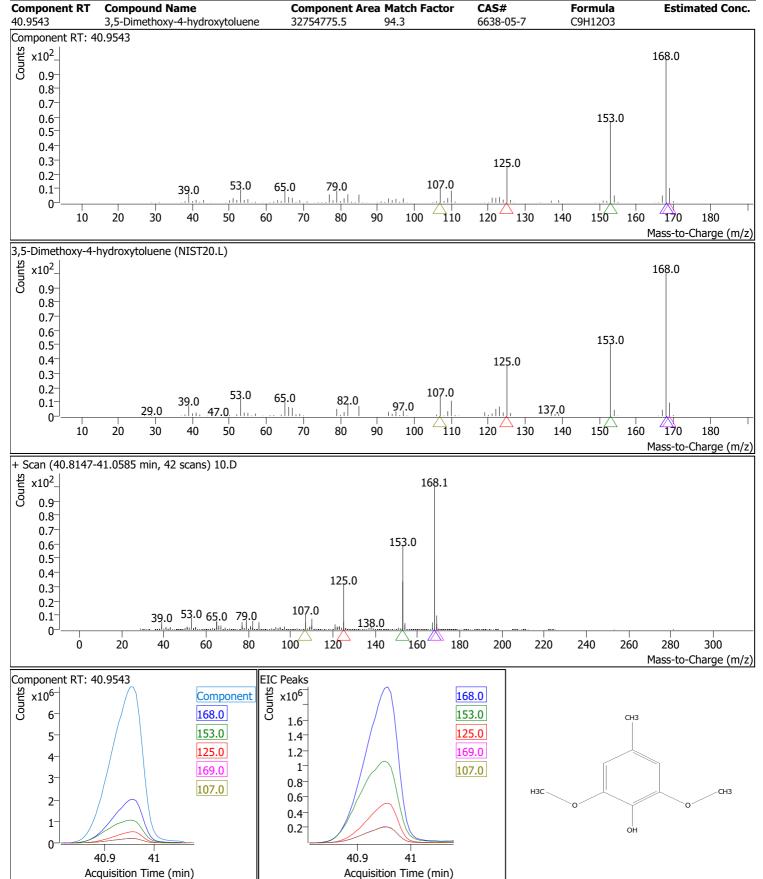
## --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 40.9515 2-Cyclohexen-3-ol-1-one, 2-[1-13629249.6 81.5 1000131-52-4 C8H11NO2 iminoethyl]-Component RT: 40.9515 x10<sup>2</sup>\_ 153.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 0.1 169.1 0-90 170 30 40 80 100 110 120 130 140 150 160 Mass-to-Charge (m/z) 2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]- (NIST20.L) $x10^{2}$ 153.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 83.0 97.0 125.0 112.0 138.0 0 60 170 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (40.8028-41.0585 min, 44 scans) 10.D st x10<sup>2</sup> 0.9 168.1 0.8 0.7 153.0 0.6 0.5 0.4 125.0 0.3 0.2 107.0 39.0 53.0 65.0 79.0 0.1 138.0 Ó 20 60 80 160 200 260 100 120 140 180 220 240 280 300 Mass-to-Charge (m/z) Component RT: 40.9515 **EIC Peaks** Counts Counts x10<sup>6</sup> x10<sup>6</sup>-153.0 Component 153.0 169.1 2.25 0.8 53.0 154.1 0.7 1.75 154.1 53.0 0.6



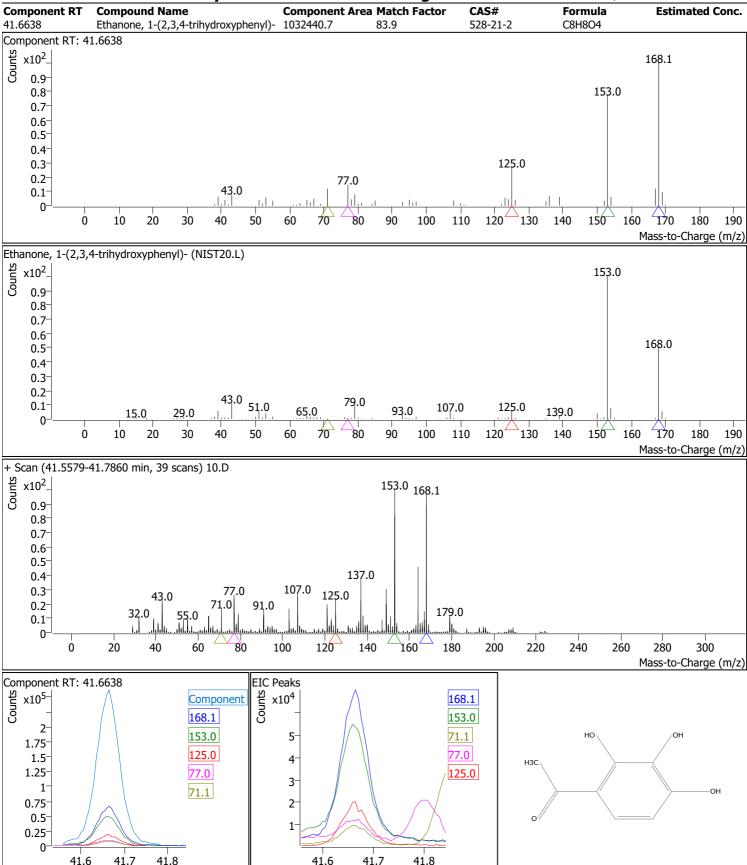




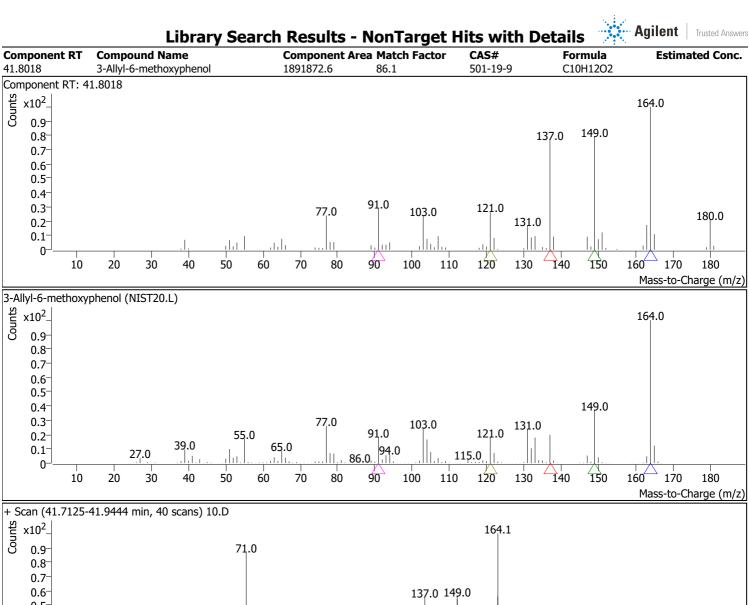


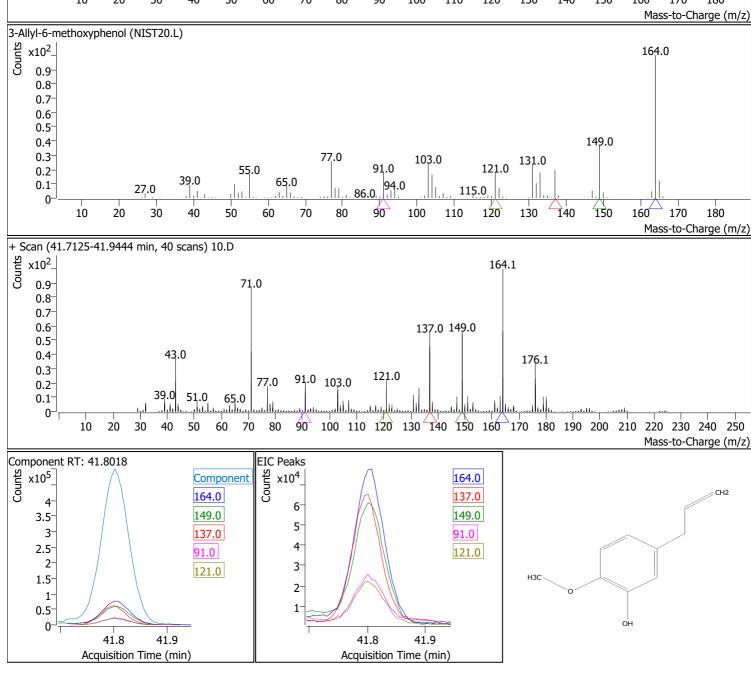






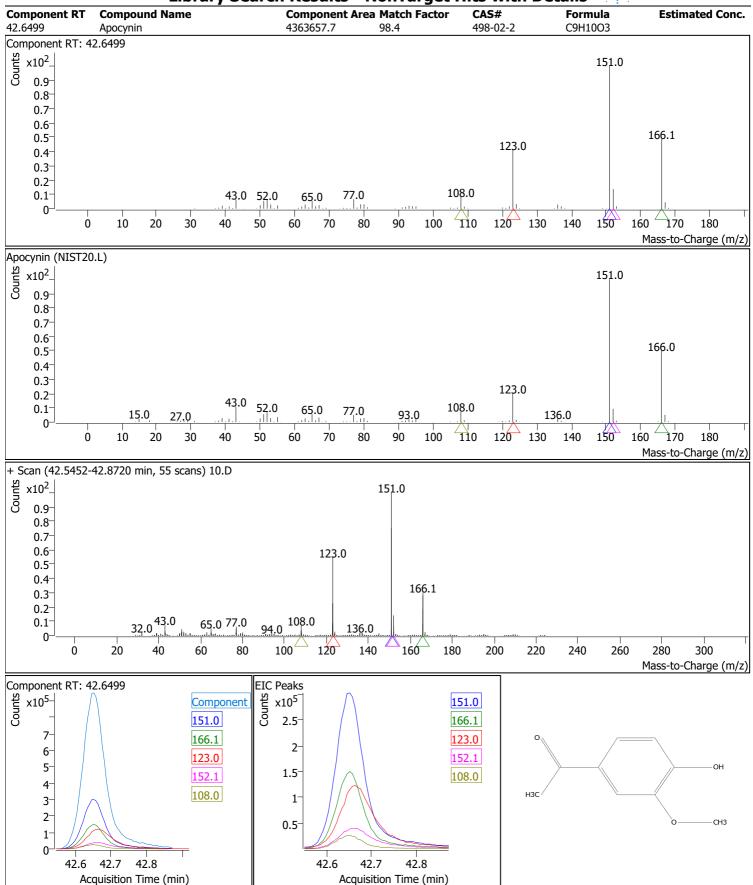
Acquisition Time (min)





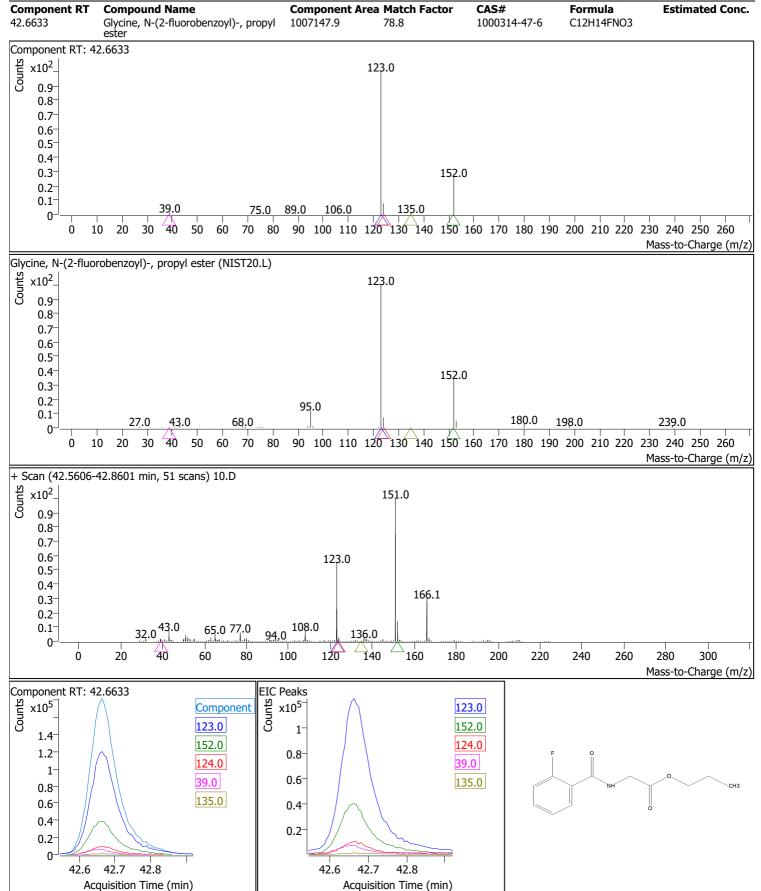






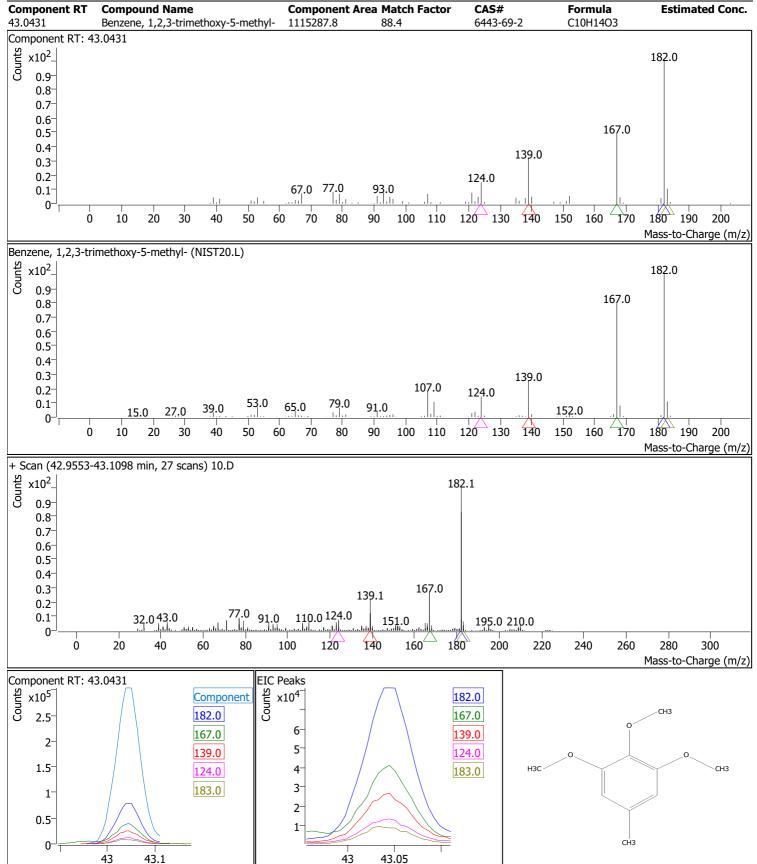
# **Library Search Results - NonTarget Hits with Details**



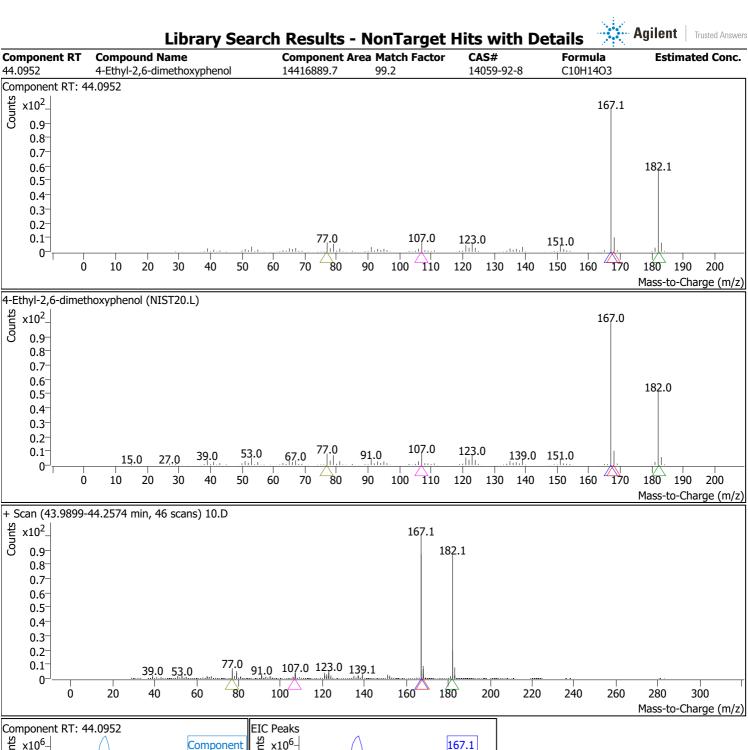


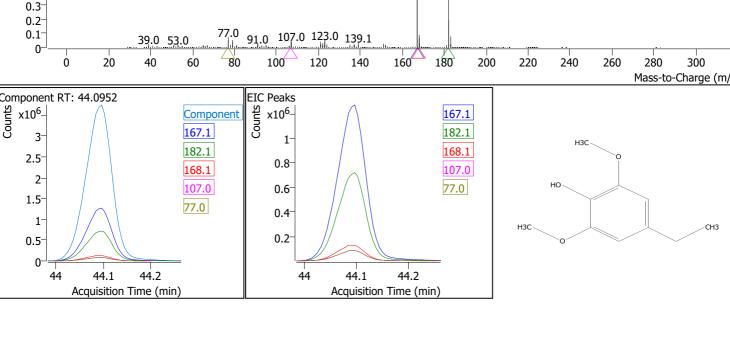






Acquisition Time (min)





#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 44.3392 2-Propanone, 1-(4-hydroxy-3-12973649.2 91.1 2503-46-0 C10H12O3 methoxyphenyl) Component RT: 44.3392 x10<sup>2</sup>\_ 137.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 $0.2^{-}$ 122.0 94.0 0.1 0-120 180 20 30 50 60 70 80 90 100 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 $0.7^{-}$ 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 66.0 85.0<sup>9</sup>1.0 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2285-44.5607 min, 56 scans) 10.D x10<sup>2</sup>. 137.1 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 180.1 74.0 87.0 0.2 43.0 55.0 122.0 0.1 94.0 153.0 171.1 0 100 140 180 Ó 20 40 60 80 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3392 **EIC Peaks** Counts Counts x10<sup>6</sup>x10<sup>6</sup> 137.1 Component 180.1 137.1 0.9 2 180.1 122.0 0.8 1.75 0.7 122.0 138.1 1.5 0.6

44.4

Acquisition Time (min)

44.5

94.0

138.1

94.0

 $0.5^{-}$ 

0.4

0.3

0.2

0.1

44.3

1.25

0.75

0.5

44.3

44.4

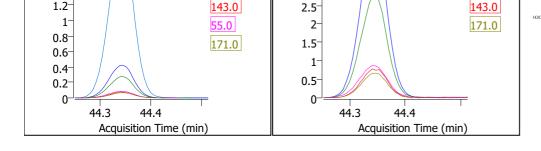
Acquisition Time (min)

44.5

0.25

1

# --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3436 Dodecanoic acid, methyl ester 6887321.2 84.4 111-82-0 C13H26O2 Component RT: 44.3436 v10<sup>2</sup> 0.9 74.0 0.8 87.0 $0.7^{-}$ 0.6 0.5 0.4 0.3 143.0 171.0 183.0 43.0 55.0 0.2 0.1 130 140 150 160 170 180 190 200 10 20 50 80 100 110 120 210 220 230 240 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 74.0 0.8 0.7 87.0 0.6 0.5 0.4 0.3 0.2 55.0 29.0 69.0 214.0 0.1 101.0 115.0 129.0 83.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) + Scan (44.2515-44.5131 min, 45 scans) 10.D st x10<sup>2</sup> 0.9 137.1 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 180.1 74.0 87.0 0.2 43.0 55.0 122.0 0.1 94.0 171.1 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3436 **EIC Peaks** x10<sup>6</sup> st x10<sup>5</sup>-74.0 Component 74.0 87.0 1.6



3

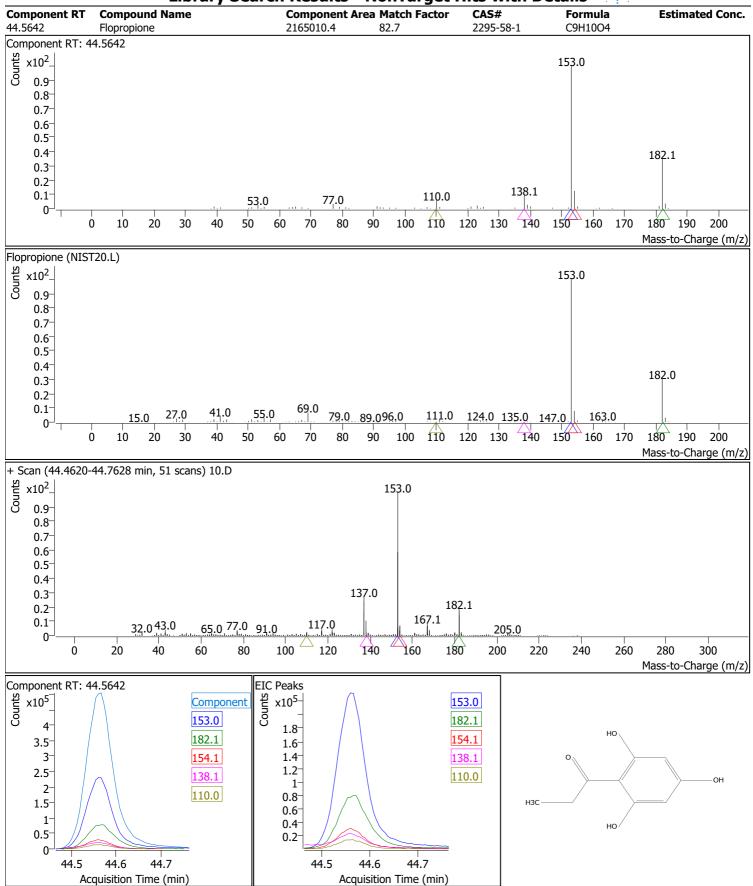
87.0

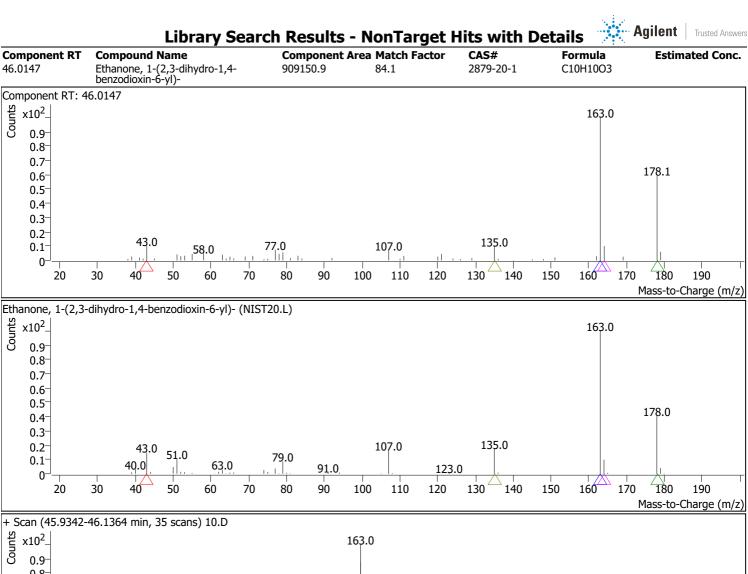
1.4

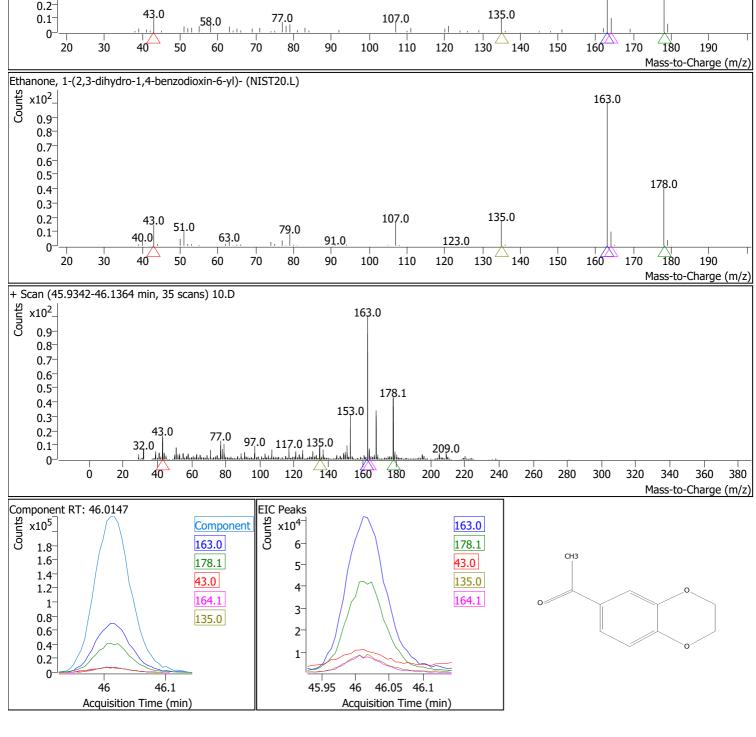
55.0











#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 1-Propanone, 1-(4-hydroxy-3-1835-14-9 46.5177 1286737.8 89.2 C10H12O3 methoxyphenyl)-Component RT: 46.5177 $x10^{2}$ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 $0.2^{-}$ 123.0 108.0 0.1 65.0 77.0 170.1 0-110 180 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 180.0 123.0 0.2 108.0 77.0 93.0 0.1 52.0 65.0 29.0 39.0 136.0 164.0 0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (46.4218-46.5942 min, 30 scans) 10.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 180.1 0.2 0.1 65.0 77.0 91.0 108.0 32.043.0 164.0 195.0 0 Ó 40 60 80 100 120 180 20 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 46.5177 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup> 151.0 Component СНЗ 180.1 151.0 1-180.1 123.0 2 123.0 0.8 152.1

46.5 46.55

Acquisition Time (min)

108.0

1.5

1

46.45 46.5 46.55 46.6

Acquisition Time (min)

0.5

152.1

108.0

0.6

0.4

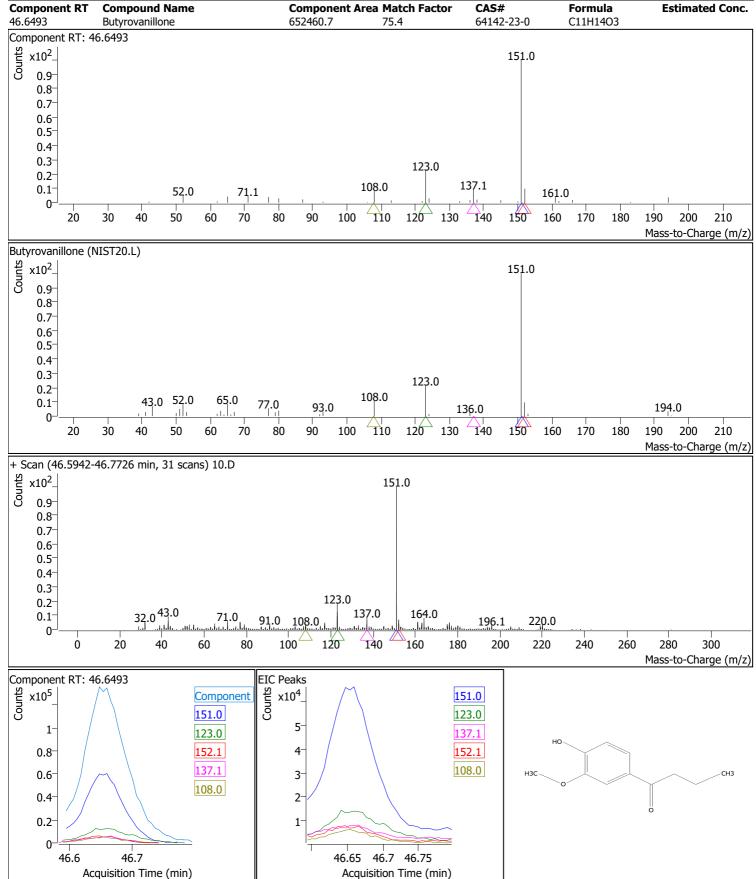
0.2

46.45

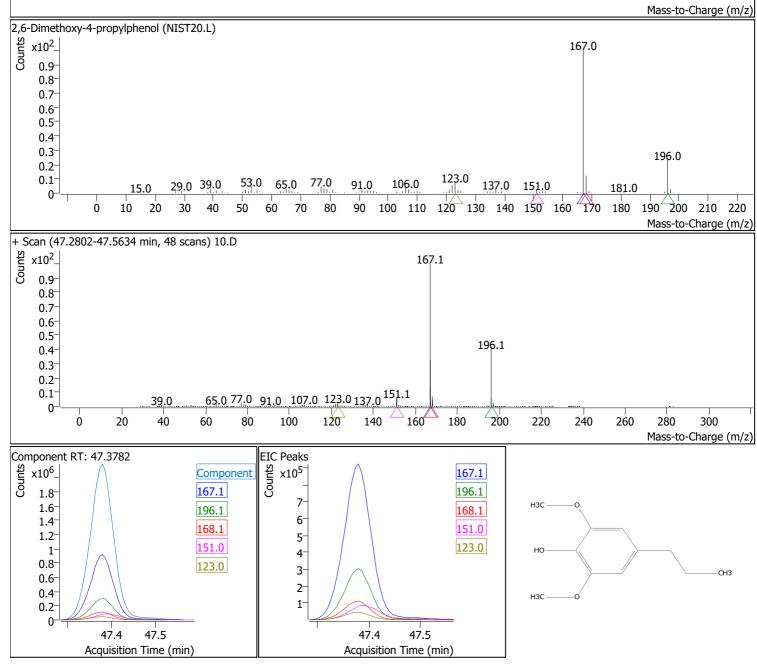
нзс







### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 6766-82-1 47.3782 2,6-Dimethoxy-4-propylphenol 8188459.8 95.8 C11H16O3 Component RT: 47.3782 y x10<sup>2</sup> 0.9 167.1 0.8 0.7 0.6 0.5 0.4 196.1 0.3 0.2 151.0 0.1 123.0 77.0 106.0 53.0 190 200 100 110 120 130 140 150 160 170 10 20 60 70 90 210 2,6-Dimethoxy-4-propylphenol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 167.0 0.8 0.7 0.6 0.5 0.4 0.3 196.0 0.2 0.1 77.0 53.0 29.0 39.0 106.0 91.0 151.0 181.0 120 130 140 150 160 170 180 190 200 10 20 50 60 70 80 100 110 + Scan (47.2802-47.5634 min, 48 scans) 10.D st x10<sup>2</sup> 0.9 167.1 0.8 $0.7^{-}$



#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 48.9922 Benzenepropanol, 4-hydroxy-3-3282726.2 89.4 C10H14O3 methoxy-Component RT: 48.9922 x10<sup>2</sup>\_ 137.1 0.9 8.0 0.7 0.6 0.5 182.1 0.4 0.3 $0.2^{-}$ 158.1 122.0 77.0 91.0 107.0 0.1 0-**140** 180 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 122.0 0.2 77.0 91.0 65.0 106.0 0.1 31.0 39.0 53.0 149.0 164.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (48.9019-49.2462 min, 58 scans) 10.D x10<sup>2</sup>. 137.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 182.1 0.3 0.2 65.0 77.0 91.0 107.0 122.0 158.1 0.1 32.043.0 194.1 0 Ó 40 60 120 140 180 260 20 80 100 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 48.9922 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup>– 137.1 Component 182.1 137.1 1.4 5 182.1 138.1 1.2 4 122.0 138.1 1 158.1 158.1 3 0.8



49

49.1

Acquisition Time (min)

49.2

122.0

2

1

49

49.1

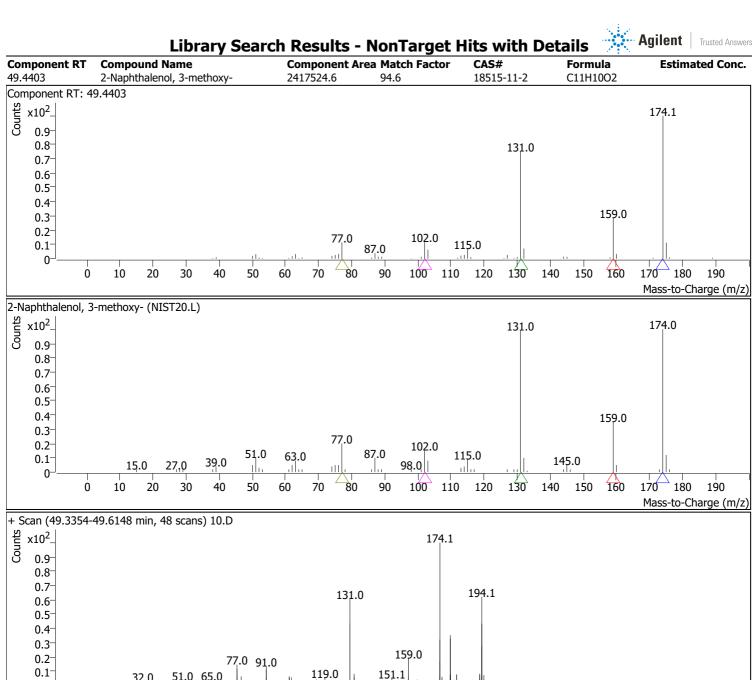
Acquisition Time (min)

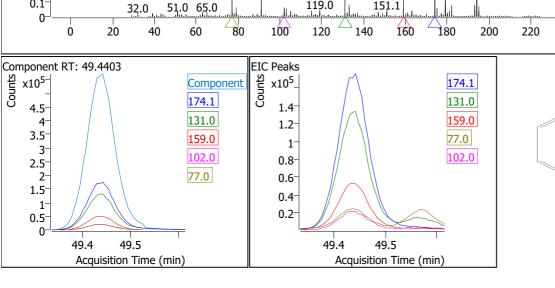
49.2

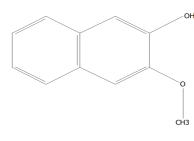
0.6

 $0.4^{\circ}$ 

0.2







260

280

300 Mass-to-Charge (m/z)

240

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 49.5695 (E)-2,6-Dimethoxy-4-(prop-1-en-1-2781323.1 88.0 C11H14O3 yl)phenol Component RT: 49.5695 x10<sup>2</sup>\_ 194.0 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 91.0 $0.2^{-}$ 119.0 133.0 77.0 151.0 163.0 0.1 0-0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 200 210 220 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 97.0 85.0 0 90 180 20 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4781-49.6505 min, 30 scans) 10.D st x10<sup>2</sup> 0.9 194.1 0.8 0.7 0.6 0.5 179.1 0.4 0.3 0.2 131.0 65.0 77.0 105.0119.0 151.1 32.043.0 0.1 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.5695 **EIC Peaks** Counts Counts x10<sup>5</sup> $x10^{5}$ 194.0 Component 179.0 194.0 1.4 5 **Н3С** 179.0 91.0 1.2 193.0 91.0 4 1-193.0 119.0 0.8 НО 3 119.0 0.6 2

49.6

Acquisition Time (min)

49.7

0.4

0.2

49.5

1

49.5

49.6

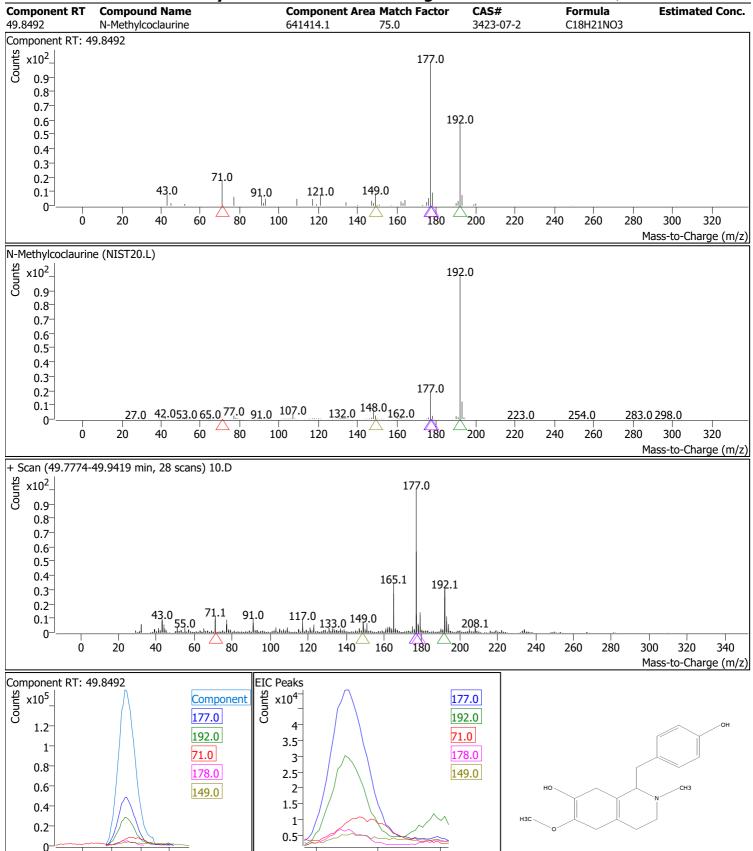
Acquisition Time (min)

49.7

НЗС







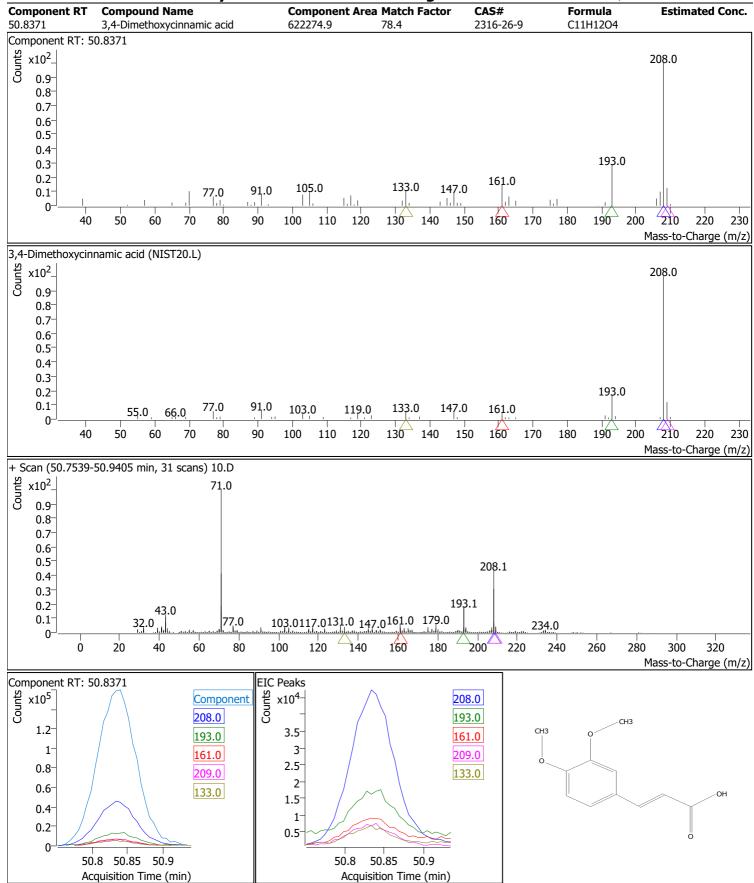
Acquisition Time (min)

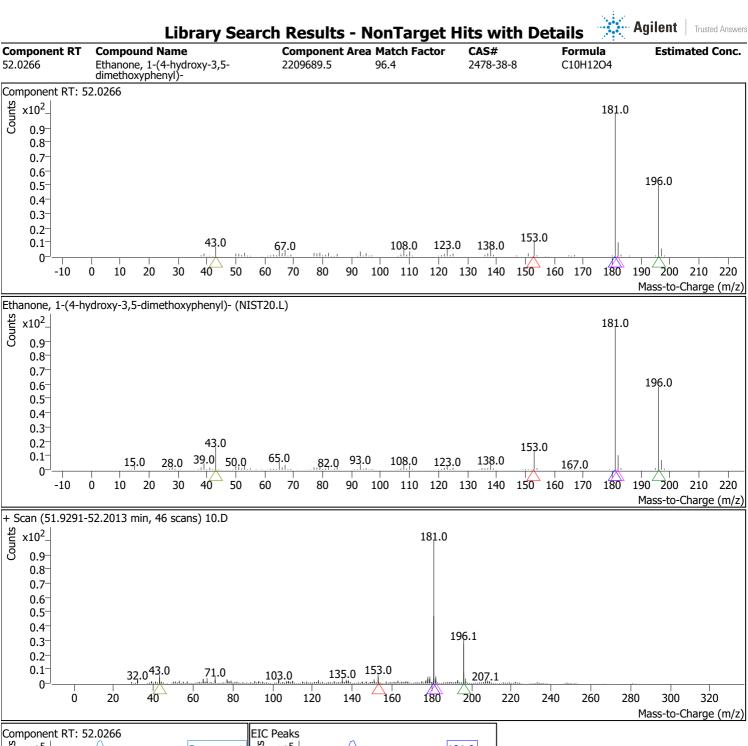
49.8

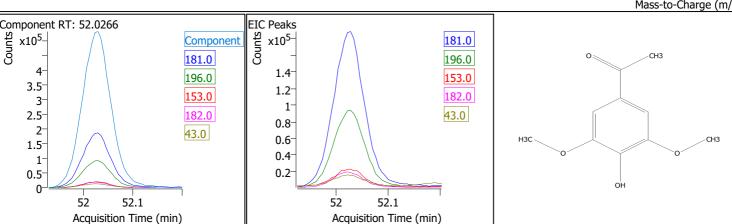
49.7 49.8 49.9

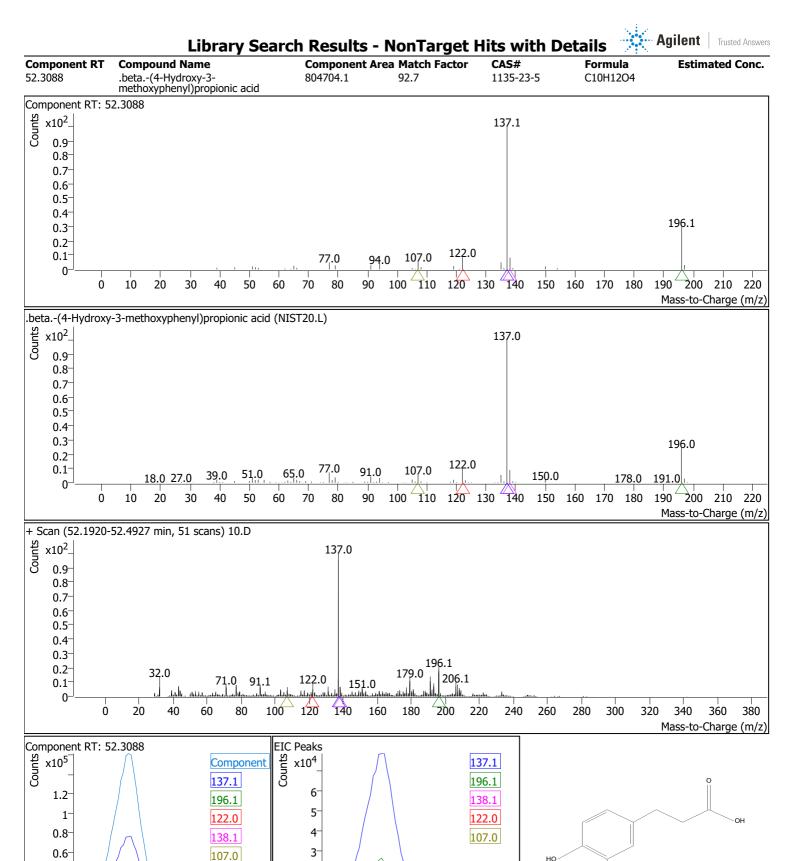












52.4

Acquisition Time (min)

2

0.4

0.2

52.3

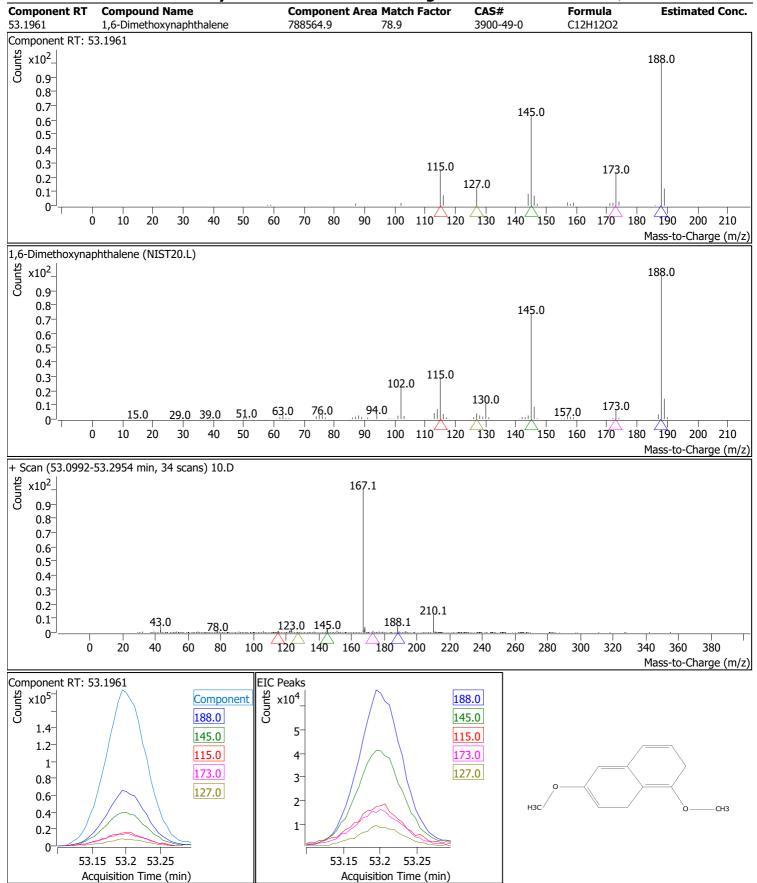
52.4

Acquisition Time (min)

СНЗ

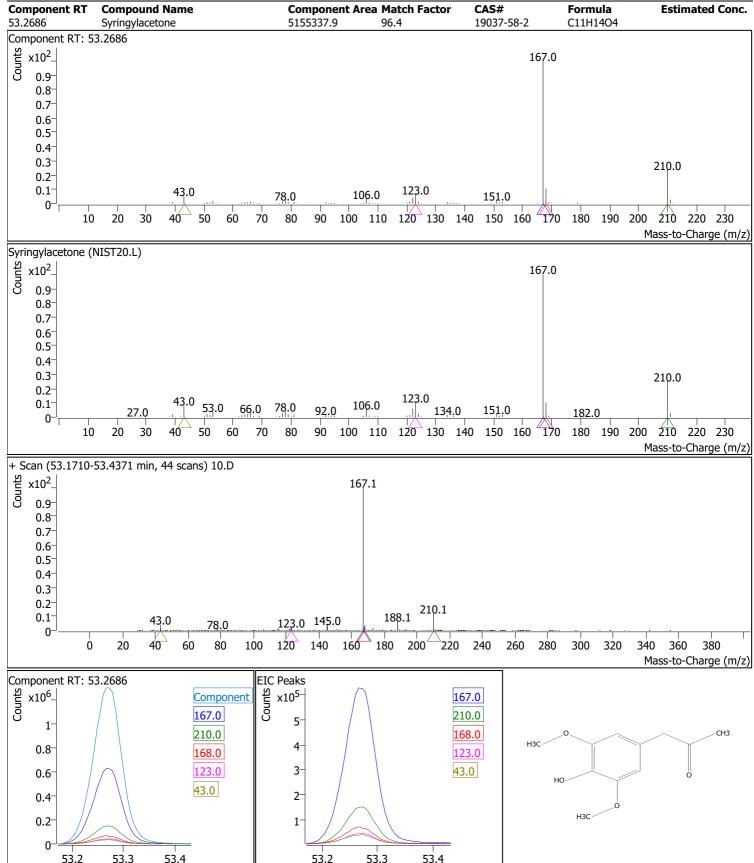


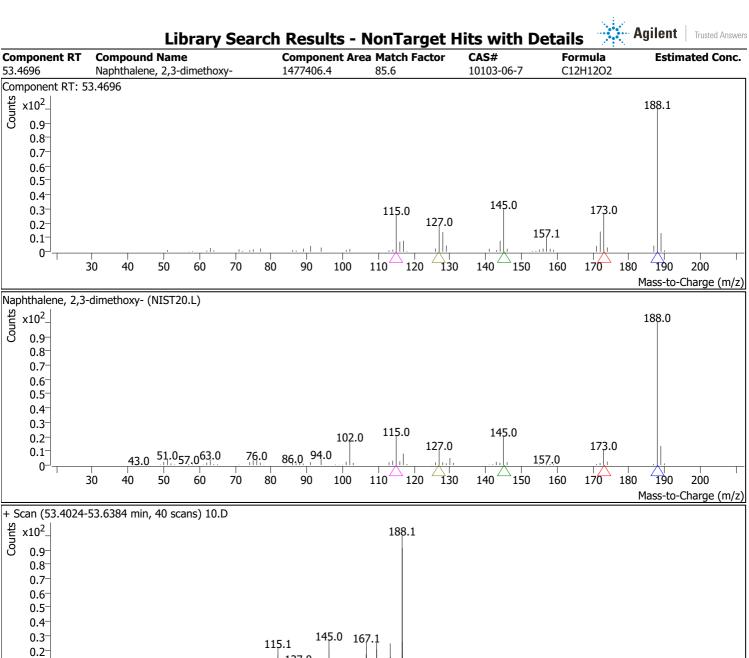


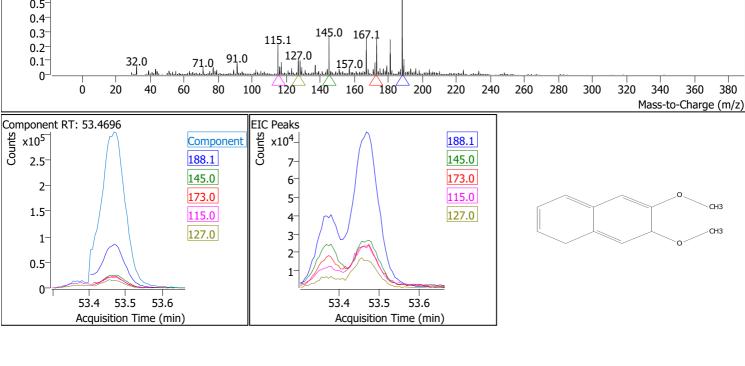






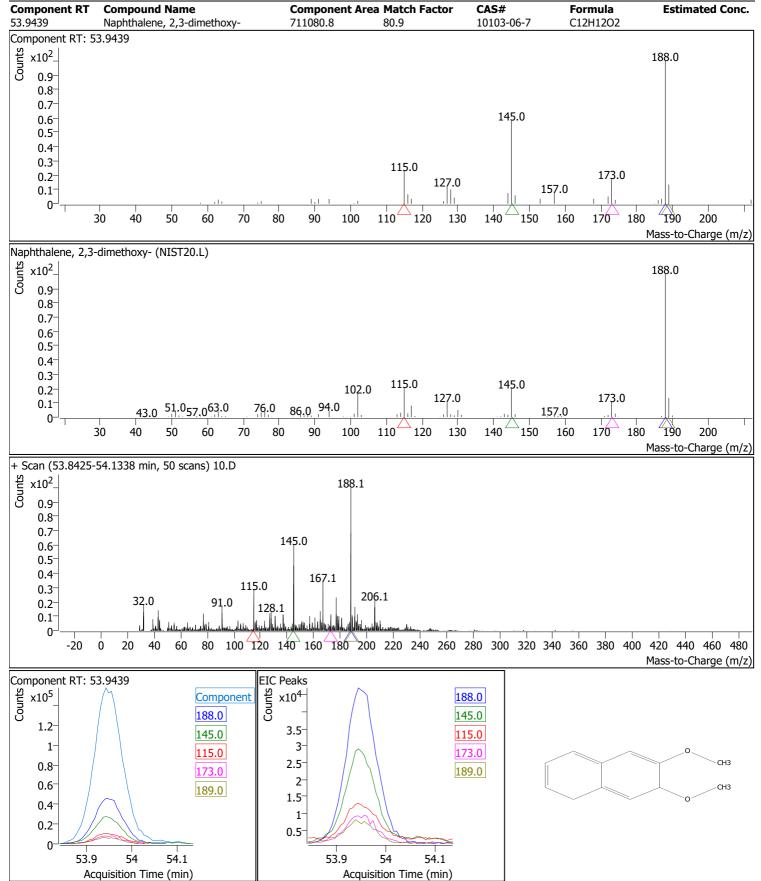






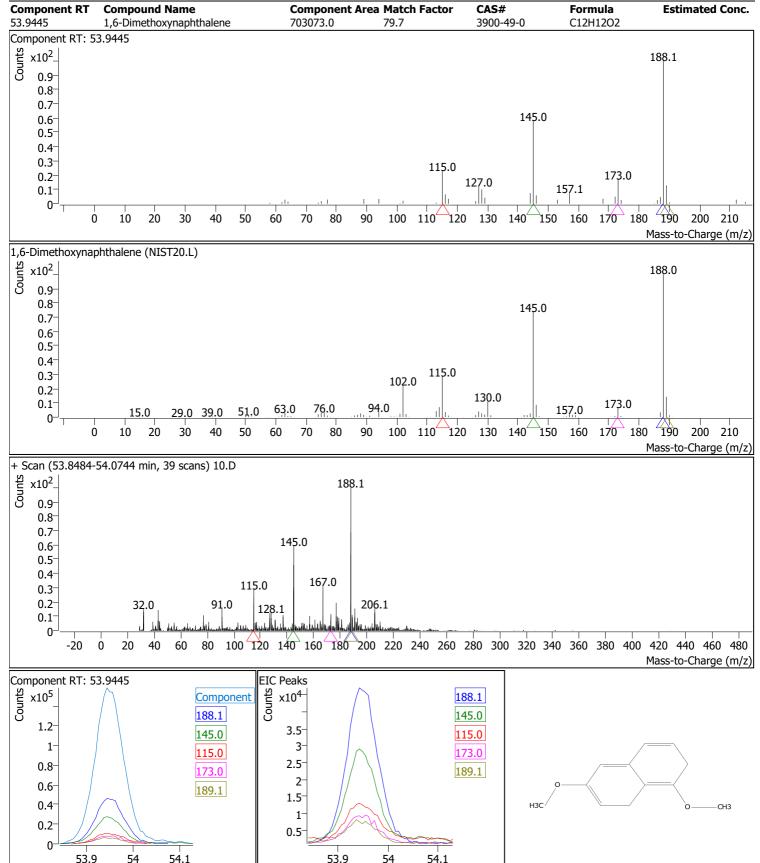




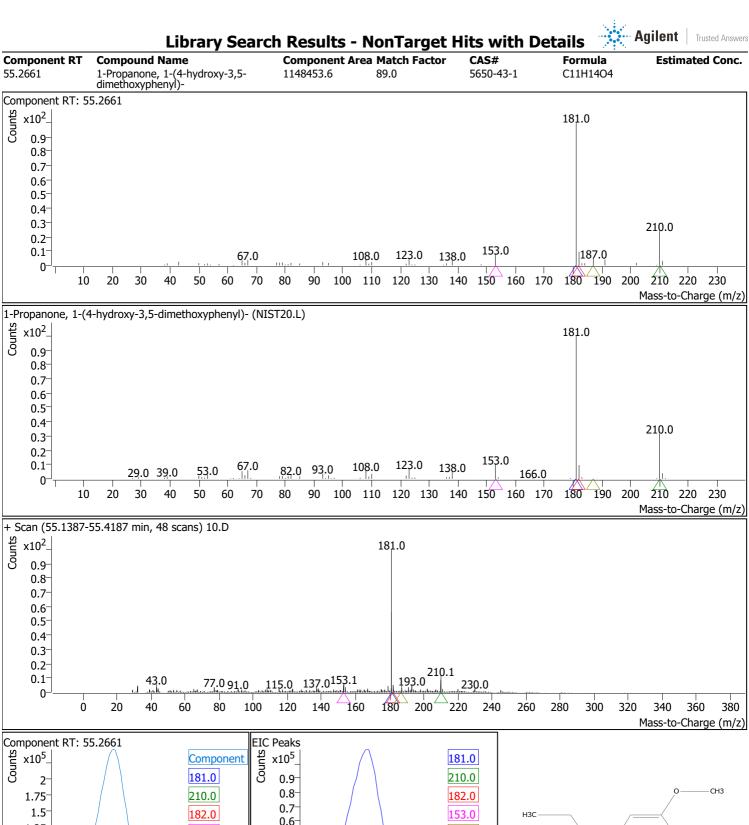


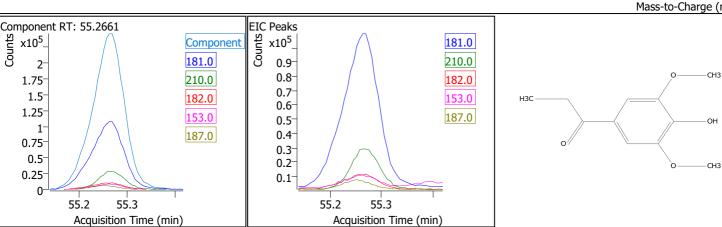
## **Library Search Results - NonTarget Hits with Details**





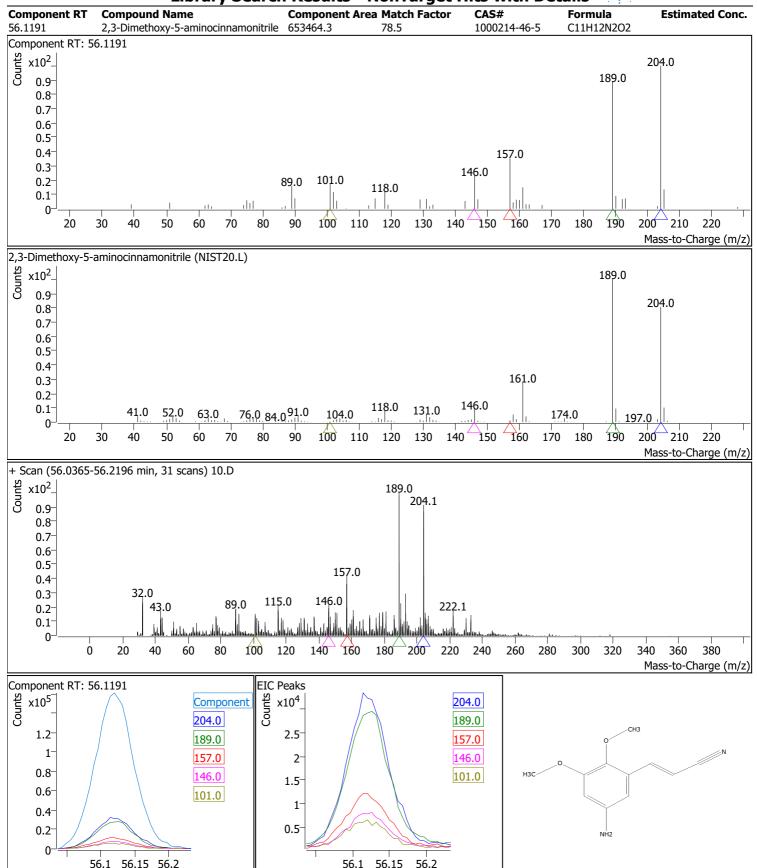
Acquisition Time (min)





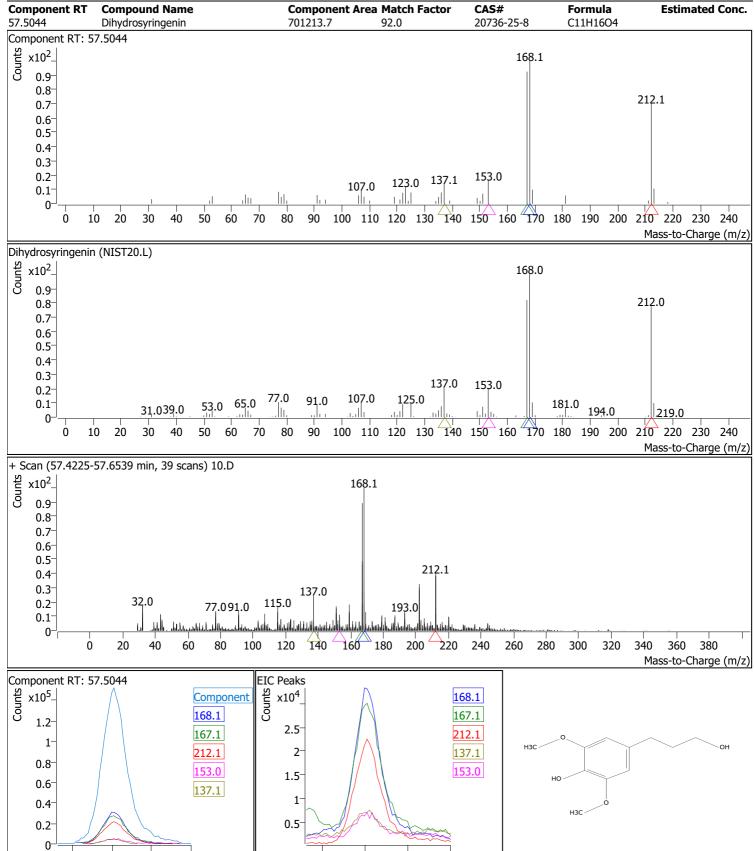












57.6

Acquisition Time (min)

57.4

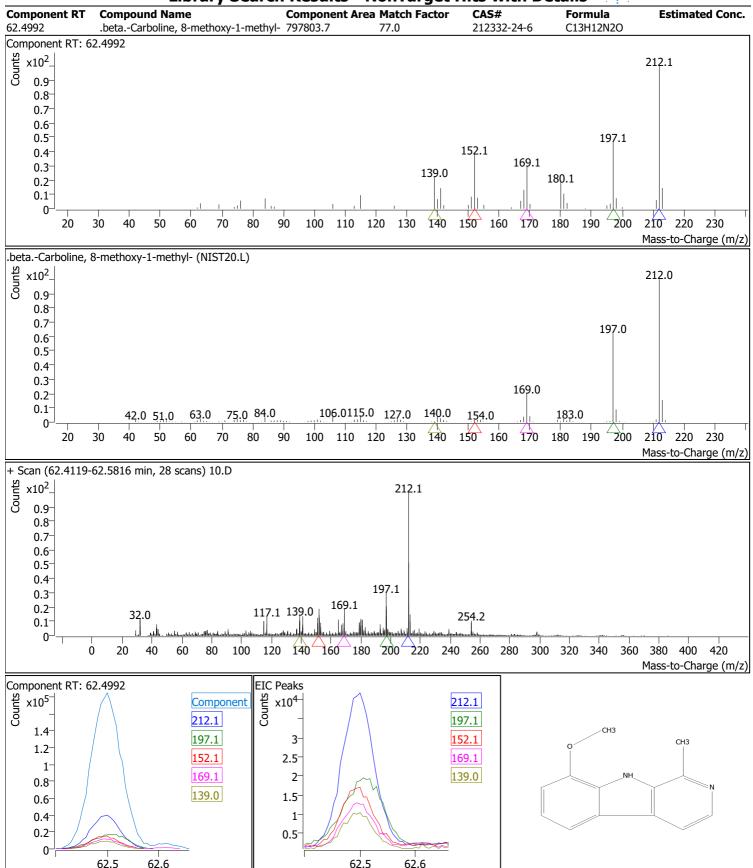
57.4

57.5

57.6

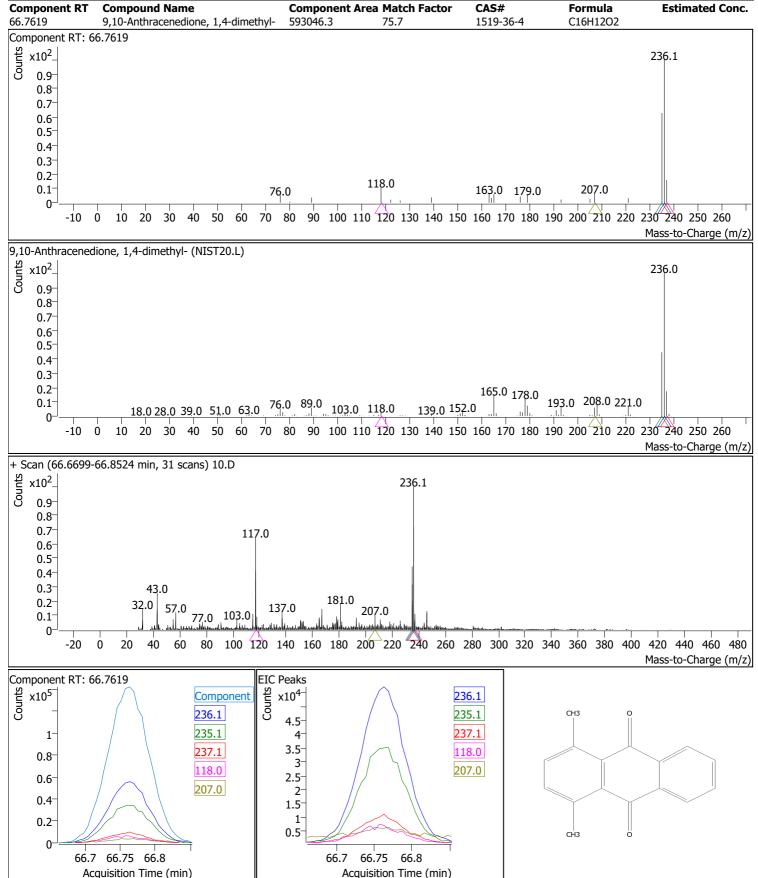






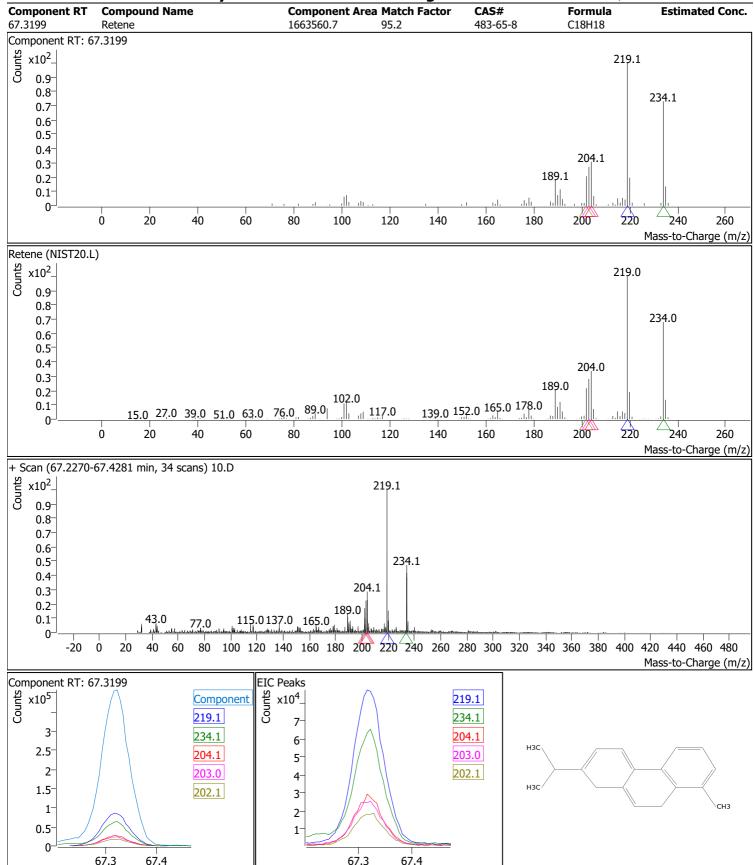






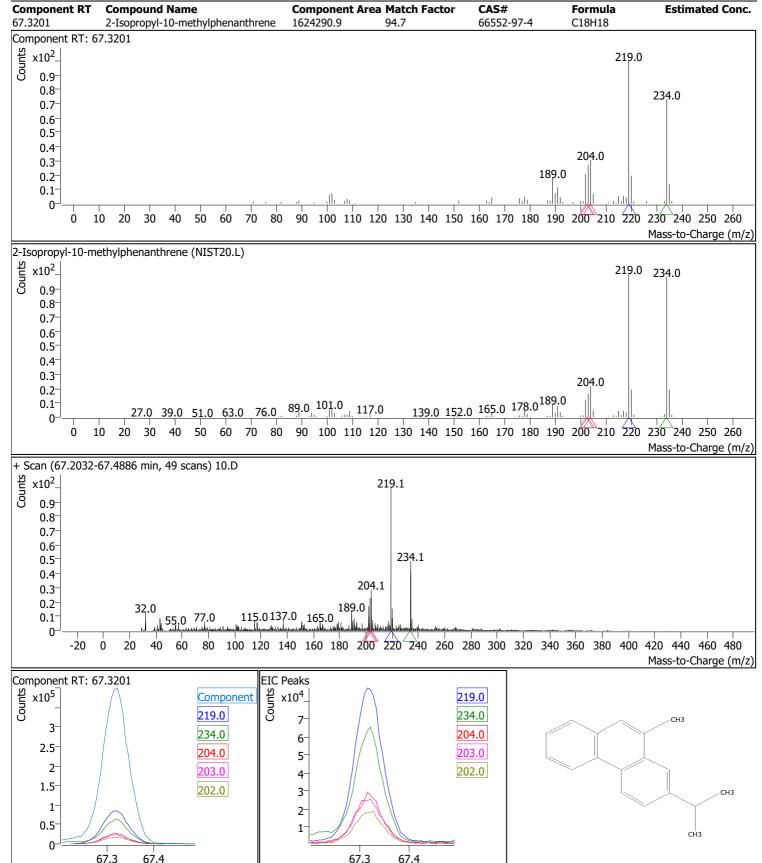






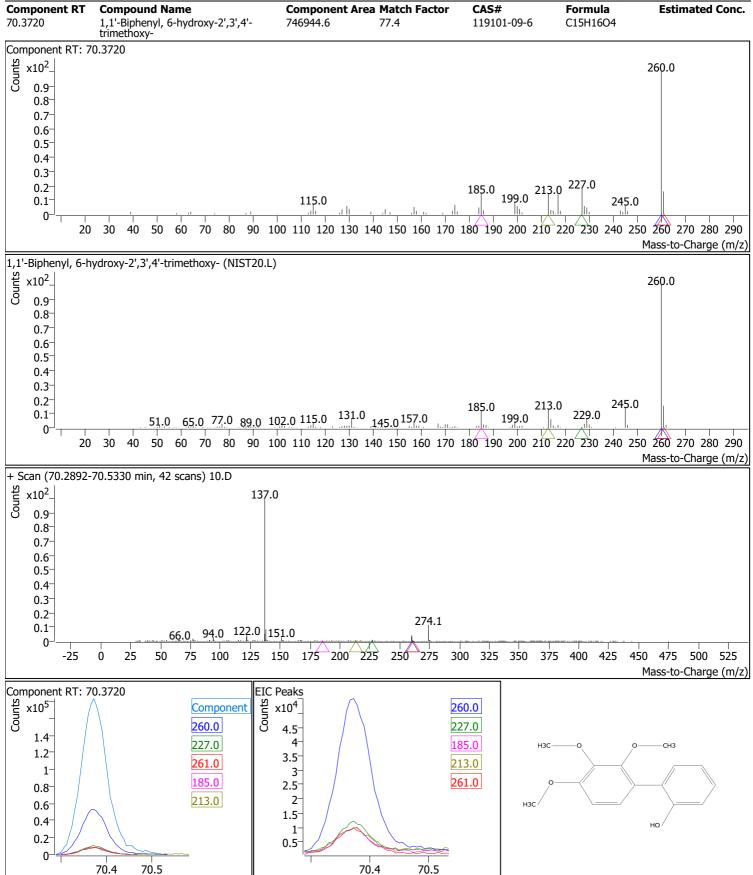






# **Library Search Results - NonTarget Hits with Details**

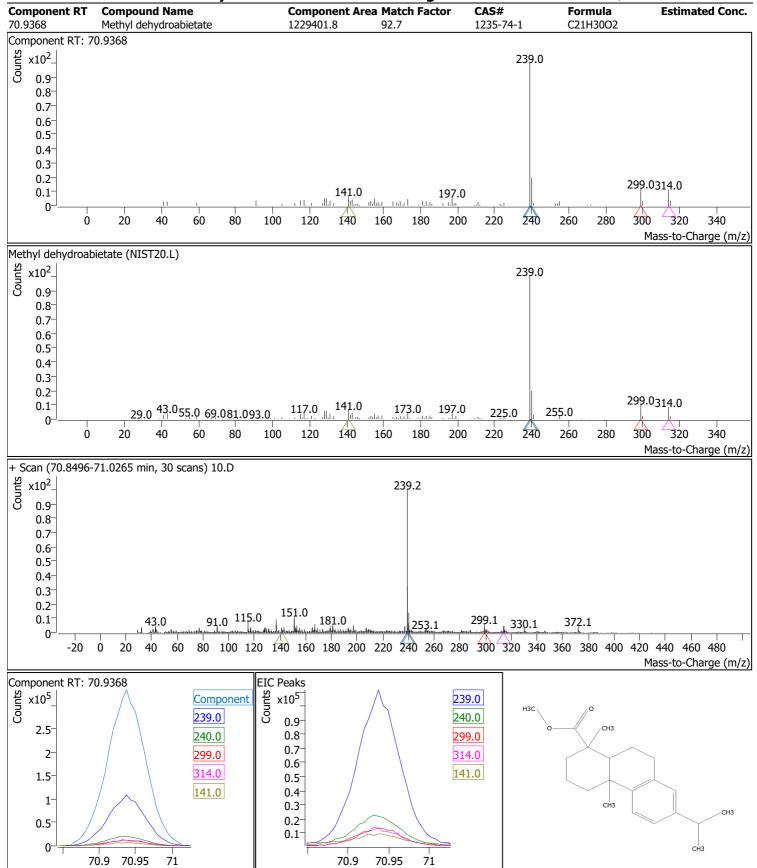


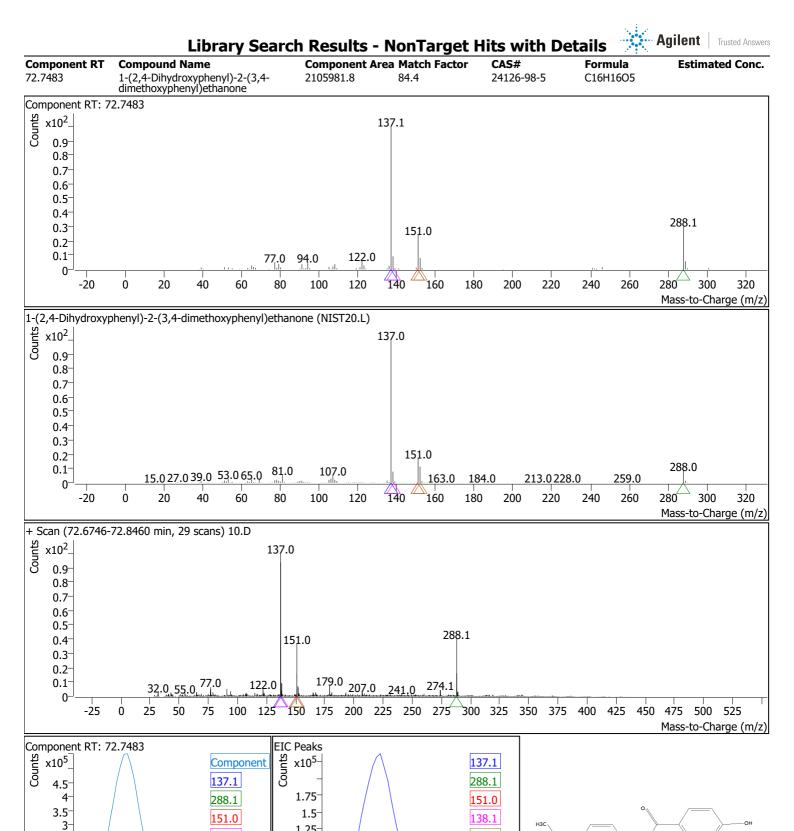


Acquisition Time (min)









Acquisition Time (min)

152.1

1.25

0.75

0.5 0.25

72.7

1

138.1

152.1

2.5

1.5

0.5

72.7

72.8

Acquisition Time (min)

2

Acquisition Time (min)

73.8

141.0

300.1

141.0

0.8

0.6

0.4

0.2

73.6

0.6

0.4

0.2

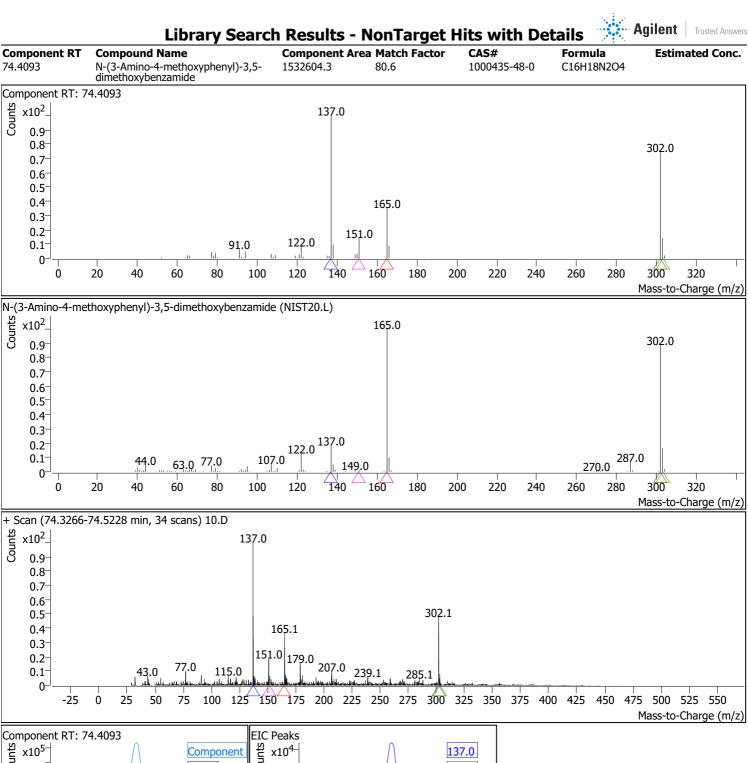
73.6

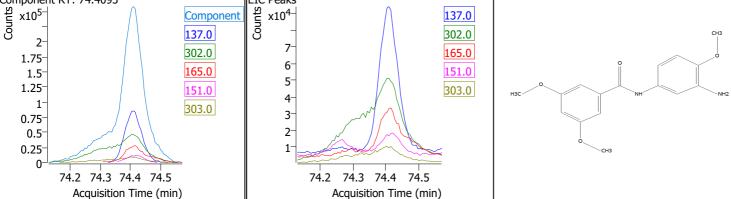
73.7

Acquisition Time (min)

73.8

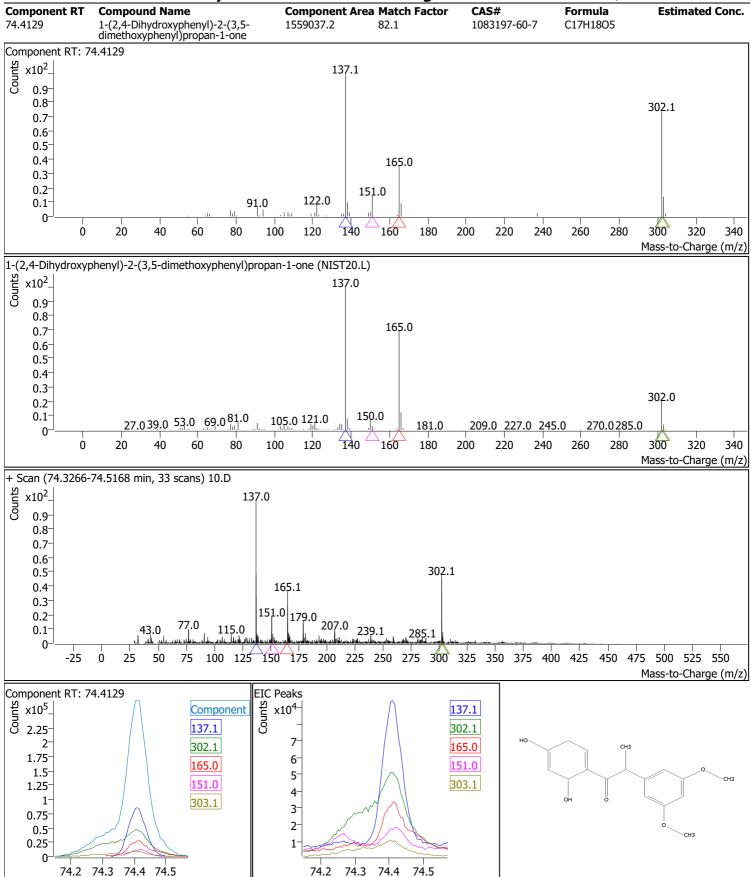
СНЗ



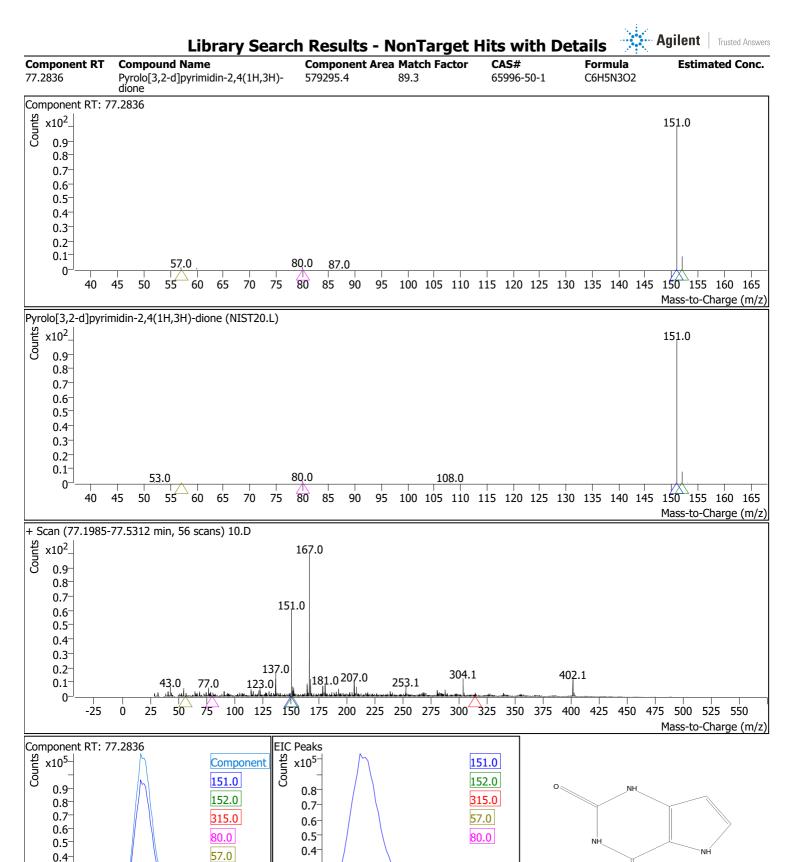


# **Library Search Results - NonTarget Hits with Details**





Acquisition Time (min)





Acquisition Time (min)

77.5

77.3

0.3

0.2

0.1

0.3

0.2

0.1

77.2

77.4