

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** 15.D **Path Name Sample Name** 15 **Sample Type** Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

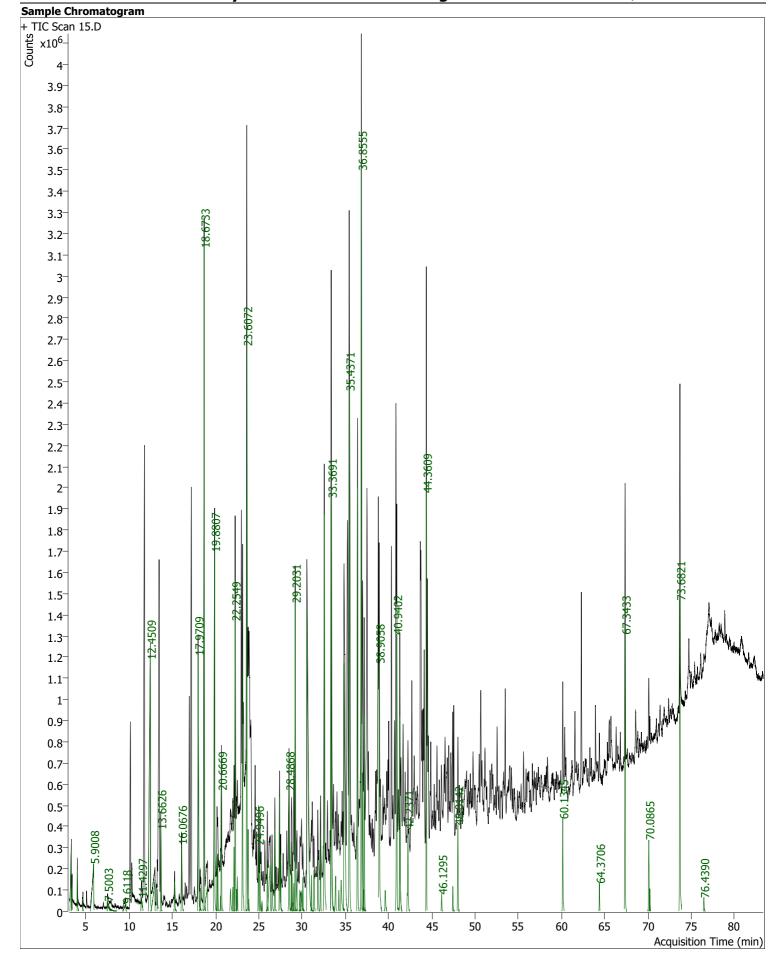
Acq. Date-Time 5/2/2024 9:17:32 AM **Instrument Name** GCMSD Dil. 1

| Component R | Γ Compound Name | CAS# | Formula | Component Area | Match Factor | Estimated Conc. |
|-------------|--|------------------------|------------------|-------------------|--------------|--------------------|
| 3.3165 | Propanoic acid | 79-09-4 | C3H6O2 | 1344443.4 | 97.7 | |
| 3.4054 | 2-Propenoic acid | 79-10-7 | C3H4O2 | 232828.2 | 87.2 | |
| 4.0054 | Propylene Glycol | 57-55-6 | C3H8O2 | 549350.3 | 88.4 | |
| 4.6609 | Propanoic acid, 2-methyl- | 79-31-2 | C4H8O2 | 157512.9 | 87.7 | |
| 5.9008 | Butanoic acid | 107-92-6 | C4H8O2 | 2572279.7 | 94.6 | |
| 7.4992 | Trimethylene oxide | 503-30-0 | C3H6O | 496165.7 | 86.0 | |
| 7.5003 | 1,3-Propanediol | 504-63-2 | C3H8O2 | 695898.1 | 85.2 | |
| 9.6118 | Butanoic acid, 2-methyl- | 116-53-0 | C5H10O2 | 369696.9 | 86.1 | |
| 11.4297 | Ethanol, 2,2'-oxybis- | 111-46-6 | C4H10O3 | 539968.4 | 91.5 | |
| 11.4303 | Methylal | 109-87-5 | C3H8O2 | 502169.0 | 89.2 | |
| 12.4509 | Butyrolactone | 96-48-0 | C4H6O2 | 9899495.5 | 97.7 | |
| 12.9909 | Pentanoic acid | 109-52-4 | C5H10O2 | 1885123.3 | 95.1 | |
| 13.2568 | Methyltartronic acid | 595-98-2 | C4H6O5 | 386988.3 | 93.0 | |
| 13.6626 | 2,5-Hexanedione | 110-13-4 | C6H10O2 | 1466424.5 | 94.6 | |
| 15.2585 | 2(3H)-Furanone, dihydro-5-methyl- | 108-29-2 | C5H8O2 | 674136.2 | 94.1 | |
| 16.0676 | 2-Cyclopenten-1-one, 3-methyl- | 2758-18-1 | C6H8O | 1559356.4 | 98.0 | |
| 17.9709 | Phenol | 108-95-2 | C6H6O | 5949135.3 | 97.5 | |
| 18.2187 | 2-Cyclopenten-1-one, 2,3-dimethyl- | 1121-05-7 | C7H10O | 434331.4 | 90.2 | |
| 18.6733 | 1,3-Dioxolane-4-methanol, 2-ethyl- | 53951-44-3 | C6H12O3 | 13578997.9 | 86.0 | |
| 19.0611 | Pentanoic acid | 109-52-4 | C5H10O2 | 1435408.7 | 89.2 | |
| 19.8807 | 1,3-Dioxolane-4-methanol, 2-ethyl- | 53951-44-3 | C6H12O3 | 7758870.6 | 94.8 | |
| 20.1635 | 3,6-Heptanedione | 1703-51-1 | C7H12O2 | 985528.1 | 87.7 | |
| 20.2516 | 2-Cyclopenten-1-one, 2-hydroxy-3-methyl- | 80-71-7 | C6H8O2 | 1512958.6 | 90.5 | |
| 20.5770 | 2-Acetyl-5-methylfuran | 1193-79-9 | C7H8O2 | 278734.2 | 85.2 | |
| 20.6669 | 2-Cyclopenten-1-one, 2,3-dimethyl- | 1121-05-7 | C7H10O | 2435274.1 | 95.6 | |
| 21.7216 | 2(3H)-Furanone, dihydro-3-methyl- | 1679-47-6 | C5H8O2 | 638090.1 | 86.3 | |
| 21.9934 | 2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl- | 21835-00-7 | C7H10O2 | 475887.6 | 86.3 | |
| 22.1267 | 2-Cyclopenten-1-one, 3,4,5-trimethyl- | 55683-21-1 | C8H12O | 1181804.8 | 94.0 | |
| 22.2549 | Phenol, 2-methyl- | 95-48-7 | C7H8O | 5361966.1 | 98.5 | |
| 22.4317 | Acetophenone | 98-86-2 | C8H8O | 670685.4 | 89.0 | |
| 22.5151 | Pentanoic acid, 4-oxo-, ethyl ester | 539-88-8 | C7H12O3 | 596223.2 | 91.6 | |
| 23.1102 | 1-Octanol | 111-87-5 | C8H18O | 4899098.9 | 94.7 | |
| 23.6072 | Phenol, 2-methoxy- | 90-05-1 | C7H8O2 | 10847074.2 | 97.5 | |
| 23.7576 | 2-Cyclopenten-1-one, 2,3,4-trimethyl- | 28790-86-5 | C8H12O | 1879891.8 | 85.5 | |
| 23.8333 | 3,3-Diisopropyl-N-methylazetidin-2,4-dione | 1000305-99-4 | C10H17NO2 | 213482.6 | 85.0 | |
| 24.9496 | Phenol, 2,6-dimethyl- | 576-26-1 | C8H10O | 1172958.7 | 96.3 | |
| 25.1193 | 2-Oxepanone | 502-44-3 | C6H10O2 | 1405285.7 | 90.4 | |
| 25.2360 | Benzenemethanol, .alphamethyl- | 98-85-1 | C8H10O | 125876.7 | 87.0 | |
| 25.3677 | 1,3-Benzenediamine, 4-methoxy- | 615-05-4 | C7H10N2O | 154012.0 | 86.5 | |
| 25.9845 | 5-Ethyl-2-furaldehyde | 23074-10-4 | C7H8O2 | 1088595.0 | 89.2 | |
| 26.3112 | Pentanoic acid, 2-methyl-4-oxo- | 6641-83-4 | C6H10O3 | 2293524.1 | 89.7 | |
| 26.5265 | 3,3-Dimethylcyclohexanone | 2979-19-3 | C8H14O | 1229432.6 | 87.8 | |
| 26.8530 | Phenol, 2-ethyl- | 90-00-6 | C8H10O | 1440345.0 | 94.6 | |
| 27.3873 | Phenol, 2,4-dimethyl- | 105-67-9 | C8H10O | 1986020.1 | 97.9 | |
| 27.5164 | Phenol, 2,5-dimethyl- | 95-87-4 | C8H10O | 1059980.7 | 96.1 | |
| 28.4868 | 2-Methoxy-5-methylphenol | 1195-09-1 | C8H10O2 | 2300364.1 | 93.7 | |
| 28.7656 | Naphthalene | 91-20-3 | C10H8 | 1269718.1 | 93.8 | |
| 28.8332 | Phenol, 3,5-dimethyl- | 108-68-9 | C8H10O | 852935.7 | 89.1 | |
| 28.9564 | 7-Chloro-1-(4-fluorophenyl)heptan-1-one | 17135-47-6 | C13H16CIFO | 144694.5 | 86.3 | |
| 29.0471 | 2-Chloroethyl benzoate | 939-55-9 | C9H9ClO2 | 589719.2 | 85.3 | |
| 29.2031 | 2-Methoxy-5-methylphenol | 1195-09-1 | C8H10O2 | 5624516.3 | 98.6 | |
| 29.4084 | Octanoic acid | 124-07-2 | C8H16O2 | 1080701.5 | 88.3 | |
| 29.7404 | Phenol, 3,4-dimethyl- | 95-65-8 | C8H10O | 407488.5 | 88.2 | |
| 29.9192 | Propanoic acid, anhydride | 123-62-6 | C6H10O3 | 1289168.4 | 85.3 | |
| 29.9198 | Propanoic acid, annydride | 123-62-6 | C6H10O3 | 593423.4 | 92.7 | |
| 30.0917 | Phenol, 3,4,5-trimethyl- | 527-54-8 | C9H12O | 646726.3 | 89.2 | |
| 30.5509 | Catechol | 120-80-9 | C6H6O2 | 14962815.9 | 96.1 | |
| 31.0853 | Phenol, 4-propyl- | 645-56-7 | C9H12O | 637771.2 | 91.8 | |
| 31.3789 | Phenol, 4-propyi- Phenol, 2-ethyl-4-methyl- | 3855-26-3 | C9H12O C9H12O | 1046524.7 | 91.8 91.4 | |
| 31.8232 | Benzene, 1-ethyl-4-methoxy- | 1515-95-3 | C9H12O C9H12O | 1093050.4 | 90.3 | |
| | | 1515-95-3 1450-72-2 | | 1367848.8 | | |
| 32.1304 | Ethanone, 1-(2-hydroxy-5-methylphenyl)- | 1450-72-2 934-00-9 | C9H10O2 | 9709701.1 | 92.1 97.2 | |
| 32.5610 | 1,2-Benzenediol, 3-methoxy- | | C7H8O3 | | 97.2 86.1 | |
| 33.3371 | 1,2-Benzenediol, 3-methyl- | 488-17-5 | C7H8O2 | 9201686.0 | 86.1 | |
| 33.3691 | Phenol, 4-ethyl-2-methoxy- | 2785-89-9 | C9H12O2 | 9933698.5 | 95.5 | |

| Agilent |
|---------|
| 9 |

Trusted Answers

| Component R | T Compound Name | CAS# | Formula | Component Area | Match Factor | Estimated Conc. |
|-------------|--|--------------|-----------|-------------------|--------------|-----------------|
| 33.8864 | Nonanoic acid | 112-05-0 | C9H18O2 | 917992.5 | 86.7 | |
| 34.2548 | Naphthalene, 2-methyl- | 91-57-6 | C11H10 | 381449.1 | 90.2 | |
| 34.5116 | Hydroquinone | 123-31-9 | C6H6O2 | 1171954.3 | 88.6 | |
| 34.8424 | 1,2-Benzenediol, 3-methyl- | 488-17-5 | C7H8O2 | 10000448.5 | 93.4 | |
| 35.4371 | 2,3-Dimethylhydroquinone | 608-43-5 | C8H10O2 | 12044118.4 | 86.8 | |
| 36.4071 | 3,4-Dimethoxyphenol, 2-methylpropionate | 1000447-30-5 | C12H16O4 | 8291983.8 | 85.8 | |
| 36.8555 | Phenol, 2,6-dimethoxy- | 91-10-1 | C8H10O3 | 14455261.2 | 96.6 | |
| 36.9699 | 4-Ethylcatechol | 1124-39-6 | C8H10O2 | 3043824.4 | 86.4 | |
| 37.1191 | Ethanone, 1-(2-hydroxy-6-methoxyphenyl)- | 703-23-1 | C9H10O3 | 405177.8 | 89.7 | |
| 37.1741 | 3,4-Dimethoxyphenol, 2-methylpropionate | 1000447-30-5 | C12H16O4 | 3912079.6 | 87.4 | |
| 38.9058 | 4-Ethylcatechol | 1124-39-6 | C8H10O2 | 6138391.9 | 91.8 | |
| 39.6021 | Acetophenone, 4'-hydroxy- | 99-93-4 | C8H8O2 | 595504.7 | 88.6 | |
| 40.9402 | 3,5-Dimethoxy-4-hydroxytoluene | 6638-05-7 | C9H12O3 | 6495841.4 | 91.9 | |
| 41.2982 | Phenol, 4-ethyl-2-methoxy- | 2785-89-9 | C9H12O2 | 4132134.9 | 88.8 | |
| 41.2983 | 3-Isopropyl-1,2-benzenediol | 2138-48-9 | C9H12O2 | 4145204.1 | 88.3 | |
| 42.2371 | Ethyl Vanillin | 121-32-4 | C9H10O3 | 1923021.2 | 85.6 | |
| 44.3609 | Dodecanoic acid, methyl ester | 111-82-0 | C13H26O2 | 6695897.0 | 90.5 | |
| 46.1295 | Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione | 65996-50-1 | C6H5N3O2 | 315462.0 | 90.5 | |
| 47.4301 | Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione | 65996-50-1 | C6H5N3O2 | 462252.6 | 95.6 | |
| 48.0142 | 1-Methyl-2-naphthol | 1076-26-2 | C11H10O | 1835032.9 | 91.8 | |
| 60.1345 | n-Hexadecanoic acid | 57-10-3 | C16H32O2 | 1804063.3 | 88.5 | |
| 64.3706 | Nonane, 2-methyl-5-propyl- | 31081-17-1 | C13H28 | 477323.0 | 86.1 | |
| 67.3433 | Retene | 483-65-8 | C18H18 | 5425518.1 | 96.3 | |
| 70.0865 | 8-Isopropyl-1,3-dimethylphenanthrene | 135886-06-5 | C19H20 | 1533057.2 | 88.8 | |
| 70.1995 | Sulfurous acid, 2-ethylhexyl isohexyl ester | 1000309-19-0 | C14H30O3S | 395497.8 | 90.8 | |
| 70.2001 | Decane, 2,3,7-trimethyl- | 62238-13-5 | C13H28 | 392395.4 | 91.0 | |
| 73.6821 | 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1- methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- | 5155-70-4 | C20H28O2 | 7483069.3 | 92.4 | |
| 76.4390 | 2H-Phenanthro[9,10-b]pyran | 217-67-4 | C17H12O | 308910.3 | 87.2 | |



--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 79-09-4 3.3165 Propanoic acid 1344443.4 97.7 C3H6O2 Component RT: 3.3165 y x10² 0.9 74.0 0.8 0.7 45.0 29.0 0.6 0.5 0.4 57.0 0.3 55.0 0.2 42.0 0.1 15 20 55 70 10 25 35 40 45 50 65 80 Mass-to-Charge (m/z) Propanoic acid (NIST20.L) Square x10² 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 10 20 25 30 35 40 45 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.1316-3.3488 min, 37 scans) 15.D st x10² 0.9 29.1 74.0 0.8 0.7 0.6 45.0 0.5 0.4 0.3 57.0 0.2 0.1 0-60 20 40 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.3165 St x10⁴ x10⁵ Component 74.0 74.0 45.0 2.25 ОН 73.0 29.0 1.75 73.0 45.0 1.5 57.0 29.0 3-

1.25

0.75 0.5

0.25

3.2 3.25

3.3

Acquisition Time (min)

57.0

2-

1

3.15

3.2

3.25

Acquisition Time (min)

3.3

CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 232828.2 79-10-7 C3H4O2 3.4054 2-Propenoic acid 87.2 Component RT: 3.4054 y x10² 0.9 72.1 0.8 0.7 55.0 0.6 0.5 0.4 0.3 45.0 0.2 0.1 53.0 5 25 35 45 65 70 10 15 20 30 40 60 80 Mass-to-Charge (m/z) 2-Propenoic acid (NIST20.L) S x10² 0.9 27.0 0.8 0.7 0.6 72.0 55.0 0.5 0.4 0.3 0.2 45.0 0.1 48.0 38.0 53.0 55 70 10 15 20 25 30 35 40 45 50 60 65 80 Mass-to-Charge (m/z) + Scan (3.3397-3.4440 min, 18 scans) 15.D st x10² 0.9 72.0 0.8 55.0 0.7 0.6 0.5 41.0 0.4^{-} 31.0 0.3 0.2 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.4054 Counts Counts x10⁵ x10⁴ Component 72.1 H2C 72.1 55.0 4 0.8 55.0 3.5 45.0 0.7 3-53.0 45.0 0.6 2.5 53.0 73.0 0.5 2 0.4 73.0 1.5 0.3 0.2 1

3.36 3.38 3.4 3.42 Acquisition Time (min)

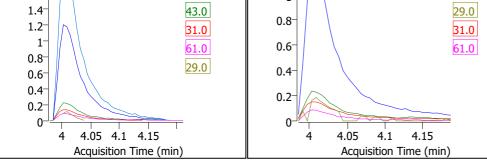
0.5

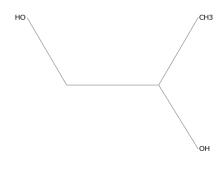
0.1

3.4

3.5

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 549350.3 57-55-6 4.0054 Propylene Glycol 88.4 C3H8O2 Component RT: 4.0054 v10² 0.9 45.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 43.0 0.2 31.0 61.0 0.1 33.0 40.0 15 30 35 45 70 75 5 10 20 25 40 50 55 60 65 80 Mass-to-Charge (m/z) Propylene Glycol (NIST20.L) Square x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 27.0 31.0 15.0 _{18.0} 0.1 41.0 33.0 76.0 75 5 10 15 20 25 30 35 40 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.9793-4.1872 min, 35 scans) 15.D st x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 29.0 0.1 61.0 0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 4.0054 EIC Peaks Counts st x10⁵-1.6x10⁵ 45.0 Component 45.0 43.0 1.6 1 1.4 43.0 29.0 0.8





-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 79-31-2 4.6609 Propanoic acid, 2-methyl-157512.9 87.7 C4H8O2 Component RT: 4.6609 v10² 0.9 43.0 0.8 0.7 0.6 41.0 73.0 0.5 0.4 0.3 39.0 0.2 45.0 88.0 0.1 53.0 25 45 85 10 15 20 30 35 40 50 55 60 65 70 80 90 95 Mass-to-Charge (m/z) Propanoic acid, 2-methyl- (NIST20.L) st x10²_ 0.9-43.0 0.8 0.7 0.6 0.5 41.0 0.4 0.3 73.0 27.0 0.2 39.0 88.0 45.0 0.1 29.0 55.0 15.0 60.0 71.0 5 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (4.5522-4.7402 min, 32 scans) 15.D st x10² 0.9 43.1 0.8 0.7 0.6 0.5 0.4^{-} 32.0 57.0 73.0 0.3 0.2 88.0 0.1 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 4.6609 Counts Counts x10⁴ 43.0 Component 43.0 41.0 1.6 3.5 41.0 73.0 1.4 3 39.0 73.0 1.2 Н3С < 2.5

4.65

4.7 Acquisition Time (min)

45.0

1

0.8

0.6

0.4

39.0

45.0

2

1

4.6

4.65

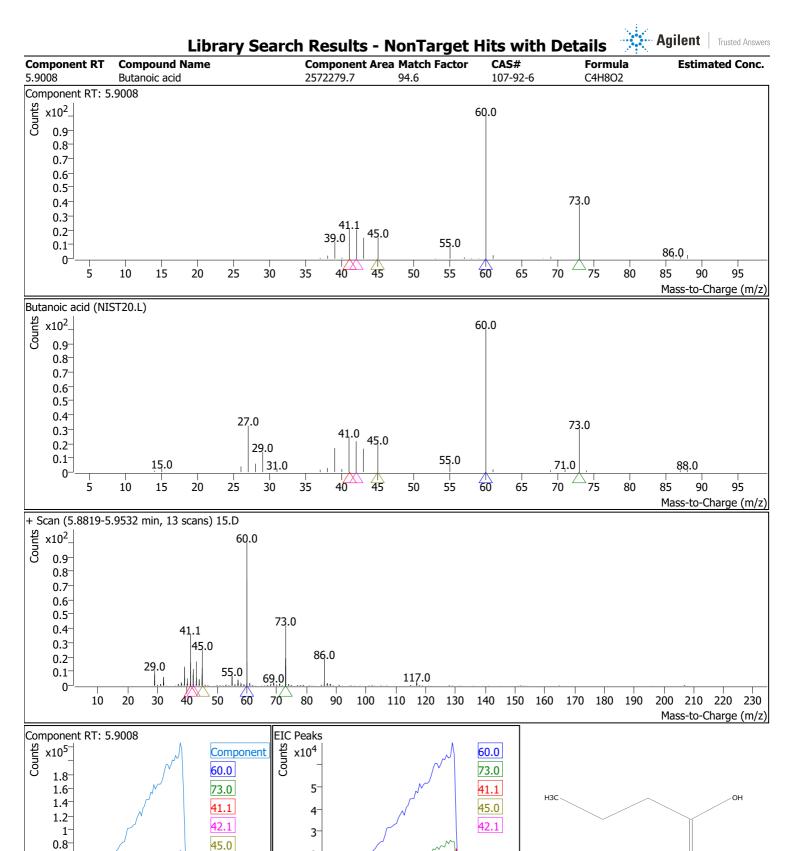
Acquisition Time (min)

4.7

1.5

0.5

СНЗ



2-

1

5.6

5.7

5.8

Acquisition Time (min)

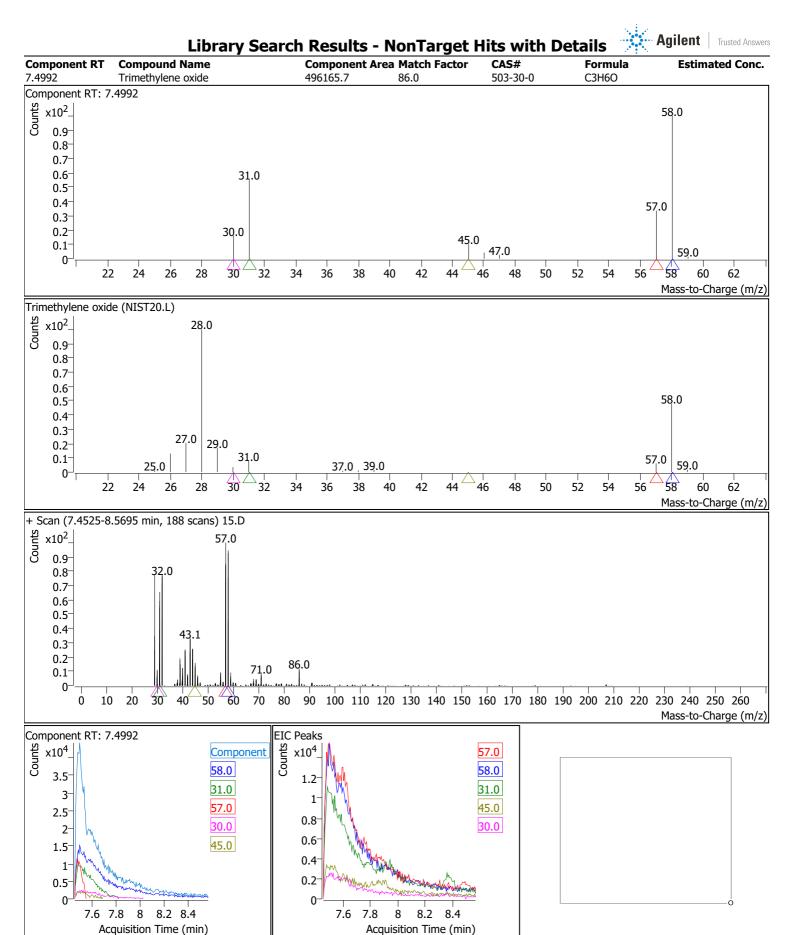
5.9

0.6⁻ 0.4⁻

0.2

5.6

5.7 5.8 5.9



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 504-63-2 7.5003 1,3-Propanediol 695898.1 85.2 C3H8O2 Component RT: 7.5003 v10² 0.9 57.0 0.8 0.7^{-} 31.0 0.6 0.5 0.4 0.3 0.2 45.0 0.1 45 15 25 55 70 75 10 20 30 35 40 50 80 85 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10²_ 0.9 28.0 58.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 45.0 0.2 0.1 15.0 18.0 41.0 55.0 49.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (7.4525-8.5695 min, 188 scans) 15.D St x10² 0.9 32.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 86.0 71.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 Mass-to-Charge (m/z) EIC Peaks Component RT: 7.5003 Counts Counts x10⁴ 57.0 Component 57.0 58.0 1.2 3.5 58.0 31.0 3 1 31.0 45.0 2.5 0.8 30.0 30.0

8.2 8.4

Acquisition Time (min)

8

0.6

0.4

0.2

0

7.6 7.8

45.0

2

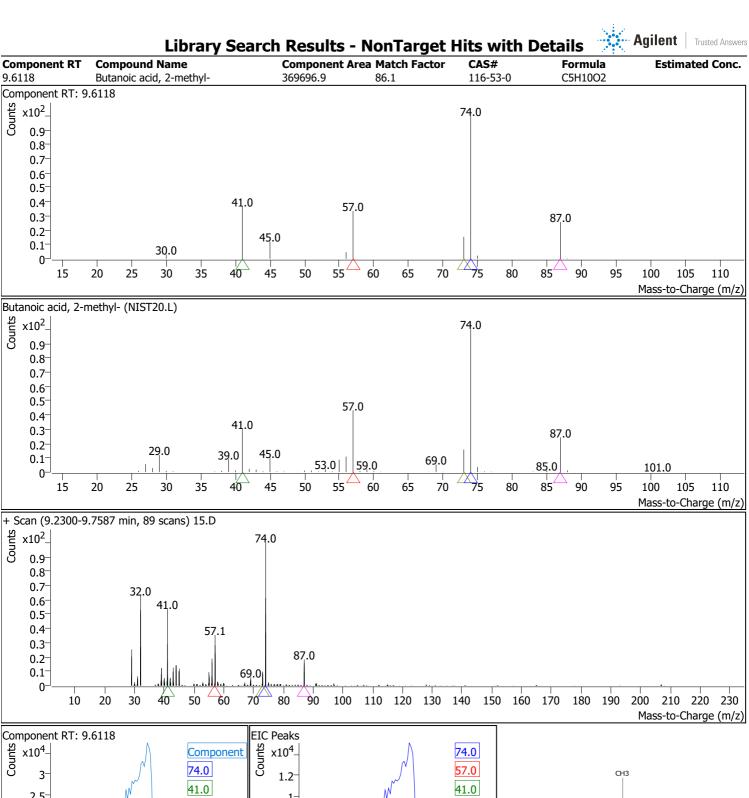
1.5

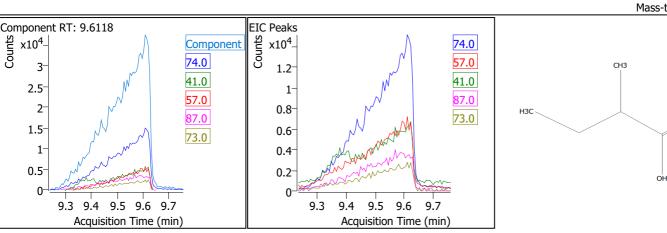
0.5

1

7.6 7.8 8

8.2 8.4





··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 539968.4 11.4297 Ethanol, 2,2'-oxybis-91.5 111-46-6 C4H10O3 Component RT: 11.4297 $x10^{2}$ 45.0 0.9 0.8 0.7 0.6 75.0 0.5 0.4 43.0 0.3 31.0 0.2 0.1 47.0 58.0 0 25 45 70 10 15 20 30 50 55 65 80 Mass-to-Charge (m/z) Ethanol, 2,2'-oxybis- (NIST20.L) Counts x10²_ 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 75.0 0.2 29.0 43.0 0.1 19.0 15.0 58.0 75 45 10 15 20 25 30 35 40 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (11.3306-11.6257 min, 50 scans) 15.D St x10² 0.9 45.0 0.8 0.7 0.6 31.0 0.5 0.4 75.0 0.3 0.2 103.0 61.0 87.0 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: 11.4297 **EIC Peaks** Counts Counts x10⁴ 45.0 Component 45.0 43.0 5 31.0 75.0 2 4 75.0 43.0 1.5

11.5

Acquisition Time (min)

3

2

1

11.4

11.6

Acquisition Time (min)

31.0 76.0

11.8

1 0.5

11.4

76.0

11.6

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 109-87-5 11.4303 Methylal 502169.0 89.2 C3H8O2 Component RT: 11.4303 y x10² 0.9 45.0 0.8 0.7 0.6 75.0 0.5 0.4 43.0 0.3 31.0 0.2 0.1 47.0 25 45 65 70 10 15 20 30 35 55 60 80 85 Mass-to-Charge (m/z) Methylal (NIST20.L) st x10² 0.9 45.0 0.8 0.7 0.6 0.5 75.0 0.4 29.0 15.0 0.3 0.2 31.0 0.1 47.0 18.0 75 5 10 15 20 25 30 35 40 50 55 60 65 70 80 85 Mass-to-Charge (m/z) + Scan (11.3306-11.6257 min, 50 scans) 15.D St x10² 0.9 45.0 0.8 0.7 0.6 31.0 0.5 0.4^{-} 75.0 0.3 0.2 103.0 61.0 87.0 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: 11.4303 **EIC Peaks** Counts Counts x10⁴-45.0 Component 45.0 43.0 2.25 31.0 75.0 75.0 43.0 1.75 3

42.1

11.6

1.5

1.25

 0.75^{-}

0.5 0.25

11.4

11.5

Acquisition Time (min)

31.0

42.1

11.6

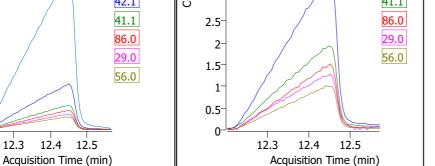
2

1

11.4

11.5

-- 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 12.4509 Butyrolactone 9899495.5 97.7 C4H6O2 Component RT: 12.4509 v10² 0.9 42.1 0.8 0.7 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 0.1 0 25 55 75 20 30 35 40 50 65 70 80 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) Counts x10²_ 0.9 42.0 0.8 0.7 0.6 28.0 0.5 86.0 0.4 56.0 0.3 0.2 39.0 0.1 53.0 0-20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (12.2040-12.5593 min, 60 scans) 15.D St x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 29.0 86.0 0.3 56.0 0.2 0.1 60.0 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: 12.4509 EIC Peaks Counts Counts x10⁶ x10⁵ 42.1 Component 42.1 41.1 41.1 86.0 2.5 0.8



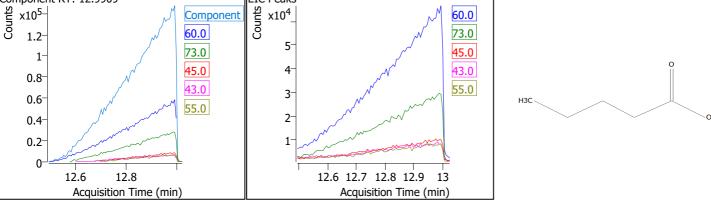
0.6

0.4

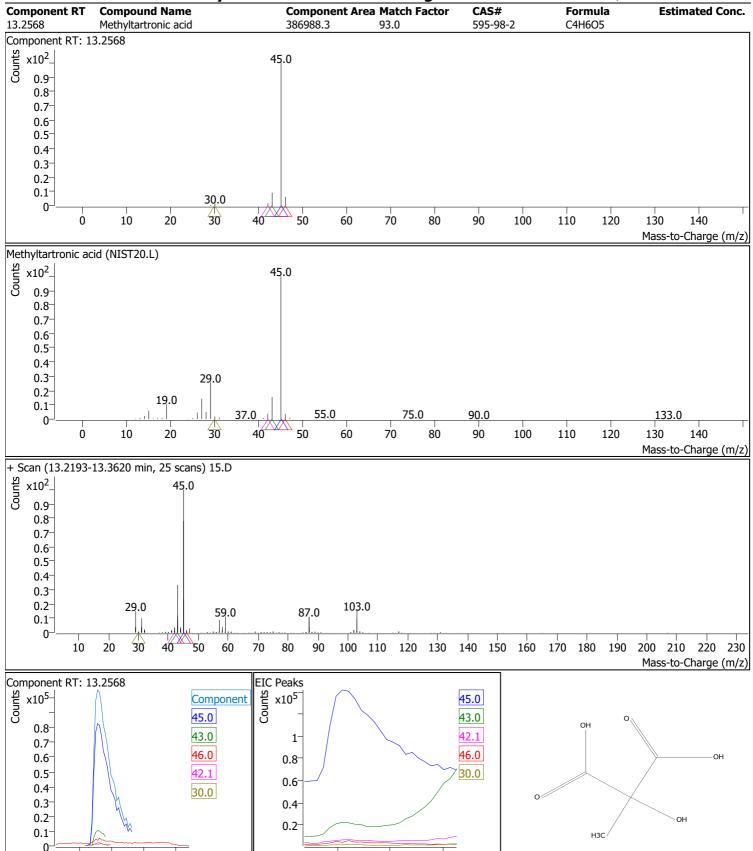
0.2

12.3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 109-52-4 12.9909 Pentanoic acid 1885123.3 95.1 C5H10O2 Component RT: 12.9909 v10² 0.9 60.0 0.8 0.7^{-} 0.6 73.0 0.5 0.4 0.3 0.2 55.0 0.1 25 55 10 15 20 30 35 40 65 70 80 85 90 95 Mass-to-Charge (m/z) Pentanoic acid (NIST20.L) st x10²_ 0.9-60.0 0.8 0.7 0.6 0.5 0.4 73.0 0.3 27.0 0.2 45.0 39.0 55.0 0.1 15.018.0 31.0 87.0 55 60 85 5 10 15 20 25 30 35 40 45 50 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (12.4949-13.0049 min, 85 scans) 15.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 73.0 0.3 0.2 29.1 0.1 55.0 86.0 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: 12.9909 **EIC Peaks** Counts stuno x10⁵x10⁴ 60.0 Component 60.0 73.0 1.2 5 73.0 45.0 1







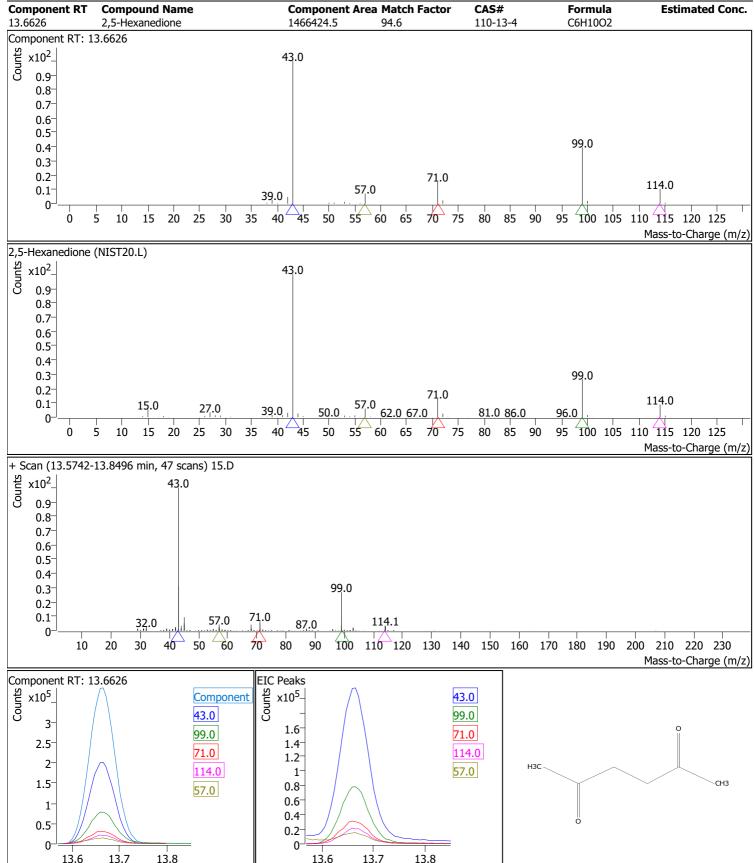
13.25

13.3

Acquisition Time (min)

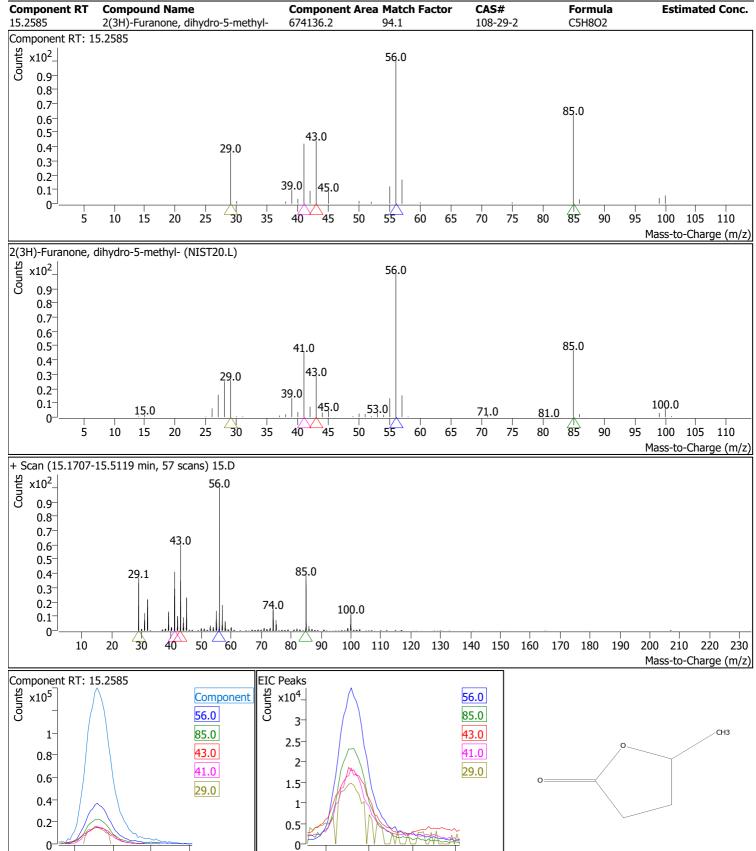
13.2 13.3 13.4 13.5





Acquisition Time (min)





15.3

15.4

Acquisition Time (min)

15.2

15.3

15.4

Acquisition Time (min)

15.2

--- 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 16.0676 2-Cyclopenten-1-one, 3-methyl-1559356.4 98.0 C6H8O Component RT: 16.0676 v10² 0.9 96.0 0.8 0.7 67.0 0.6 0.5 53.0 81.0 0.4 39.0 0.3 0.2 51.0 0.1 10 15 20 25 30 35 45 50 55 60 65 75 80 85 90 100 105 110 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3-methyl- (NIST20.L) Counts x10²_ 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 (15.9961-16.2896 min, 49 scans) 15.D st x10² 0.9 96.0 0.8 0.7 0.6 67.0 0.5 81.0 0.4^{-} 39.0 0.3 53.1 0.2 0.1 57.0 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: 16.0676 **EIC Peaks** st x10⁵-Counts x10⁴_ 96.0 Component 96.0 67.0 6 2.5 67.0 53.0 CH3 5 2 81.0 53.0



39.0

4

3-

2-

1

16

16.1

16.2

Acquisition Time (min)

81.0

39.0

1.5

1

0.5

16

16.1

--- 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 17.9709 Phenol 5949135.3 97.5 C6H6O Component RT: 17.9709 v10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 63.0 55.0 50.0 ⁴95 25 10 15 20 30 35 40 45 50 55 60 65 75 85 90 100 105 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10²_ 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 63.0 42.0 74.0 79.0 95 10 15 20 25 30 35 40 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) + Scan (17.9108-18.2913 min, 64 scans) 15.D st x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 66.0 0.2 39.0 110.1 0.1 32.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 70 Mass-to-Charge (m/z) Component RT: 17.9709 **EIC Peaks** Counts Counts x10⁶ x10⁵ 94.0 Component 94.0 66.0 66.0 65.0 3.5 0.8 39.0 65.0 3-

95.0

2.5

1.5 1

0.5

18

18.1

18.2 Acquisition Time (min)

2

39.0

95.0

0.6

0.4

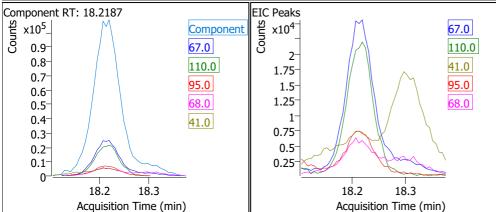
0.2

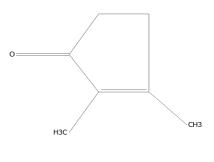
17.9

18

18.1 18.2

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 18.2187 2-Cyclopenten-1-one, 2,3-dimethyl-434331.4 90.2 1121-05-7 C7H10O Component RT: 18.2187 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 0.3 41.0 55.0 0.2 60.0 0.1 110 15 20 25 30 35 40 45 50 55 60 65 85 95 100 105 115 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 67.0 0.8 110.0 0.7 0.6 0.5 0.4 0.3 39.0 95.0 27.0 0.2 53.0 81.0 0.1 51.0 65.0 32.0 91.0 99.0 110 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (18.1248-18.3626 min, 41 scans) 15.D St x10² 67.0 0.8 110.1 0.7 0.6 0.5 94.0 0.4^{-} 0.3 32.0 0.2 103.0 117.0 81.1 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: 18.2187 **EIC Peaks** Counts 0.9 Counts x10⁴ 67.0 Component 67.0 110.0 2-8.0 110.0 41.0 1.75 0.7^{-1}





-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 18.6733 1,3-Dioxolane-4-methanol, 2-ethyl-13578997.9 86.0 53951-44-3 C6H12O3 Component RT: 18.6733 v10² 0.9 103.0 57.0 0.8 43.0 0.7^{-} 0.6 0.5 70.1 0.4 29.0 0.3 0.2 0.1 100 130 Ó 10 20 30 40 50 70 80 90 110 120 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10²_ 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 (18.5826-18.7967 min, 37 scans) 15.D St x10² 0.9 103.0 43.1 0.8 0.7 57.0 0.6 0.5 0.4^{-} 71.1 0.3 29.0 0.2 0.1 83.0 131.0 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: 18.6733 **EIC Peaks** Counts x10⁶ x10⁵ 103.0 Component 103.0 57.0 2.5 57.0 43.0 3.5 2 43.0 3 70.1



18.7

Acquisition Time (min)

18.8

101.1

2.5

1.5

0.5

18.6

2-

70.1

101.1

1.5

1

0.5

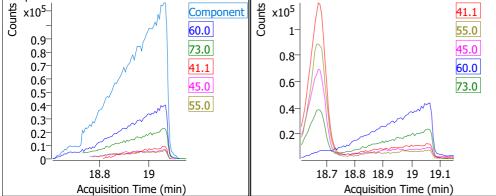
18.6

18.7

Acquisition Time (min)

18.8

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 109-52-4 19.0611 Pentanoic acid 1435408.7 89.2 C5H10O2 Component RT: 19.0611 v10² 0.9 60.0 0.8 0.7^{-} 0.6 73.0 0.5 0.4 0.3 41.1 45.0 0.2 55.0 87.0 0.1 25 55 85 10 15 20 30 35 40 50 65 70 80 90 95 Mass-to-Charge (m/z) Pentanoic acid (NIST20.L) st x10²_ 0.9-60.0 0.8 0.7 0.6 0.5 0.4 73.0 0.3 27.0 0.2 45.0 39.0 55.0 0.1 15.018.0 31.0 87.0 ^{__}75 55 60 85 10 15 20 25 30 35 40 45 50 65 70 80 90 95 Mass-to-Charge (m/z) + Scan (18.6075-19.1189 min, 86 scans) 15.D St x10² 0.9 103.0 43.1 0.8 0.7 57.0 0.6 0.5 0.4 71.1 0.3 29.0 0.2 0.1 83.0 131.0 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: 19.0611 Counts x10⁵ x10⁵ Component 41.1 60.0 55.0 1 0.9 45.0 73.0 0.8 0.8



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 19.8807 1,3-Dioxolane-4-methanol, 2-ethyl-7758870.6 C6H12O3 Component RT: 19.8807 v10² 0.9 103.0 57.0 0.8 0.7^{-} 0.6 0.5 0.4 43.0 0.3 29.0 0.2 47.0 0.1 40 100 120 130 Ó 10 20 30 50 70 80 90 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10²_ 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 (19.7460-20.0572 min, 53 scans) 15.D St x10² 0.9 103.0 0.8 57.0 0.7 0.6 0.5 43.0 0.4^{-} 0.3 31.0 0.2 0.1 83.0 95.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 19.8807 x10⁶-Counts x10⁵ 103.0 Component 103.0 57.0 1.4 3.5 1.2 57.0 43.0 3 1 43.0 29.0



19.9

Acquisition Time (min)

20

101.1

2.5

1.5

0.5

1

19.8

2

29.0

101.1

0.8

0.6

0.4

0.2

19.8

19.9

Acquisition Time (min)

20

Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 1703-51-1 20.1635 3,6-Heptanedione 985528.1 87.7 C7H12O2 Component RT: 20.1635 v10² 0.9 99.0 0.8 0.7^{-} 43.0 0.6 57.0 0.5 0.4 0.3 71.0 29.0 0.2 0.1 81.0 85.0 [∠]45 30 100 35 50 55 85 20 25 40 60 65 70 75 80 90 95 105 Mass-to-Charge (m/z) 3,6-Heptanedione (NIST20.L) Counts x10²_ 0.9 43.0 0.8 0.7 57.0 99.0 0.6 29.0 0.5 0.4 0.3 0.2 71.0 0.1 55.0 39.0 81.0 85.0 95.0 67.0 100 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 105 Mass-to-Charge (m/z) + Scan (20.0776-20.3174 min, 40 scans) 15.D st x10² 0.9 43.0 0.8 0.7 0.6 0.5 61.0 112.0 0.4 0.3 99.0 0.2 31.0 69.0 0.1 83.0 0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.1635 Counts Counts x10⁴ 99.0 Component 99.0 43.0 8 2 43.0 57.0 7 1.75 57.0 6 29.0 1.5



20.2 Acquisition Time (min)

71.0

5

4

3

2

1

20.1

71.0

29.0

1.25

0.75⁻

0.25

20.2

Acquisition Time (min)

20.3

1

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 80-71-7 20.2516 2-Cyclopenten-1-one, 2-hydroxy-3-1512958.6 90.5 C6H8O2 Component RT: 20.2516 x10²_ 112.0 0.9 8.0 0.7 0.6 0.5 55.0 0.4 69.0 0.3 83.0 41.0 0.2^{-} 39.0 0.1 103.0 73.0 0-55 30 35 45 50 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2-hydroxy-3-methyl- (NIST20.L) $x10^{2}$ 112.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 69.0 41.0 55.0 0.2 43.0 83.0 39.0 0.1 53.0 97.0 66.0 0 55 30 35 40 45 50 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (20.1227-20.4259 min, 51 scans) 15.D $x10^{2}$ 0.9 0.8 0.7 61.0 0.6 0.5 112.0 0.4 0.3 99.0 0.2 31.0 69.0 0.1 83.0 0 Ó 40 80 200 220 260 20 60 100 120 140 160 180 240 280 300 Mass-to-Charge (m/z) Component RT: 20.2516 EIC Peaks Counts Counts $x10^{4}$ x10⁵-112.0 Component 55.0 112.0 5 2 55.0 69.0 1.75 41.0 69.0 1.5 83.0 83.0 1.25 3нзс 41.0

20.3

Acquisition Time (min)

20.4

2

20.2

0.75 0.5 0.25

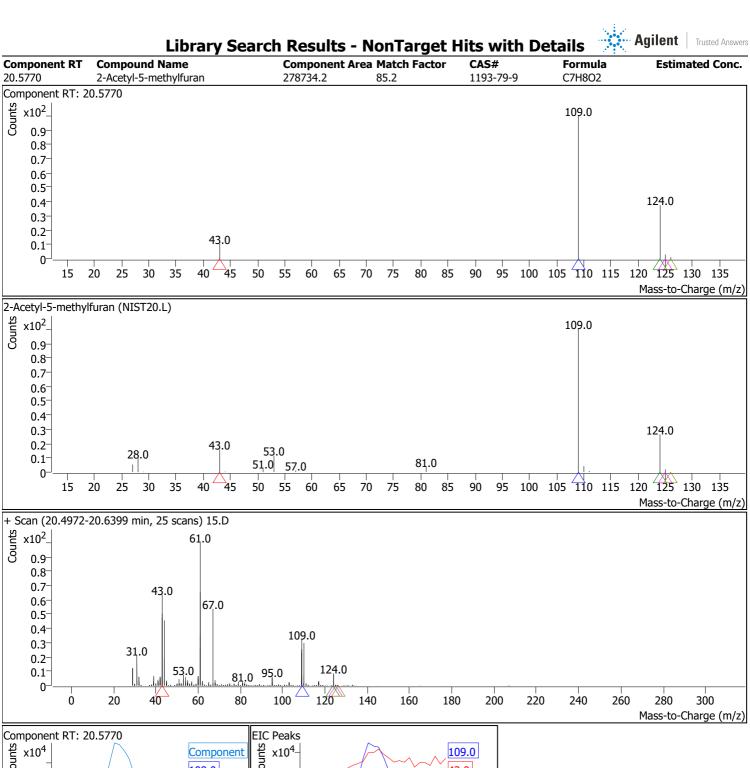
20.2

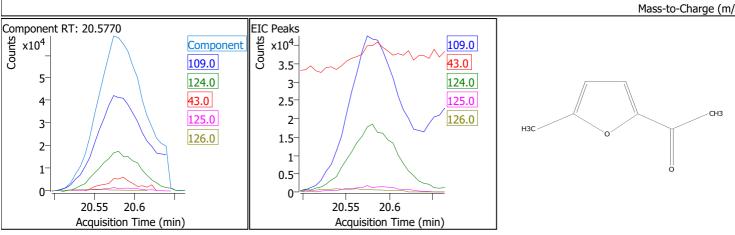
20.3

Acquisition Time (min)

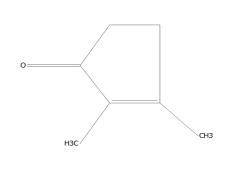
20.4

ОН





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.6669 2-Cyclopenten-1-one, 2,3-dimethyl-2435274.1 95.6 1121-05-7 C7H10O Component RT: 20.6669 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 0.3 39.0 0.2 54.0 81.0 0.1 110 95 15 20 25 30 35 40 45 50 55 60 65 80 85 90 100 105 115 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 67.0 0.8 110.0 0.7 0.6 0.5 0.4 0.3 39.0 95.0 27.0 0.2 53.0 81.0 0.1 51.0 65.0 32.0 91.0 99.0 110 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (20.5686-20.8897 min, 55 scans) 15.D Counts $x10^{2}$ 61.0 43.0 0.9 0.8 67.0 0.7 110.1 0.6 0.5 0.4^{-} 0.3 31.0 95.0 0.2 54.0 0.1 124.0 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.6669 Counts Counts x10⁵ 67.0 Component 67.0 110.0 4.5 110.0 109.0 1 3.5 95.0 95.0



20.7

20.8

Acquisition Time (min)

39.0

0.8

0.6

0.4

0.2

20.6

39.0

109.0

3

2.5

1.5 1

20.6

20.7

20.8

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 21.7216 2(3H)-Furanone, dihydro-3-methyl-638090.1 86.3 1679-47-6 C5H8O2 Component RT: 21.7216 v10² 0.9 42.0 0.8 0.7^{-} 56.0 0.6 0.5 0.4 100.0 39.0 0.3 0.2 0.1 10 15 20 25 30 35 55 75 85 90 100 105 Mass-to-Charge (m/z) 2(3H)-Furanone, dihydro-3-methyl- (NIST20.L) st x10²_ 0.9-41.0 56.0 0.8 0.7 0.6 0.5 27.0 0.4 39.0 100.0 0.3 0.2 0.1 31.0 71.0 66.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (21.6291-21.8760 min, 41 scans) 15.D st x10² 0.9 0.8 0.7 43.0 0.6 0.5 0.4^{-} 0.3 29.0 0.2 0.1 56.0 85.0 100.0 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: 21.7216 **EIC Peaks** Counts Counts x10⁴ 42.0 Component 42.0 41.0 3 8.0 41.0 56.0 0.7^{-1} 2.5 56.0 39.0



21.8

Acquisition Time (min)

100.0

21.9

H3C

2

1.5

1

21.7

0.5

100.0

39.0

21.9

0.6

 0.5^{-}

 0.4^{-}

0.3

0.2

0.1

21.7

21.8

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 21.9934 2-Cyclopenten-1-one, 2-hydroxy-3,4-475887.6 86.3 21835-00-7 C7H10O2 dimethyl-Component RT: 21.9934 x10². 126.0 0.9 8.0 0.7 0.6 0.5 111.0 0.4 69.0 55.0 83.0 0.3 41.1 0.2^{-} 39.0 98.0 0.1 0-55 110 30 35 40 45 50 60 65 70 75 80 85 90 95 100 105 115 120 125 130 135 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl- (NIST20.L) $x10^{2}$ 126.0 0.9 0.8 0.7 0.6 0.5 111.0 0.4 69.0 83.0 0.3 41.0 55.0 0.2 98.0 0.1 70 55 110 115 125 30 35 40 45 50 60 65 75 80 85 90 95 100 105 120 130 Mass-to-Charge (m/z) + Scan (21.9093-22.1365 min, 38 scans) 15.D x10². 43.0 0.9 0.8 0.7 0.6 0.5 0.4 31.0 0.3 0.2 69.0 81.1 126.0 0.1 0 Ó 80 200 260 20 40 60 100 120 140 160 180 220 240 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 21.9934 Counts Counts x10⁴ x10⁵ 126.0 Component CH3 111.0 126.0 0.9 111.0 55.0 0.8 2 0.7 69.0 69.0 0.6 1.5

22

Acquisition Time (min)

83.0

22.1

83.0

55.0

22.1

1

0.5

 0.5^{-}

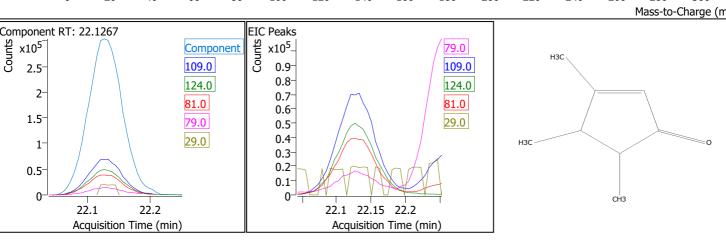
 0.4^{-}

0.3 0.2

0.1

22

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 55683-21-1 22.1267 2-Cyclopenten-1-one, 3,4,5-trimethyl-1181804.8 C8H12O Component RT: 22.1267 $x10^{2}$ 109.0 0.9 0.8 124.0 0.7^{-} 81.0 0.6 0.5 0.4 0.3 79.0 0.2-29.0 67.0 96.0 39.0 53.0 0.1 30 35 40 45 50 55 65 70 75 80 85 95 100 105 110 115 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 109.0 0.8 0.7 0.6 124.0 0.5 81.0 0.4 0.3 0.2 41.0 53.0 79.0 67.0 0.1 96.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (22.0496-22.2037 min, 26 scans) 15.D st x10² 0.9 43.0 61.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 31.0 109.0 0.2 124.1 81.1 0.1 117.0 53.0 67.0 96.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 22.1267 **EIC Peaks** stuno x10⁵ x10⁵-Component 79.0 НЗС 109.0 109.0 0.9 2.5 0.8



--- 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 22.2549 Phenol, 2-methyl-5361966.1 98.5 C7H8O Component RT: 22.2549 v10² 0.9 108.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 90.0 0.2 51.0 39.0 0.1 90 15 20 25 30 35 40 45 50 55 60 65 75 85 95 100 115 Mass-to-Charge (m/z) Phenol, 2-methyl- (NIST20.L) St x10²_ 0.9 108.0 0.8 0.7 0.6 0.5 0.4 79.0 0.3 90.0 0.2 39.0 51.0 27.0 0.1 63.0 74.0 43.0 29.0 68.0 86.0 90 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (22.1681-22.4391 min, 46 scans) 15.D st x10² 0.9 43.0 108.0 0.8 0.7 0.6 0.5 0.4^{-} 79.0 0.3 31.0 0.2 90.0 0.1 51.0 117.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 22.2549 **EIC Peaks** Counts Counts x10⁵ 108.0 Component 108.0 107.0 2.5 1 107.0 77.0 0.8 77.0 79.0 2 НО



22.3

Acquisition Time (min)

90.0

22.4

79.0

90.0

22.4

0.6

0.4

0.2

22.2

22.3

Acquisition Time (min)

1.5

1⁻

22.2

H3C

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 98-86-2 22.4317 Acetophenone 670685.4 89.0 **C8H8O** Component RT: 22.4317 y x10² 0.9 105.0 0.8 77.0 0.7^{-} 0.6 0.5 120.0 0.4 0.3 43.0 51.0 0.2 60.0 0.1 85 95 100 105 110 115 120 125 130 135 35 45 50 55 60 65 70 75 ⁻80 90 Mass-to-Charge (m/z) Acetophenone (NIST20.L) \$\frac{\psi}{0.9} \tag{0.9} 105.0 0.8 77.0 0.7 0.6 0.5 0.4 0.3 120.0 51.0 0.2 43.0 0.1 15.0 27.0 32.0 39.0 74.0 63.0 56.0 25 30 35 40 45 15 20 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (22.3583-22.5546 min, 34 scans) 15.D st x10² 0.9 43.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 31.0 0.2 0.1 77.0 89.0 105.0 129.0 <u>8</u>0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 22.4317 x10⁵ Counts x10⁵ 43.0 Component 105.0 105.0 1-0.8 77.0 77.0 0.7^{-1} 0.8 120.0 120.0 0.6



22.5

Acquisition Time (min)

51.0

нзс

0.6

0.4

0.2

0-

22.4

51.0

43.0

 0.5^{-}

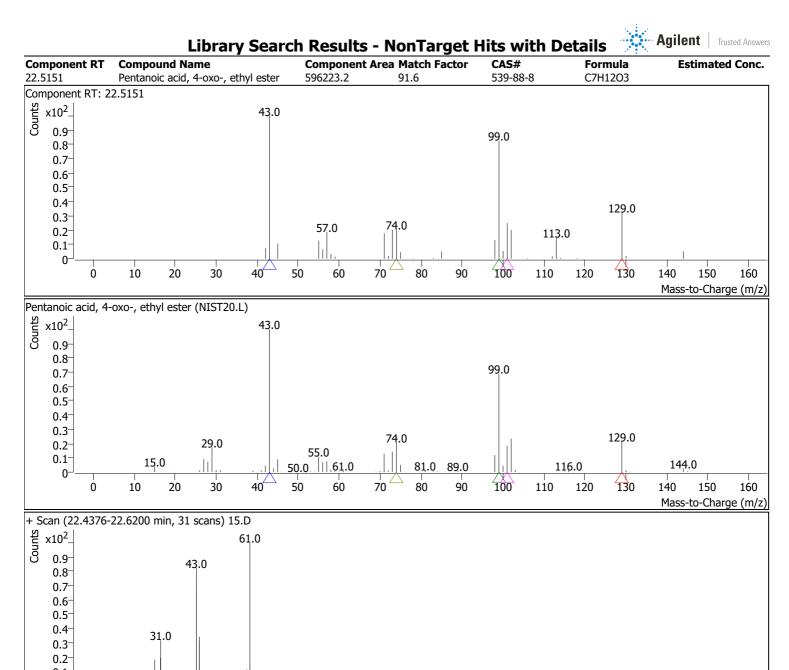
0.4

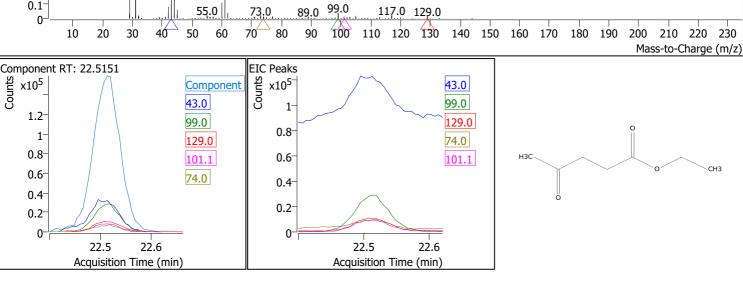
0.3⁻ 0.2⁻

0.1

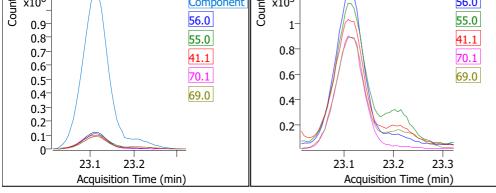
22.4

22.5





-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4899098.9 111-87-5 23.1102 1-Octanol 94.7 C8H18O Component RT: 23.1102 v10² 0.9 56.0 41.1 0.8 70.1 0.7^{-} 84.0 29.0 0.6 0.5 0.4 0.3 0.2 0.1 70 20 130 10 30 40 50 90 100 110 120 140 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10²_ 0.9 56.0 0.8 41.0 0.7 70.0 0.6 0.5 84.0 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 110 10 20 30 40 50 60 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.0124-23.3157 min, 52 scans) 15.D st x10² 0.9 0.8 0.7 43.0 0.6 0.5 0.4 0.3 31.0 0.2 103.0 70.1 83.1 0.1 110.1 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.1102 Counts Counts x10⁶ x10⁵ 56.0 Component 56.0 55.0 0.9 1 0.8 55.0 41.1 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.** 10847074.2 90-05-1 23.6072 Phenol, 2-methoxy-97.5 C7H8O2 Component RT: 23.6072 v10² 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 39.0 0.1 63.0 80 110 10 20 30 40 70 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) St x10²_ 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 15.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4881-23.6903 min, 35 scans) 15.D st x10² 0.9 109.0 61.0 124.0 0.8 0.7 43.0 0.6 81.0 0.5 0.4^{-} 0.3 0.2 31.0 53.0 0.1 90.0 117.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.6072 Counts Counts x10⁵-109.0 Component 109.0 124.0 6 2 124.0 81.0 5 1.75 81.0 53.0



23.55

23.6 23.65

Acquisition Time (min)

52.0

нзс

4

3

2-

53.0

52.0

1.5

1.25

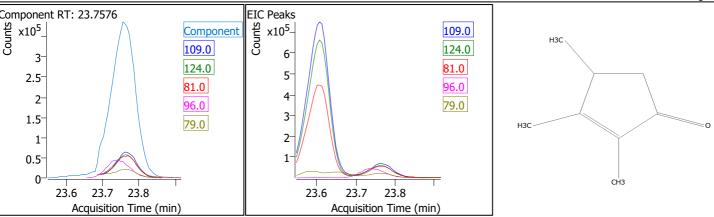
0.75

0.5 0.25

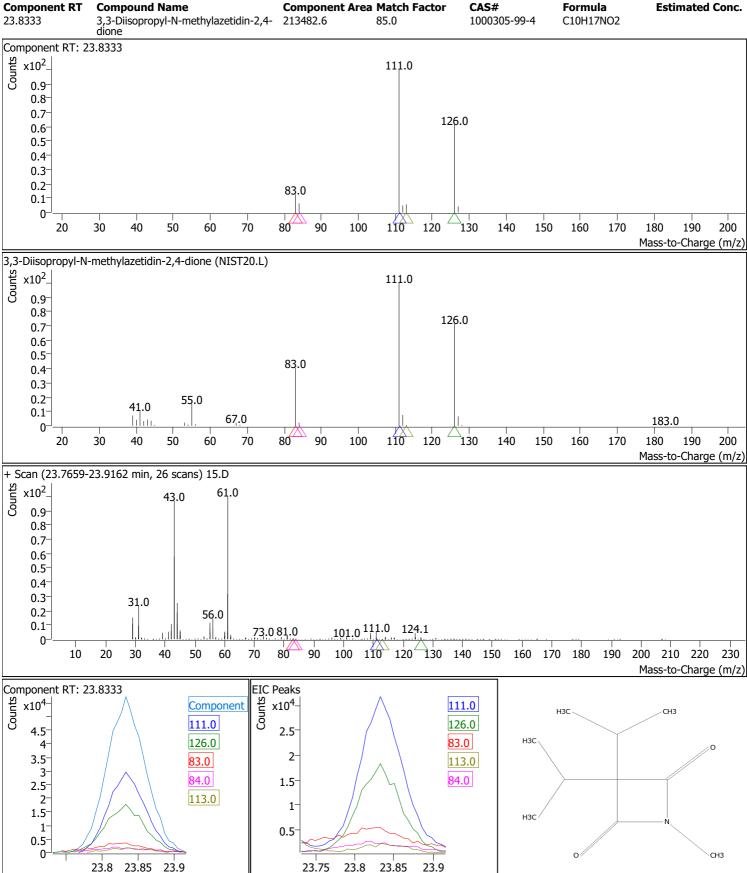
23.6

23.7

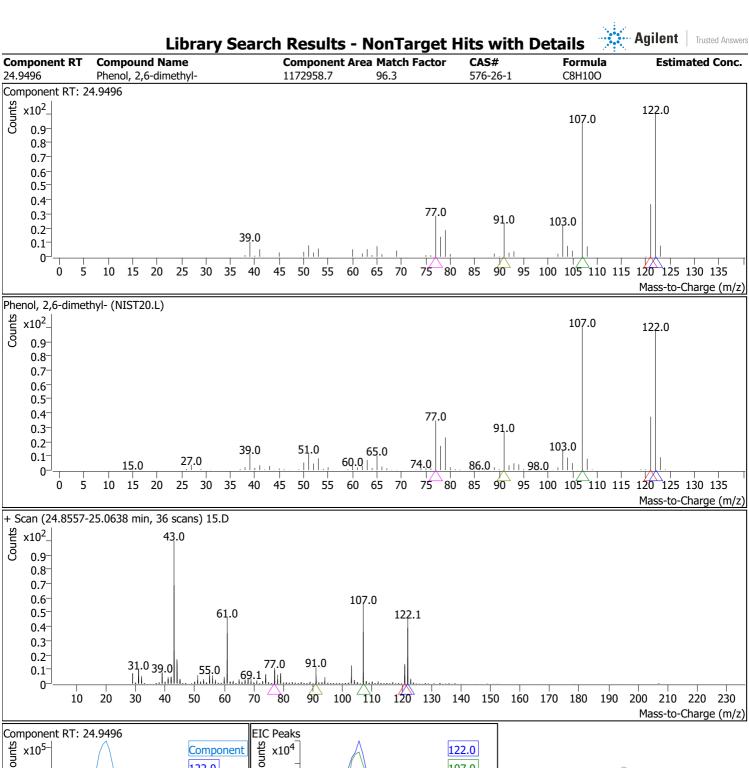
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** C8H12O 2-Cyclopenten-1-one, 2,3,4-trimethyl-1879891.8 85.5 28790-86-5 Component RT: 23.7576 v10² 0.9 109.0 124.0 81.0 0.8 96.0 0.7^{-} 0.6 0.5 0.4 79.0 0.3 67.0 41.1 0.2 0.1 30 35 45 65 70 75 95 100 105 115 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3,4-trimethyl- (NIST20.L) Counts x10²_ 0.9 109.0 0.8 0.7 0.6 81.0 0.5 124.0 0.4 0.3 0.2 79.0 96.0 67.0 0.1 53.0 91.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (23.6903-23.8508 min, 28 scans) 15.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 56.0 109.1 81.1 0.1 96.0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.7576 x10⁵-109.0 Component НЗС

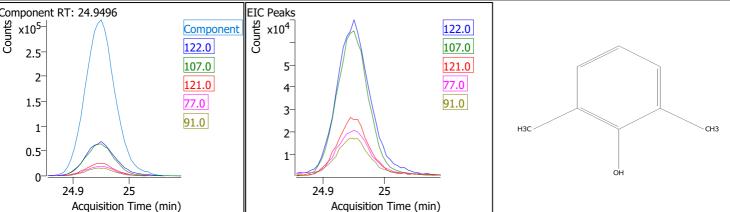


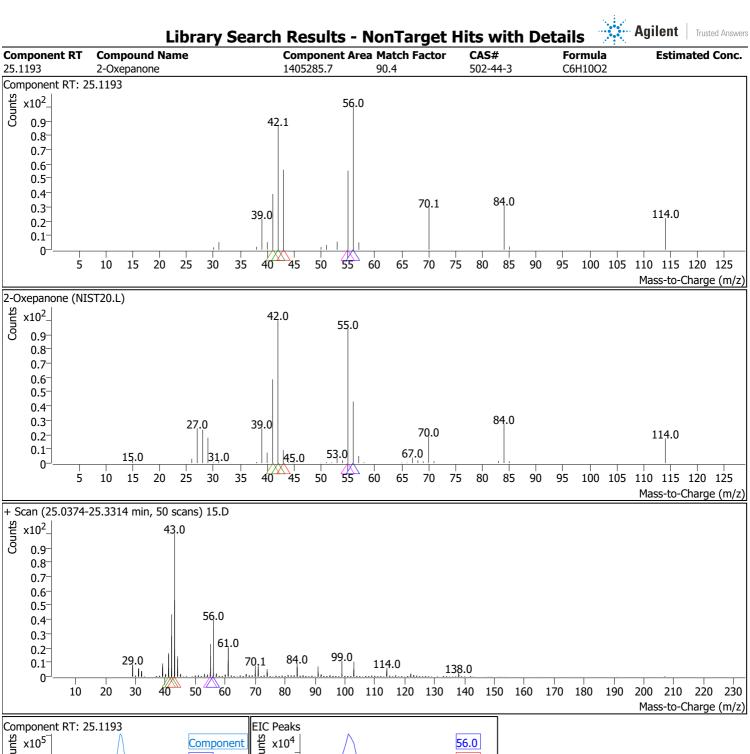
Library Search Results - NonTarget Hits with Details Agilent Trusted Answers ent RT Compound Name Component Area Match Factor CAS# Formula Estimated Conc.

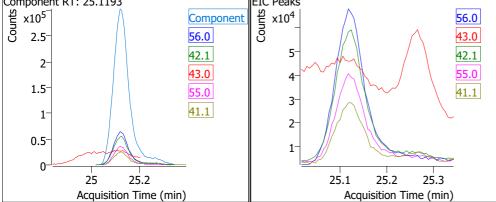


Acquisition Time (min)









--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 25.2360 Benzenemethanol, .alpha.-methyl-125876.7 87.0 98-85-1 C8H10O Component RT: 25.2360 v10² 0.9 91.0 0.8 0.7 0.6 0.5 0.4 122.1 0.3 65.0 0.2 0.1 63.0 120 125 130 135 20 25 30 35 45 55 60 65 70 75 85 100 105 110 115 Mass-to-Charge (m/z) Benzenemethanol, .alpha.-methyl- (NIST20.L) st x10²_ 0.9-92.0 0.8 0.7 122.0 0.6 0.5 0.4 0.3 0.2 0.1 65.0 78.0 104.0 31.0 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (25.1664-25.3939 min, 38 scans) 15.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 61.0 99.0 0.2 91.0 71.0 56.0 31.0 123.1 138.1 0.1 95.0 67.0 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: 25.2360 EIC Peaks x10⁴-Counts x10⁴ 91.0 Component 91.0 92.0 2.5 1.2 92.0 122.1 2 1 65.0 122.1



2 25.3
Acquisition Time (min)

63.0

0.8

0.6

 0.4°

0.2

25.2

65.0 63.0

1.5

1-

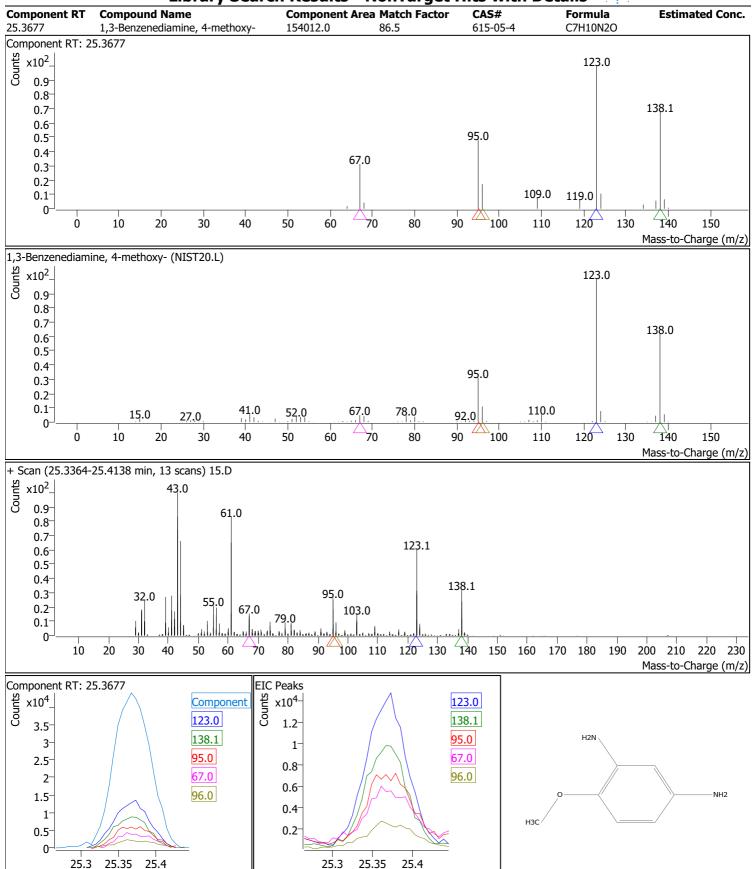
0.5

25.2

25.3

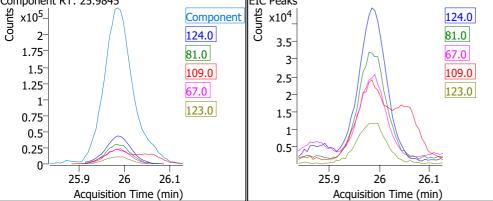
Library Search Results - NonTarget Hits with Details

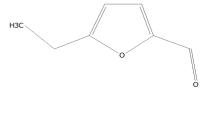




Acquisition Time (min)

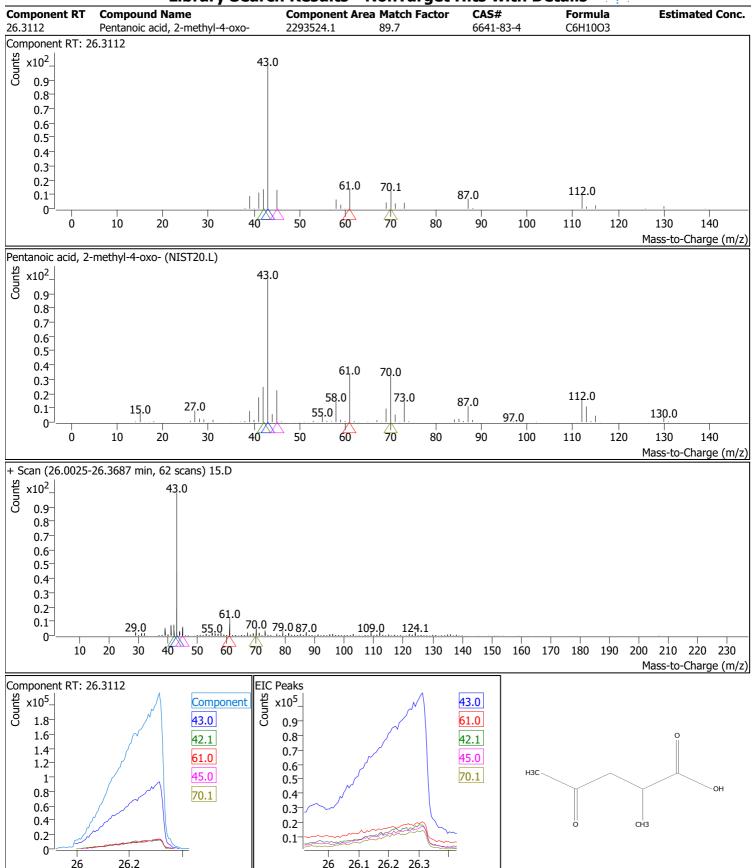
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1088595.0 23074-10-4 25.9845 5-Ethyl-2-furaldehyde 89.2 C7H8O2 Component RT: 25.9845 $x10^{2}$ 124.0 0.9 0.8 81.0 0.7^{-} 109.0 0.6 67.0 0.5 0.4 0.3 95.0 41.1 53.0 0.2 0.1 0 80 10 20 30 40 50 60 70 90 100 110 130 140 Mass-to-Charge (m/z) 5-Ethyl-2-furaldehyde (NIST20.L) Counts x10²_ 0.9 124.0 109.0 0.8 0.7 0.6 0.5 0.4 95.0 0.3 53.0 67.0 39.0 81.0 0.2 27.0 0.1 15.0 105.0 80 10 20 30 40 50 60 70 90 100 110 130 140 Mass-to-Charge (m/z) + Scan (25.9141-26.0865 min, 30 scans) 15.D St x10² 0.9 0.8 0.7 0.6 124.1 0.5 0.4^{-} 109.0 81.1 67.0 0.3 61.0 0.2 95.0 29.0 73.0 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) EIC Peaks Component RT: 25.9845 Str. x10⁵-Counts x10⁴ 124.0 Component 124.0 81.0 3.5 1.75 67.0 81.0 3





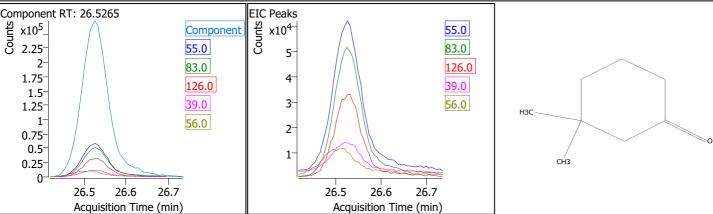
Library Search Results - NonTarget Hits with Details



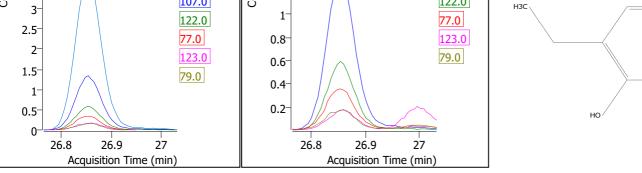


Acquisition Time (min)

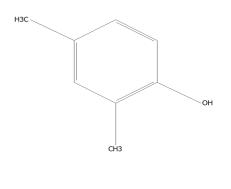
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2979-19-3 26.5265 3,3-Dimethylcyclohexanone 1229432.6 87.8 C8H14O Component RT: 26.5265 v10² 0.9 55.0 83.0 0.8 0.7 0.6 126.0 0.5 0.4 0.3 39.0 111.0 0.2 0.1 Ó 10 20 30 40 50 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) 3,3-Dimethylcyclohexanone (NIST20.L) Counts x10²_ 0.9 83.0 0.8 0.7 0.6 0.5 55.0 0.4 126.0 0.3 41.0 0.2 69.0 111.0 0.1 93.098.0 77.0 108.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (26.4262-26.7346 min, 52 scans) 15.D St x10² 0.9 55.0 83.0 0.8 0.7 0.6 43.0 0.5 126.1 0.4^{-} 0.3 0.2 29.0 111.0 69.1 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 Mass-to-Charge (m/z) EIC Peaks Component RT: 26.5265 Counts stuno 2.25 x10⁴ 55.0 Component 55.0 83.0



--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-00-6 26.8530 Phenol, 2-ethyl-1440345.0 C8H10O Component RT: 26.8530 v10² 0.9 107.0 0.8 0.7 0.6 0.5 122.0 0.4 0.3 77.0 0.2 39.0 91.0 0.1 35 55 65 75 85 90 95 100 105 110 115 Mass-to-Charge (m/z) Phenol, 2-ethyl- (NIST20.L) Counts x10²_ 0.9 107.0 0.8 0.7 0.6 122.0 0.5 0.4 0.3 77.0 0.2 86.0 ^{91.0} 0.1 39.0 51.0 103.0 27.0 65.0 18.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (26.7644-27.0260 min, 45 scans) 15.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 122.1 0.5 0.4^{-} 77.0 0.3 43.0 0.2 138.1 39.0 55.0 67.0 95.0 117.0 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) EIC Peaks Component RT: 26.8530 Counts Counts x10⁵ 107.0 Component 107.0 122.0 3 1



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 105-67-9 27.3873 Phenol, 2,4-dimethyl-1986020.1 97.9 C8H10O Component RT: 27.3873 y x10² 0.9 107.0 122.1 0.8 0.7 0.6 0.5 0.4 0.3 77.0 91.0 0.2 51.0 0.1 50 55 70 75 08 85 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) Phenol, 2,4-dimethyl- (NIST20.L) St x10²_ 0.9 122.0 107.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 0.2 91.0 0.1 103.0 74.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (27.3002-27.4601 min, 27 scans) 15.D 107.0 122.1 st x10² 0.9 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 77.0 91.0 0.2 0.1 65.0 151.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 27.3873 Counts x10⁵ Counts 107.0 Component 107.0 122.1 1 122.1 121.0 3.5 0.8 121.0 77.0



27.35

27.4

Acquisition Time (min)

91.0

3

2

77.0

91.0

 0.6^{-}

0.4

0.2

2.5

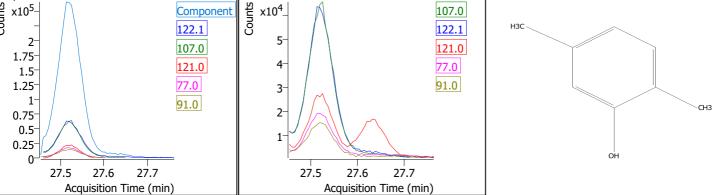
1.5 1-

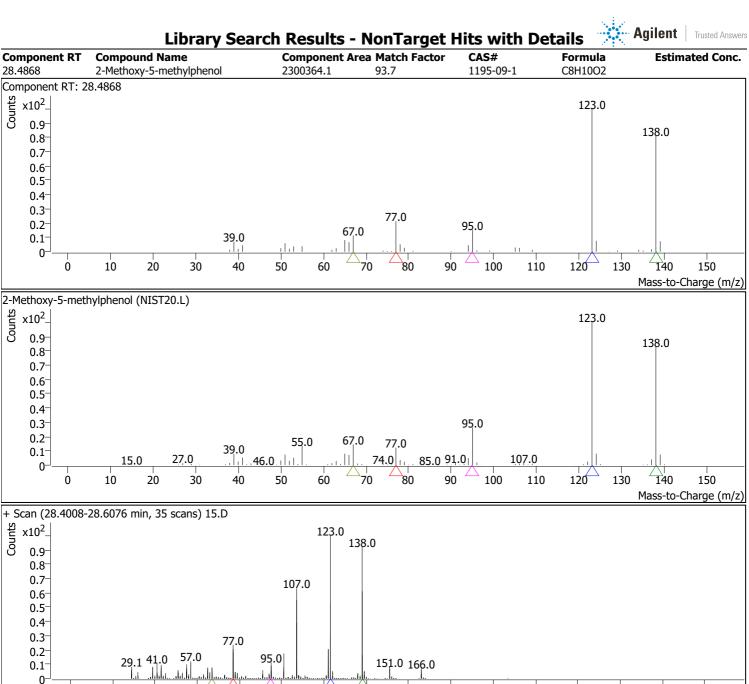
0.5

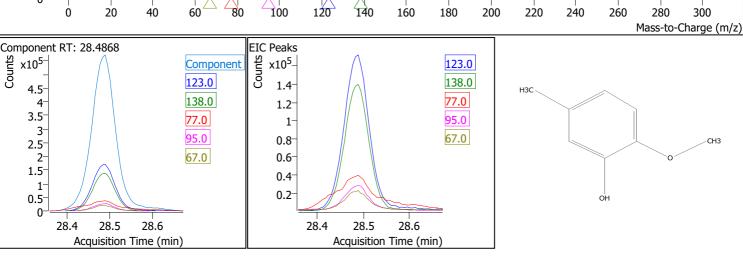
27.35

27.4

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 95-87-4 27.5164 Phenol, 2,5-dimethyl-1059980.7 96.1 C8H10O Component RT: 27.5164 v10² 0.9 122.1 107.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 91.0 0.2 0.1 50 55 75 08 85 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) Phenol, 2,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 107.0 122.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 91.0 0.2 39.0 65.0 0.1 27.0 74.0 90 95 100 105 110 115 120 125 130 135 10 15 20 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (27.4601-27.7633 min, 52 scans) 15.D st x10² 0.9 122.1 0.8 107.0 0.7^{-} 0.6 0.5 0.4^{-} 43.0 0.3 77.0 91.0 0.2 136.0 151.0 166.0 32.0 61.0 85.1 0.1 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 27.5164 Counts x10⁵ Counts x10⁴ 107.0 Component 122.1 122.1 2 107.0 121.0 1.75







--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 91-20-3 28.7656 Naphthalene 1269718.1 93.8 C10H8 Component RT: 28.7656 v10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 64.0 51.0 74.0 50 75 45 55 60 65 70 85 100 105 110 115 120 135 Mass-to-Charge (m/z) Naphthalene (NIST20.L) x10²_ 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 51.0 63.0 75.0 87.0 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 135 140 Mass-to-Charge (m/z) + Scan (28.6754-28.8990 min, 38 scans) 15.D st x10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 103.0 69.0 77.0 87.0 0.1 122.1 29.0 136.0 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 180 190 200 210 220 230 140 Mass-to-Charge (m/z) Component RT: 28.7656 EIC Peaks Counts x10⁵ Counts x10⁵ 128.0 Component 128.0 127.0 2.5 1.4 127.0 129.0 1.2 2 129.0 102.0 1 102.0 126.0 1.5



28.8

Acquisition Time (min)

0.8

0.6

0.4

0.2

28.7

126.0

1

28.7

28.8

Acquisition Time (min)

0.5

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 108-68-9 28.8332 Phenol, 3,5-dimethyl-852935.7 89.1 C8H10O Component RT: 28.8332 v10² 0.9 107.0 122.1 0.8 0.7 0.6 0.5 0.4 0.3 103.0 91.0 0.2 79.0 29.0 0.1 57.0 90 95 100 105 110 115 120 125 130 135 50 55 60 75 85 Mass-to-Charge (m/z) Phenol, 3,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 122.0 107.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 0.2 0.1 60.0 65.0 103.0 74.0 90 95 100 105 110 115 120 125 130 135 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (28.7503-28.9168 min, 29 scans) 15.D st x10² 0.9 128.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 103.0 69.0 77.0 87.0 55.0 122.1 0.1 29.0 10 20 30 50 60 70 80 100 110 120 130 150 160 170 180 190 200 210 220 230 140 Mass-to-Charge (m/z) EIC Peaks Component RT: 28.8332 x10⁵ Counts x10⁴ Component 121.0 ОН 107.0 103.0 1.4 5 122.1 107.0 1.2 121.0 122.1 1

28.9

Acquisition Time (min)

29

103.0

91.0

3

2-

28.8

0.8

0.6

0.4

28.9

Acquisition Time (min)

28.8

91.0

H3C

·CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 86.3 17135-47-6 28.9564 7-Chloro-1-(4-fluorophenyl)heptan-1-144694.5 C13H16CIFO Component RT: 28.9564 x10²_ 123.0 0.9 138.0 8.0 0.7 0.6 0.5 0.4 0.3 95.0 0.2^{-} 0.1 148.0 170.0 0-100 120 140 220 240 0 20 40 60 80 160 180 200 260 Mass-to-Charge (m/z) 7-Chloro-1-(4-fluorophenyl)heptan-1-one (NIST20.L) $x10^{2}$ 123.0 0.9 0.8 138.0 0.7 0.6 0.5 0.4 0.3 95.0 0.2 0.1 75.0 55.0 109.0 41.0 165.0177.0189.0 207.0 242.0 0 160 100 120 140 240 20 40 80 180 200 220 260 Mass-to-Charge (m/z) + Scan (28.8841-29.0120 min, 22 scans) 15.D st x10² 123.0 138.0 43.0 55.0 0.8 0.7 166.0 0.6 0.5 151.0 105.0 77.0 0.4 32.0 0.3 67.0 95.0 0.2 0.1 0 Ó 100 120 140 160 200 220 260 280 20 40 60 80 180 240 300 Mass-to-Charge (m/z) Component RT: 28.9564 **EIC Peaks** Counts Counts x10⁴ $x10^{4}$ 123.0 Component 138.0 123.0 1.6 3 138.0 95.0 1.4 2.5 1.2 95.0 139.0 2

28.95

Acquisition Time (min)

148.0

29

1

0.8

0.6

 0.4°

0.2 0

28.9

139.0

148.0

1.5

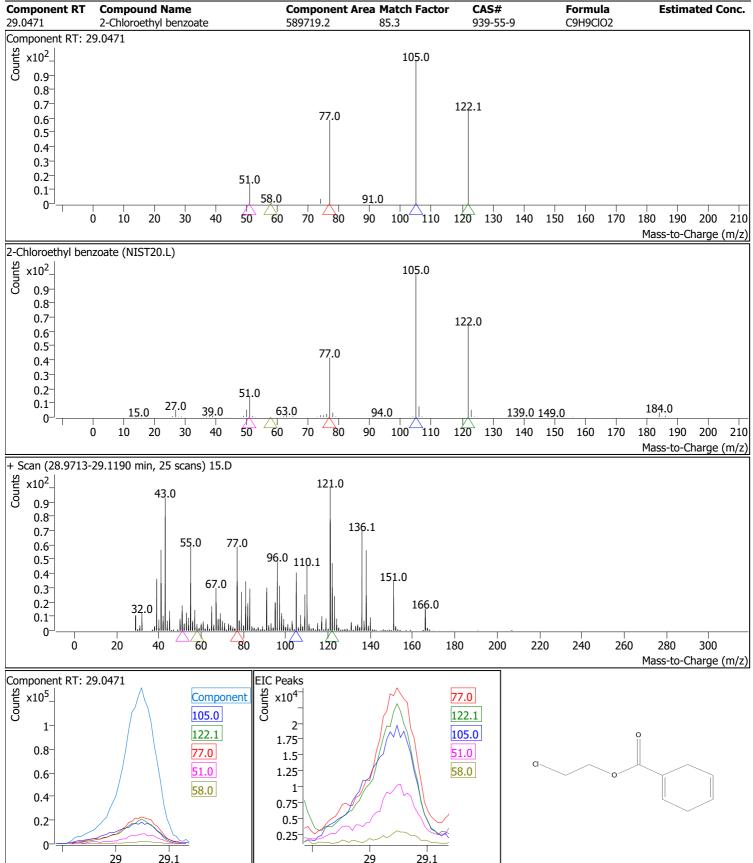
0.5

1

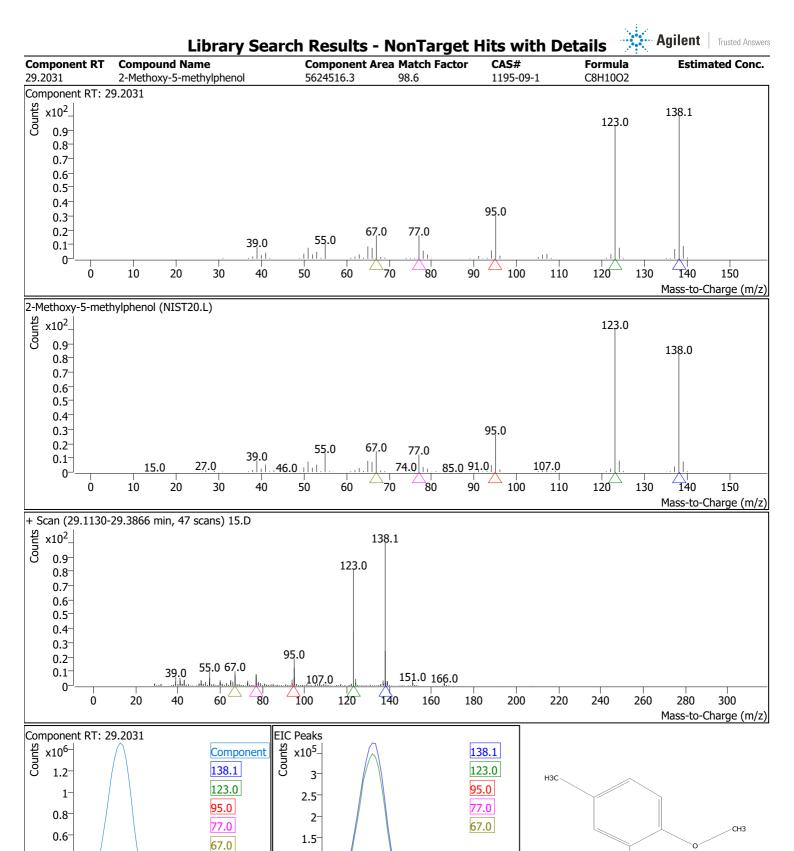
28.85 28.9 28.95







Acquisition Time (min)





29.2

29.3

Acquisition Time (min)

1

0.5

0.4

0.2

29.2

29.3

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 124-07-2 29.4084 Octanoic acid 1080701.5 88.3 C8H16O2 Component RT: 29.4084 v10² 0.9 60.0 73.0 0.8 0.7^{-} 0.6 0.5 0.4 101.0 41.0 55.0 0.3 85.0 0.2 0.1 40 60 100 10 20 30 50 80 110 120 130 140 150 160 Mass-to-Charge (m/z) Octanoic acid (NIST20.L) st x10²_ 0.9-60.0 73.0 0.8 0.7 0.6 0.5 0.4 43.0 101.0 55.0 0.3 85.0 0.2 115.0 69.0 29.0 0.1 97.0 144.0 127.0 40 60 10 20 30 50 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (29.2038-29.5055 min, 51 scans) 15.D 123.0 138.1 st x10² 0.9 0.8 0.7 0.6 0.5 0.4 0.3 95.0 41.0 55.0 67.0 0.2 151.0 166.0 0.1 107.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 29.4084 Counts Counts x10⁴ Component 55.0 60.0 60.0 3.5 1.4 73.0 73.0 3 1.2 101.0 41.0 2.5 1

29.3

29.4 Acquisition Time (min)

55.0

41.0

0.8

0.6 0.4

0.2

29.3

29.4

Acquisition Time (min)

2

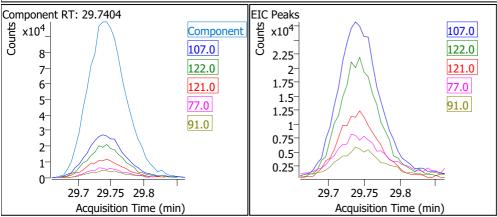
1

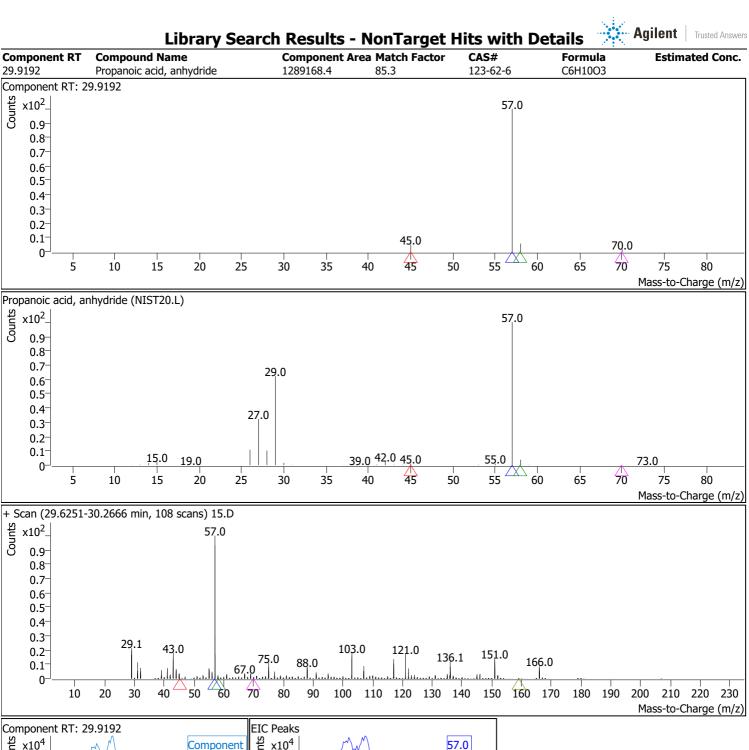
1.5

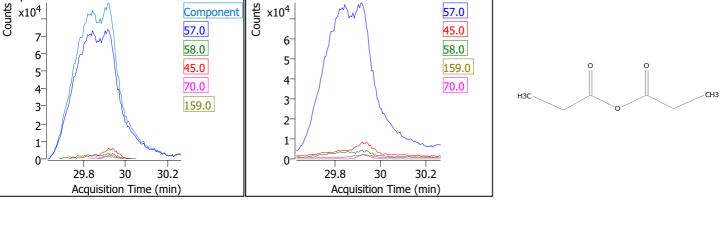
0.5

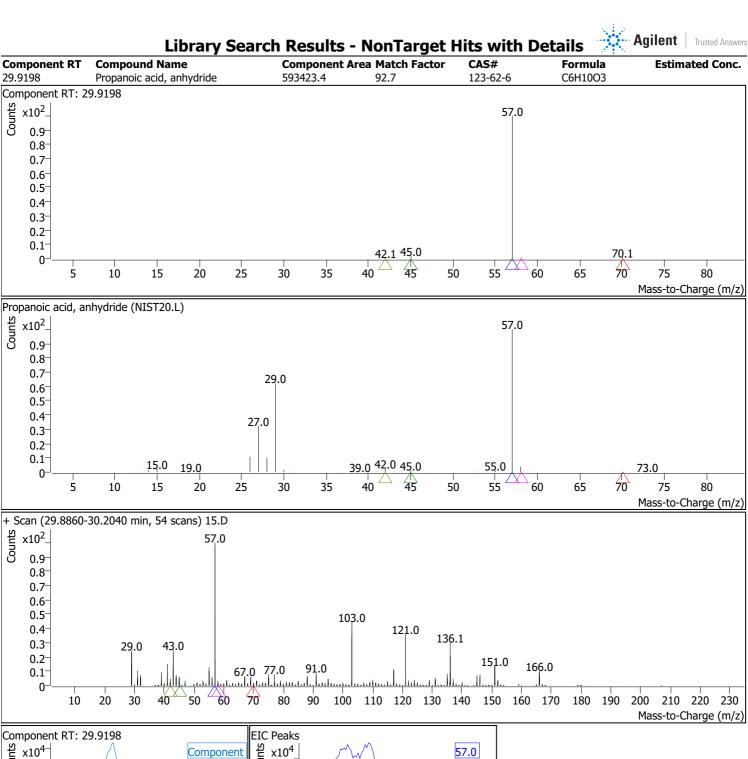
101.0

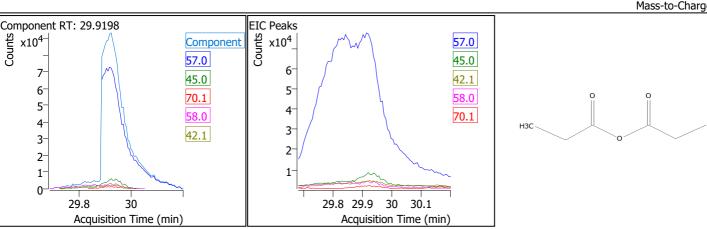
Library Search Results - NonTarget Hits with Details --- Agilent | Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 407488.5 29.7404 Phenol, 3,4-dimethyl-88.2 95-65-8 C8H10O Component RT: 29.7404 v10² 0.9 107.0 0.8 122.0 0.7 0.6 0.5 0.4 0.3 77.0 0.2 91.0 0.1 75 80 85 100 105 110 115 120 Mass-to-Charge (m/z) Phenol, 3,4-dimethyl- (NIST20.L) Counts x10²_ 0.9 107.0 122.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 0.2 91.0 51.0 60.0 65.0 0.1 27.0 103.0 74.0 15 20 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (29.6692-29.8504 min, 31 scans) 15.D st x10² 0.9 57.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 29.1 107.0 117.0 0.2 75.0 88.0 43.0 151.0 166.0 0.1 100.0 81.1 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: 29.7404 **EIC Peaks** Counts Counts x10⁴ 107.0 Component 107.0 122.0 8



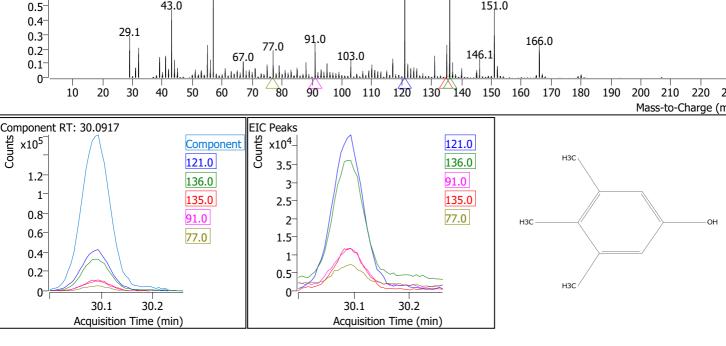








··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 30.0917 Phenol, 3,4,5-trimethyl-646726.3 89.2 527-54-8 C9H12O Component RT: 30.0917 v10² 0.9 121.0 136.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 91.0 0.2 77.0 103.0 109.0 0.1 [∠]80 20 30 40 50 60 70 90 100 110 120 130 140 150 Mass-to-Charge (m/z) Phenol, 3,4,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 136.0 121.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 91.0 77.0 39.0 0.1 27.0 51.0 65.0 103.0 117.0 59.0 86.0 120 20 30 40 50 60 70 80 90 100 110 130 140 150 Mass-to-Charge (m/z) + Scan (29.9990-30.2644 min, 45 scans) 15.D st x10² 0.9 121.0 136.1 0.8 57.0 0.7^{-} 0.6 43.0 0.5 151.0 0.4^{-} 29.1 0.3 91.0 166.0 77.0 0.2 67.0 146.1 103.0 0.1 وانستانان الماجا بابنيا المستويات والمتارين المارية والمارية والمارية والمارية والمارية والمارية والمارية والم 80 10 20 30 40 50 60 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 30.0917 Counts st x10⁴-121.0 Component НЗС 121.0 136.0 3.5 1.2



--- 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 30.5509 Catechol 14962815.9 96.1 C6H6O2 Component RT: 30.5509 v10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 110 15 20 25 30 35 45 50 55 60 65 70 75 80 85 90 95 100 105 115 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10² 0.9 110.0 0.8 0.7 0.6 0.5 64.0 0.4 0.3 81.0 0.2 27.0 92.0 39.0 53.0 0.1 42.0 46.0 79.0 .95.0 110 15 20 25 30 35 40 45 50 55 60 65 75 80 85 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (30.4985-31.0871 min, 100 scans) 15.D st x10² 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: 30.5509 **EIC Peaks** Counts Str. x10⁶ x10⁵ 110.0 Component 110.0 64.0 4.5 64.0 63.0 1 3.5 63.0 81.0 0.8 3-

81.0

92.0

0.6

0.4

0.2

30.6 30.8

31

Acquisition Time (min)

31.2

2.5

1.5⁻

0.5

30.6

30.8

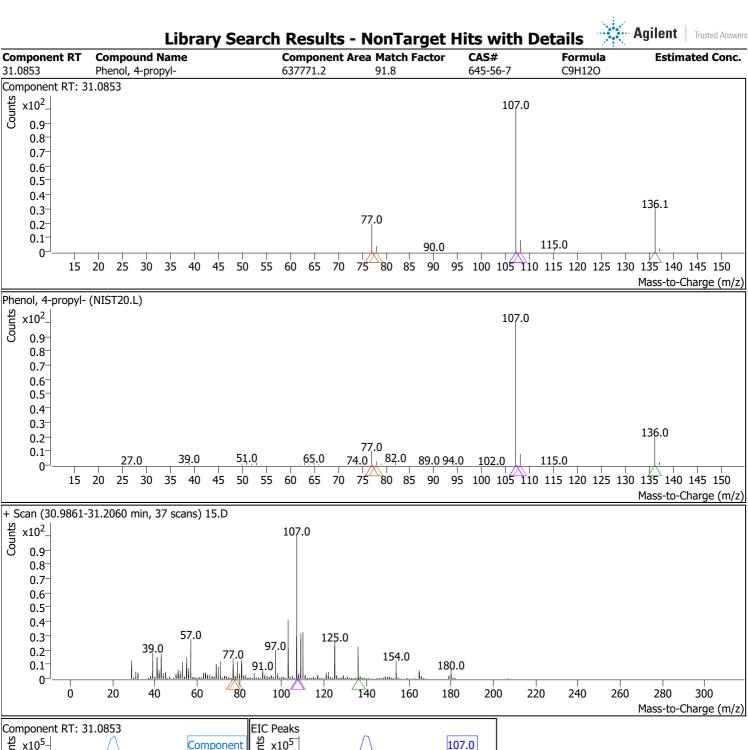
31

Acquisition Time (min)

31.2

2

92.0



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3855-26-3 31.3789 Phenol, 2-ethyl-4-methyl-1046524.7 91.4 C9H12O Component RT: 31.3789 v10² 0.9 121.0 0.8 0.7 136.0 0.6 0.5 0.4 0.3 91.0 0.2 77.0 100.0 107.0 0.1 117.0 0 120 10 20 30 40 50 60 70 100 110 140 150 Mass-to-Charge (m/z) Phenol, 2-ethyl-4-methyl- (NIST20.L) Counts x10²_ 0.9 121.0 0.8 0.7 0.6 136.0 0.5 0.4 0.3 0.2 77.0 91.0 0.1 60.065.0 39.0 46.051.0 115.0 74.0 . 83.0 10 20 30 40 60 70 80 90 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (31.2841-31.5313 min, 41 scans) 15.D St x10²_ 0.9 121.0 0.8 0.7 0.6 0.5 0.4^{-} 136.1 43.0 0.3 165.0 180.0 91.0 0.2 110.0 77.0 55.0 0.1 32.0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 31.3789 **EIC Peaks** st x10⁵-1.6-Counts x10⁴ 121.0 Component 121.0 136.0 1.6 4.5 1.4 136.0 91.0 1.2

31.4

Acquisition Time (min)

77.0

135.0

31.5

91.0

77.0

135.0

31.5

1

0.8

0.6

0.4

0.2

31.3

31.4

Acquisition Time (min)

3.5

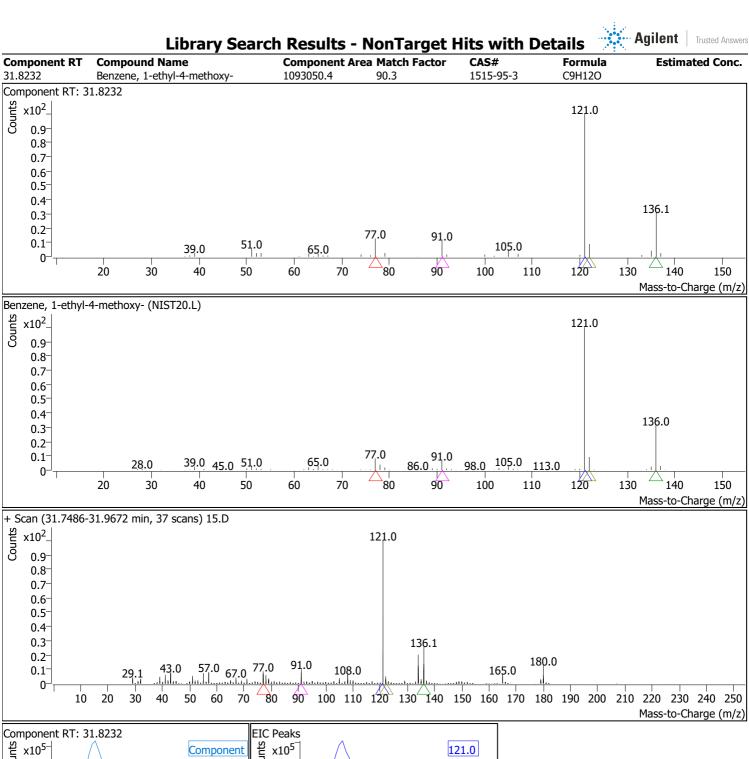
2.5

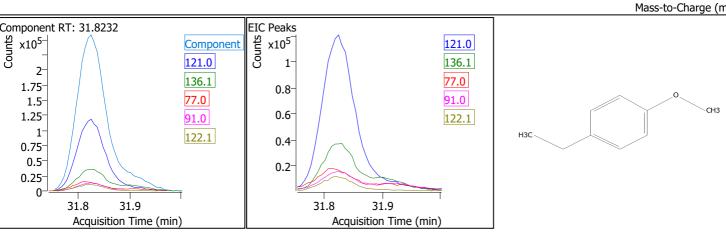
1.5

3

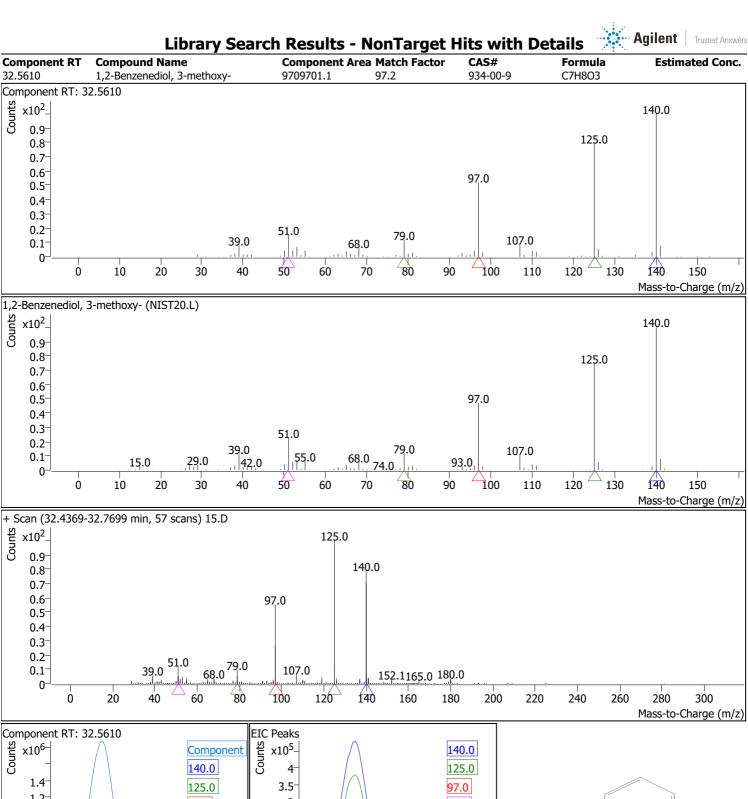
2

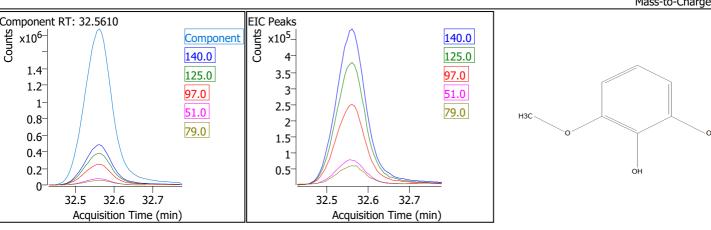
1

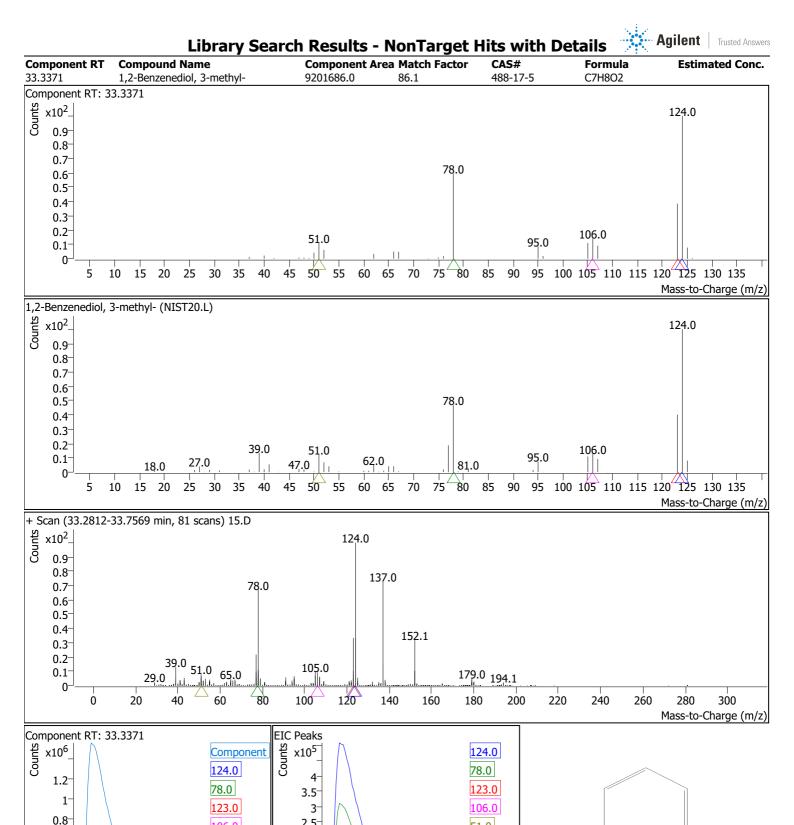




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1450-72-2 32.1304 Ethanone, 1-(2-hydroxy-5-1367848.8 92.1 C9H10O2 methylphenyl)-Component RT: 32.1304 x10²_ 135.0 0.9 8.0 0.7 0.6 0.5 150.0 0.4 0.3 77.0 0.2^{-} 0.1 51.0 107.0 0-_____80 150 0 10 20 30 40 50 60 70 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 150.0 0.5 0.4 0.3 107.0 0.2 77.0 43.0 51.0 0.1 27.0 63.0 85.091.0 131.0 121.0 0 130 150 10 20 30 40 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0444-32.2456 min, 34 scans) 15.D st x10² 0.9 135.0 0.8 0.7 0.6 0.5 150.0 0.4 0.3 77.0 121.0 0.2 165.0 180.0 43.0 96.0 110.1 0.1 32.0 51.0 67.0 0 _____80 200 260 Ó 20 40 60 100 120 140 160 180 220 240 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 32.1304 Counts Counts x10⁵ x10⁵ 135.0 Component но 135.0 150.0 2.5 150.0 1 77.0 **Н3С** 136.0 77.0 2 0.8









33.4 33.5 33.6 33.7 Acquisition Time (min)

51.0

НЗС

2.5

1.5

0.5

2-

1

106.0

51.0

0.6

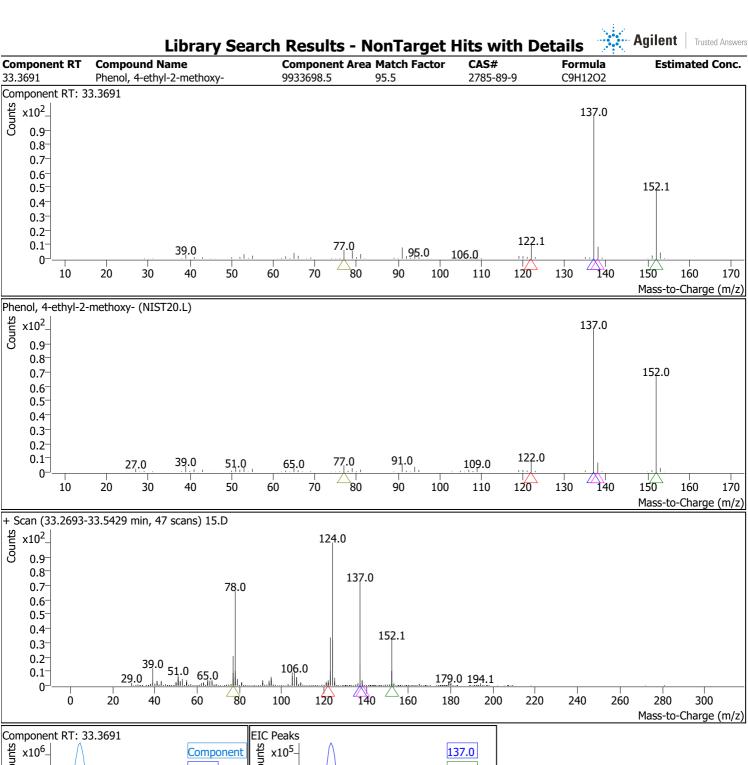
0.4

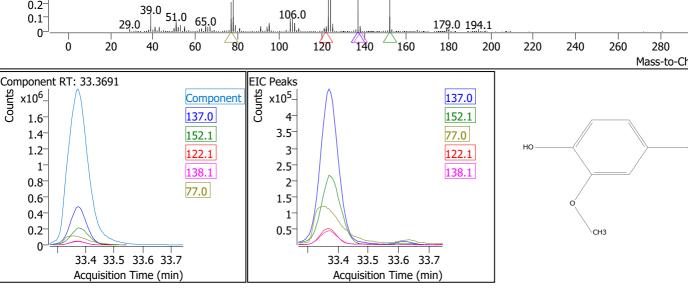
0.2

0

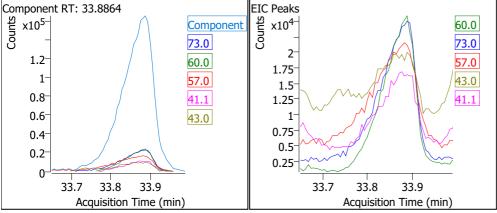
33.4

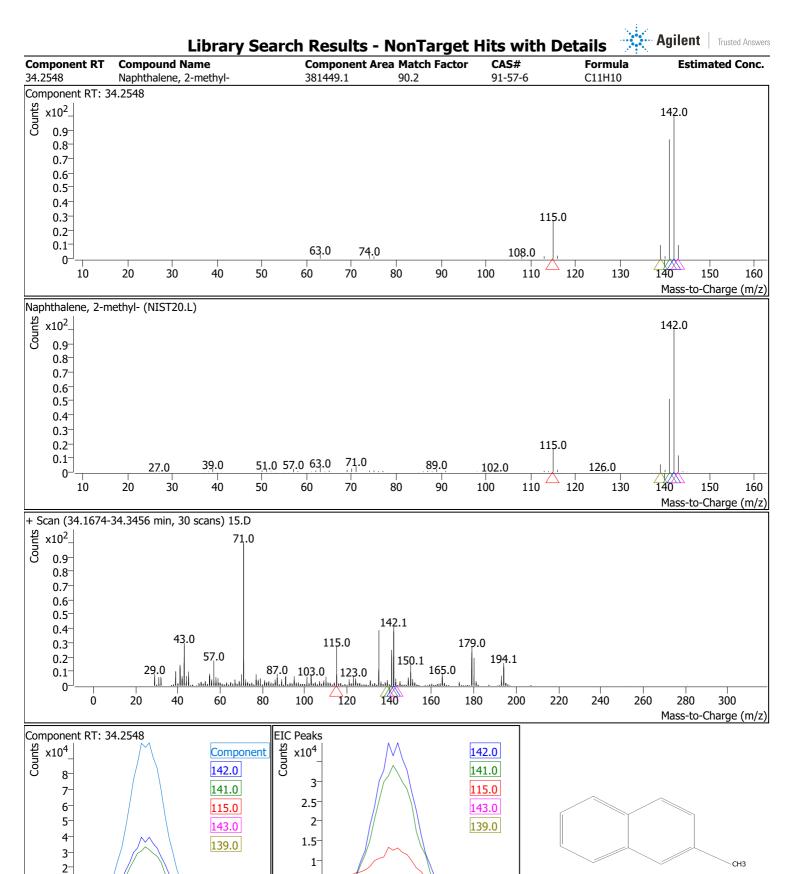
33.6





--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 112-05-0 33.8864 Nonanoic acid 917992.5 86.7 C9H18O2 Component RT: 33.8864 v10² 0.9 73.0 60.0 57.0 0.8 0.7^{-} 0.6 41.1 0.5 0.4 115.0 129.0 0.3 69.0 98.0 0.2 0.1 40 10 20 30 50 70 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Nonanoic acid (NIST20.L) st x10² 0.9 60.0 73.0 0.8 0.7 0.6 57.0 0.5 0.4 41.0 0.3 115.0 0.2 29.0 69.0 129.0 98.0 87.0 0.1 158.0 141.0 18.0 93.0 111.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (33.7093-33.9531 min, 42 scans) 15.D St x10² 0.9 179.0 43.0 0.8 57.0 0.7^{-} 73.0 0.6 194.0 0.5 29.1 121.0 0.4^{-} 115.1 0.3 83.0 103.0 0.2 149.0 0.1 <u>منالية الطائب الطائب الطباء الطالط الطائب الطائب الطائب الطائب الطالبال الطالبال الطائب الطائب الطائب الطائب ا</u> 50 60 70 80 20 30 40 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 10 Mass-to-Charge (m/z) Component RT: 33.8864 **EIC Peaks** Counts Counts x10⁴ 60.0 Component 73.0 73.0 2 1.2 60.0 57.0 1.75 1





34.25

34.3

Acquisition Time (min)

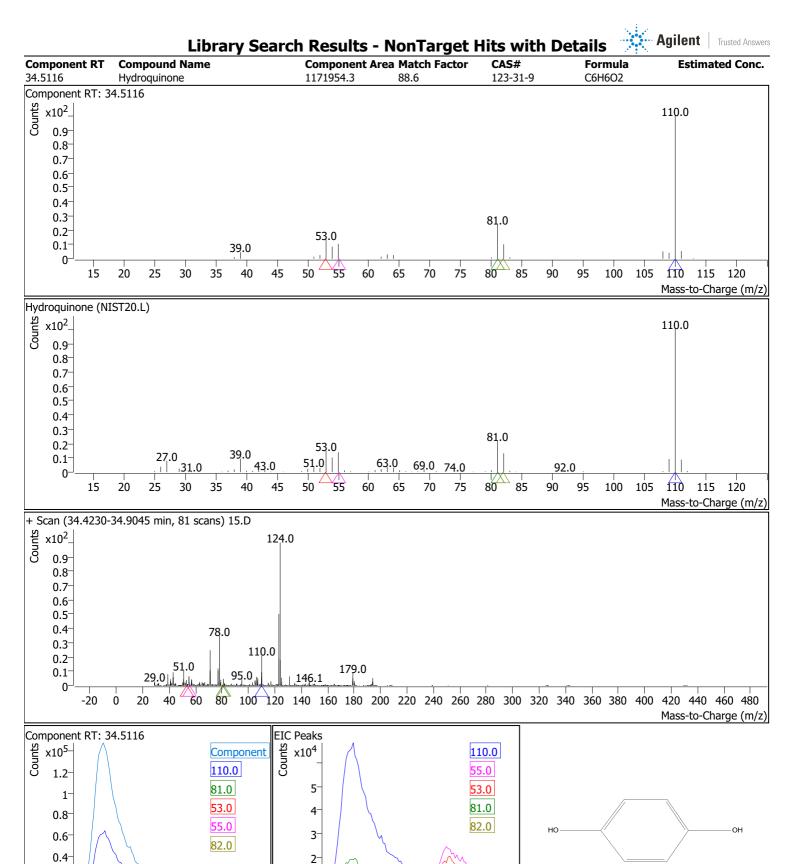
0.5

34.2

1

34.2

34.3



34.5 34.6 34.7 34.8

Acquisition Time (min)

1

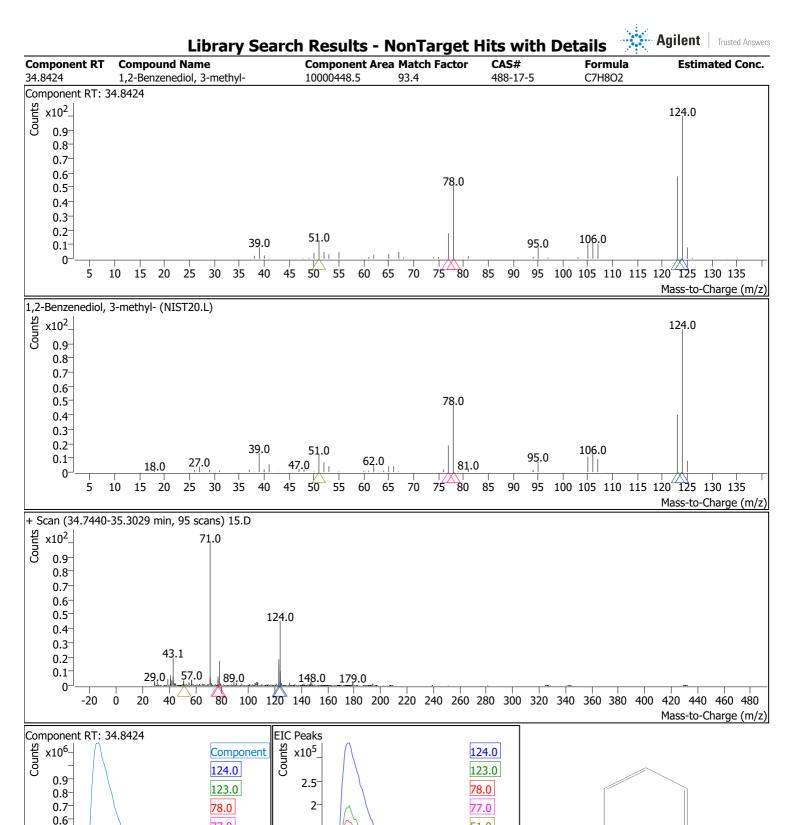
0.2

0

34.6

Acquisition Time (min)

34.8





35

Acquisition Time (min)

35.2

77.0

51.0

 0.5^{-}

0.4

0.3⁻ 0.2⁻

0

34.8

35

Acquisition Time (min)

35.2

1.5

1

34.8

0.5

51.0

НЗС

- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 608-43-5 35.4371 2,3-Dimethylhydroquinone 12044118.4 86.8 C8H10O2 Component RT: 35.4371 v10² 0.9 138.0 0.8 0.7 0.6 0.5 123.0 91.0 0.4 0.3 0.2 65.0 77.0 131.0 0.1 130 Ó 10 20 30 40 50 60 70 80 90 100 110 120 140 150 Mass-to-Charge (m/z) 2,3-Dimethylhydroquinone (NIST20.L) Counts x10²_ 0.9 138.0 0.8 0.7 0.6 123.0 0.5 0.4 0.3 0.2 53.0 109.0 39.0 67.0 0.1 27.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (35.3386-35.6953 min, 61 scans) 15.D st x10² 0.9 71.0 0.8 0.7 0.6 0.5 138.1 0.4 0.3 43.1 91.0 0.2 123.0 0.1 31.0 57.0 77.0 101.0 146.0 179.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.4371 Counts x10⁶_ x10⁵ 138.0 Component 138.0 123.0 2 4.5 1.75 123.0 91.0 3.5 1.5 91.0 137.0

35.5

35.6

Acquisition Time (min)

92.0

H3C

3-

2.5

1.5

0.5

1

137.0

92.0

1.25

0.75

0.5

35.4

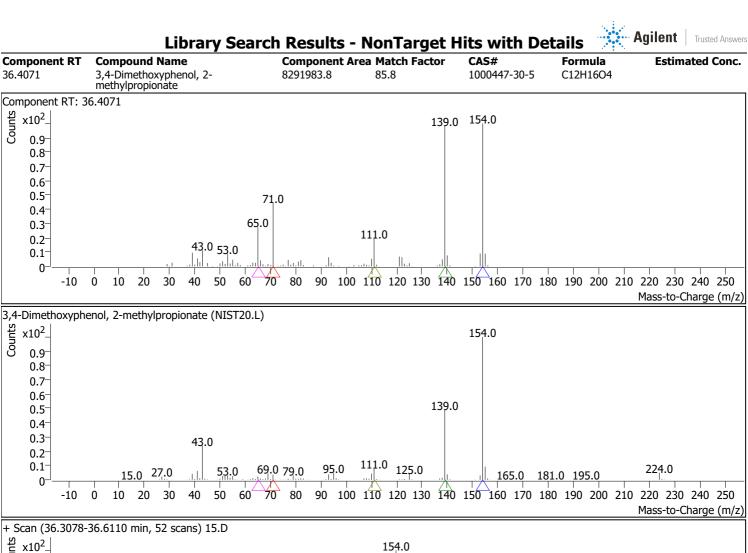
35.5

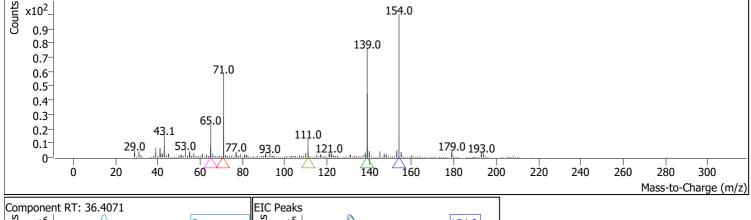
35.6

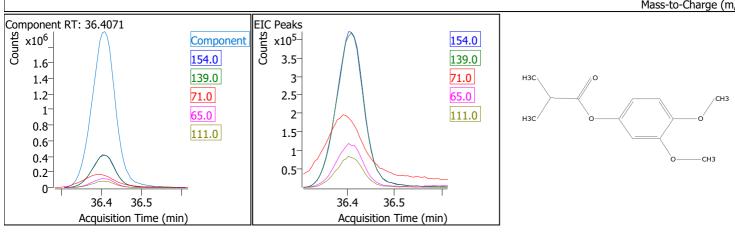
Acquisition Time (min)

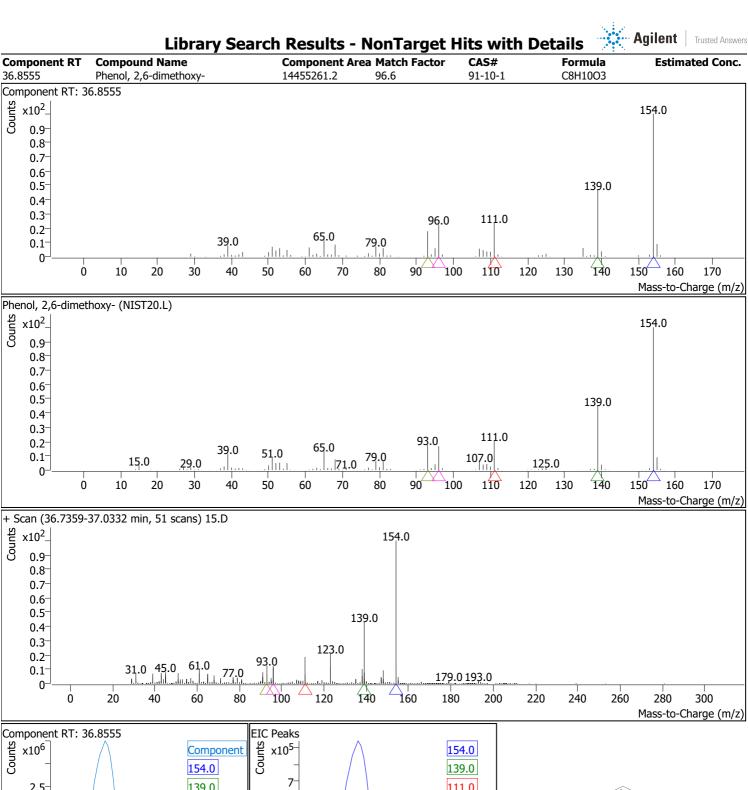
0.25

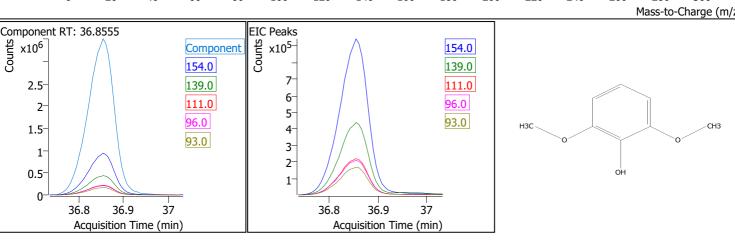
1

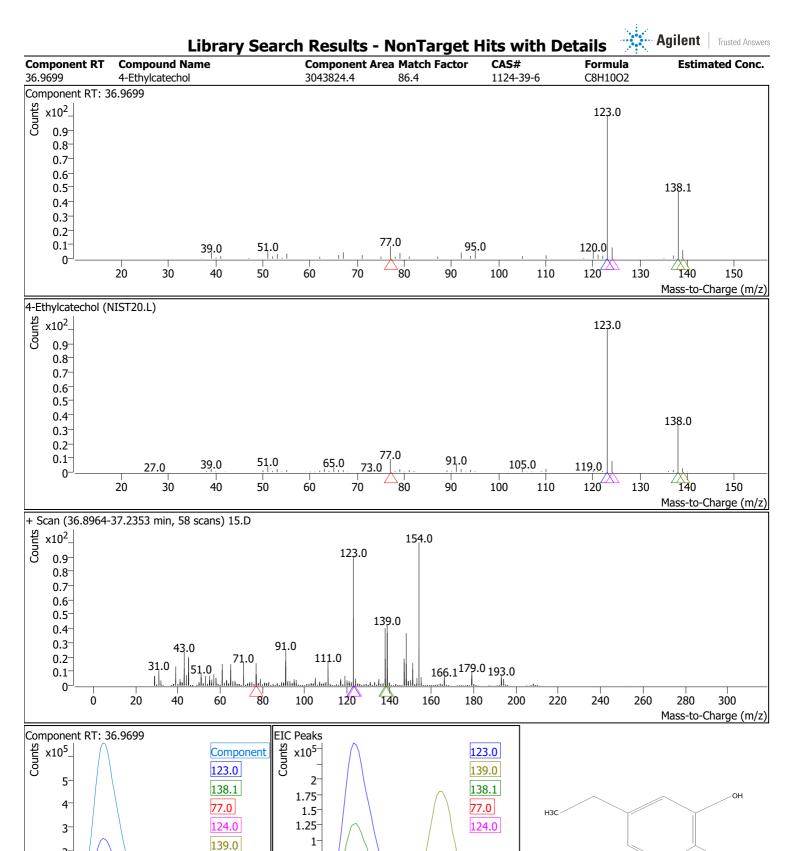














Acquisition Time (min)

37.2

0.75

0.25

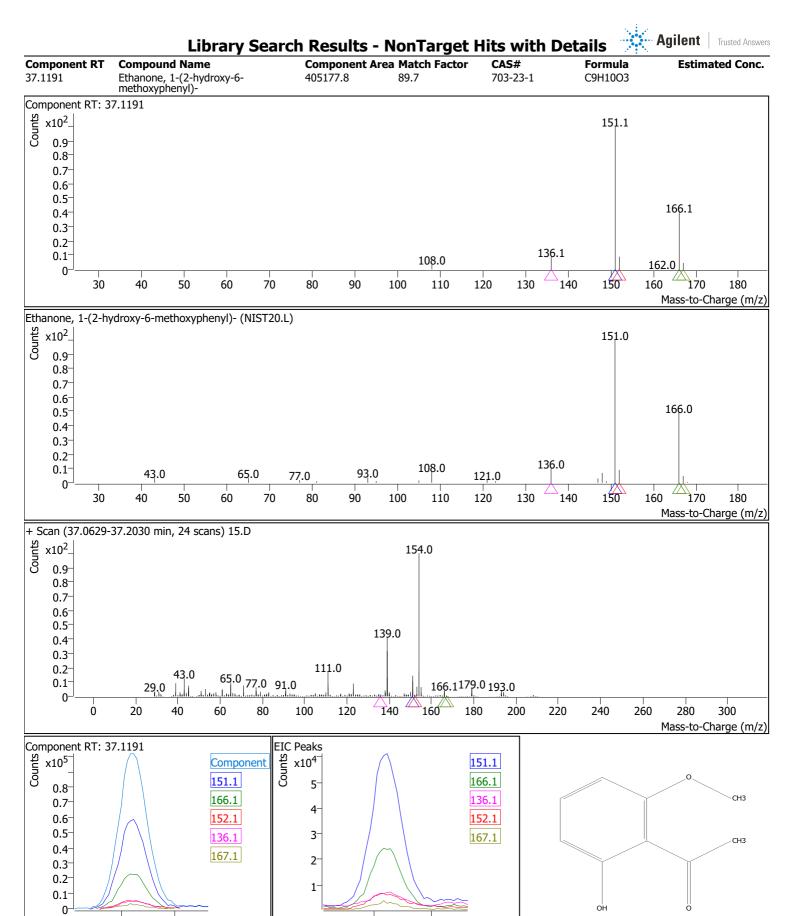
2

1

37.1

Acquisition Time (min)

37.2



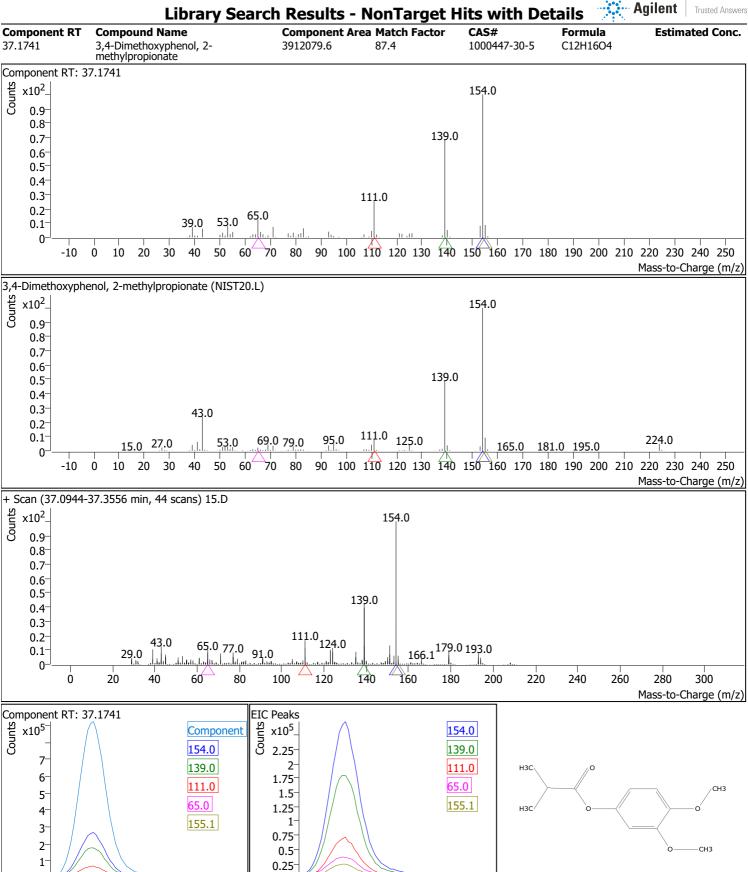
37.2

Acquisition Time (min)

37.1

37.2



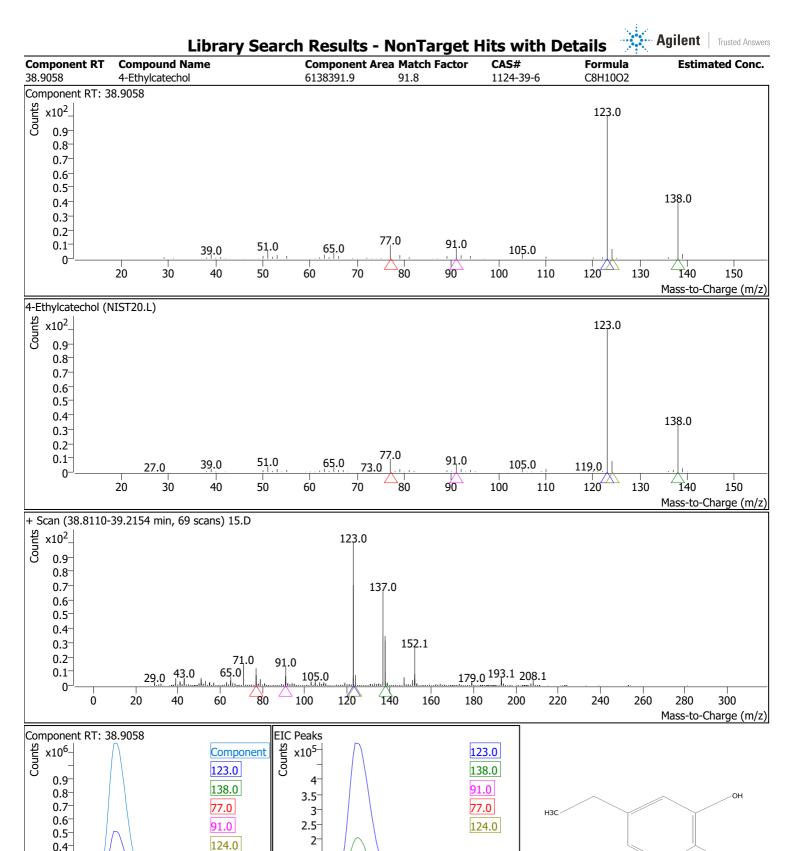


37.2

37.3

Acquisition Time (min)

37.3



0.5

1

38.9

39

39.1

Acquisition Time (min)

0.3

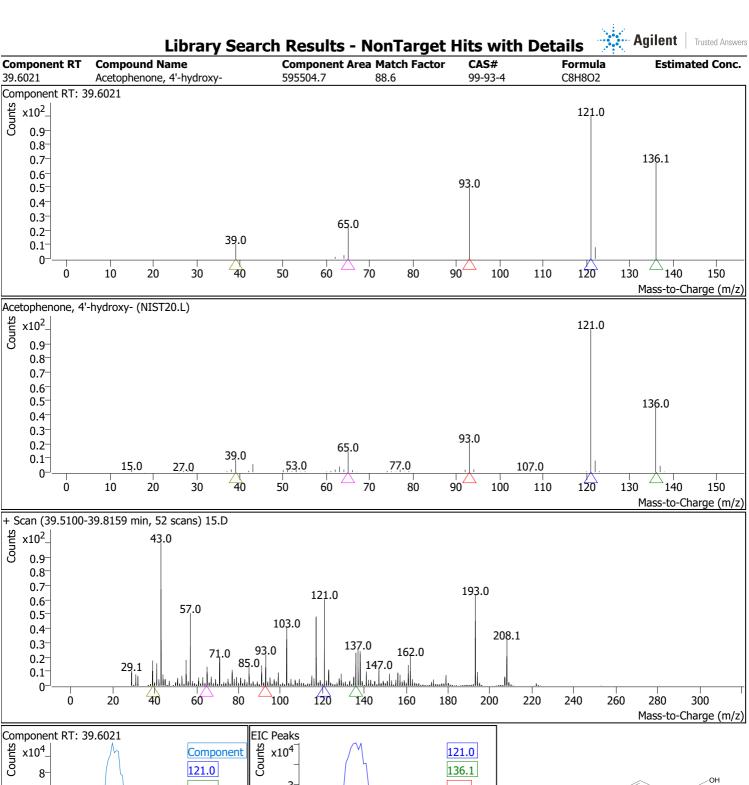
0.2

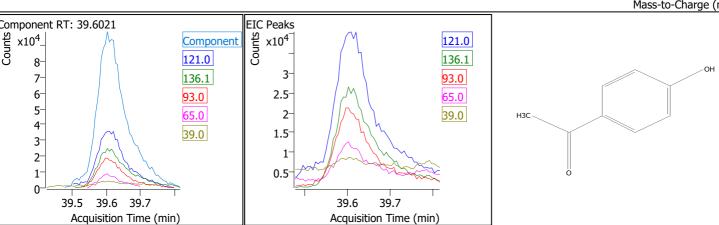
38.9

39

Acquisition Time (min)

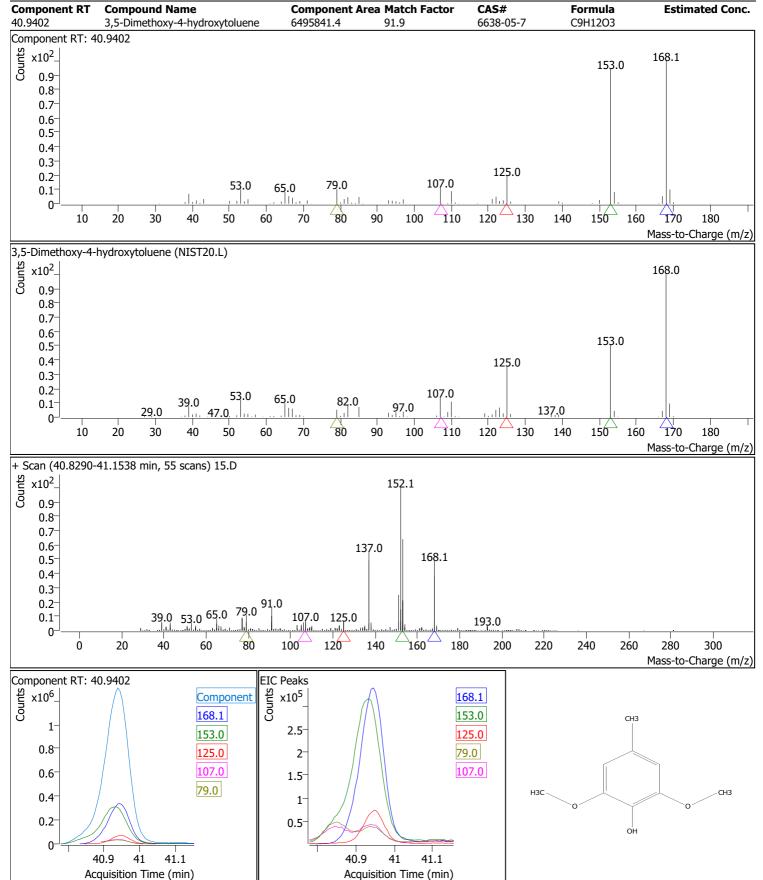
39.1

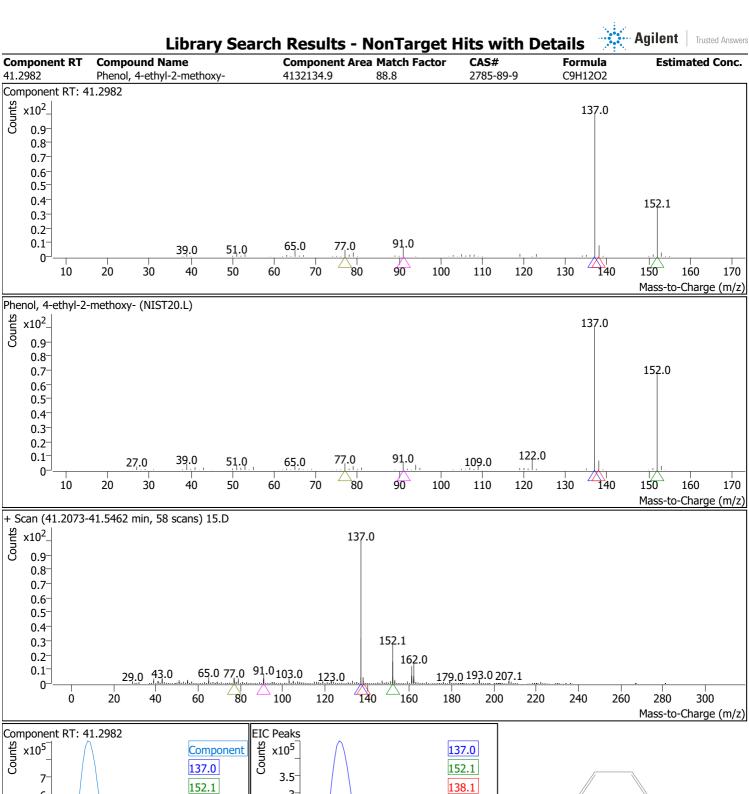


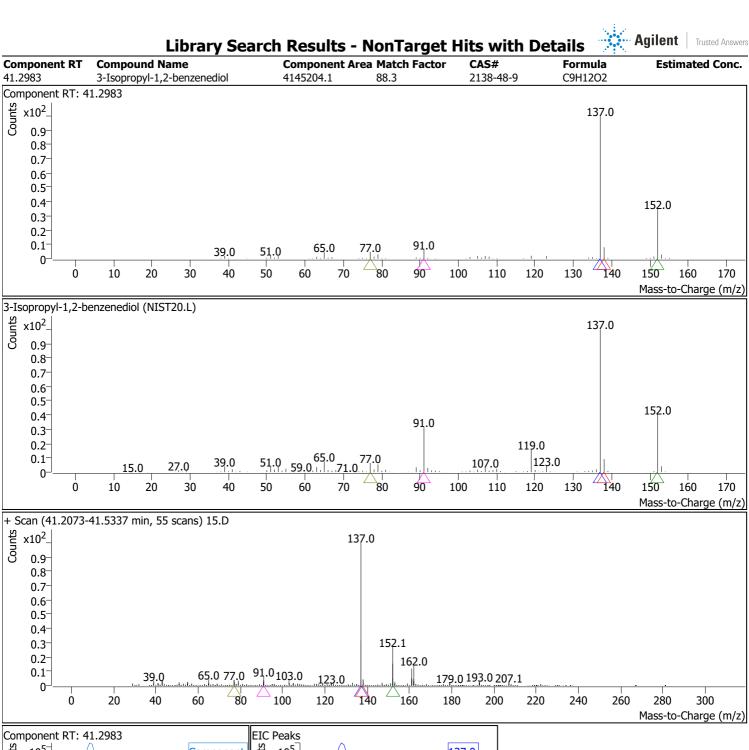


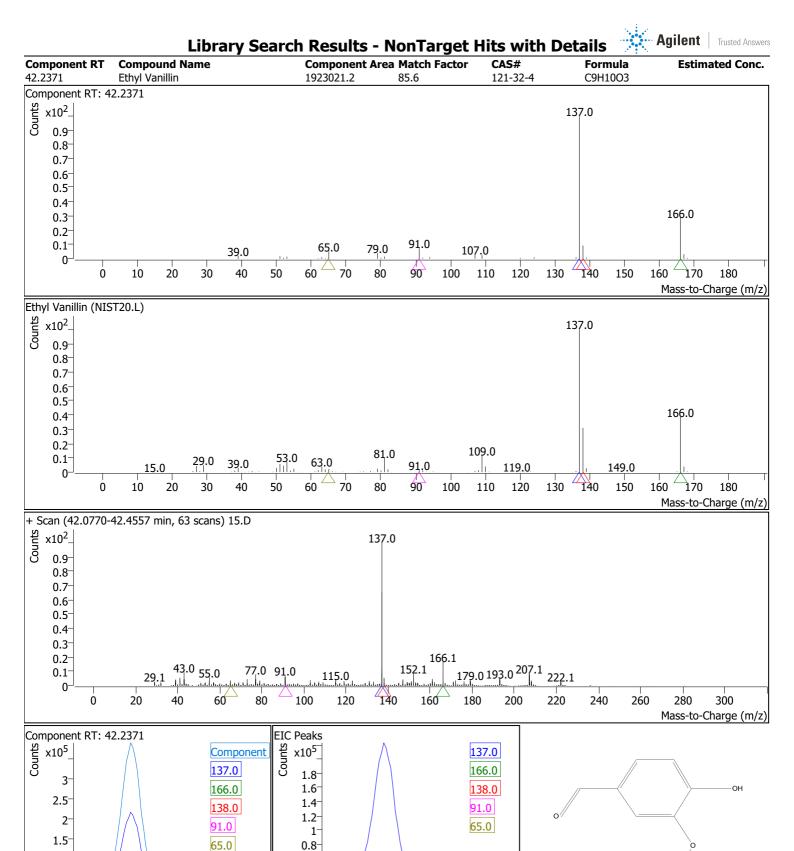














42.3

Acquisition Time (min)

42.4

0.6

0.4

1

42.2

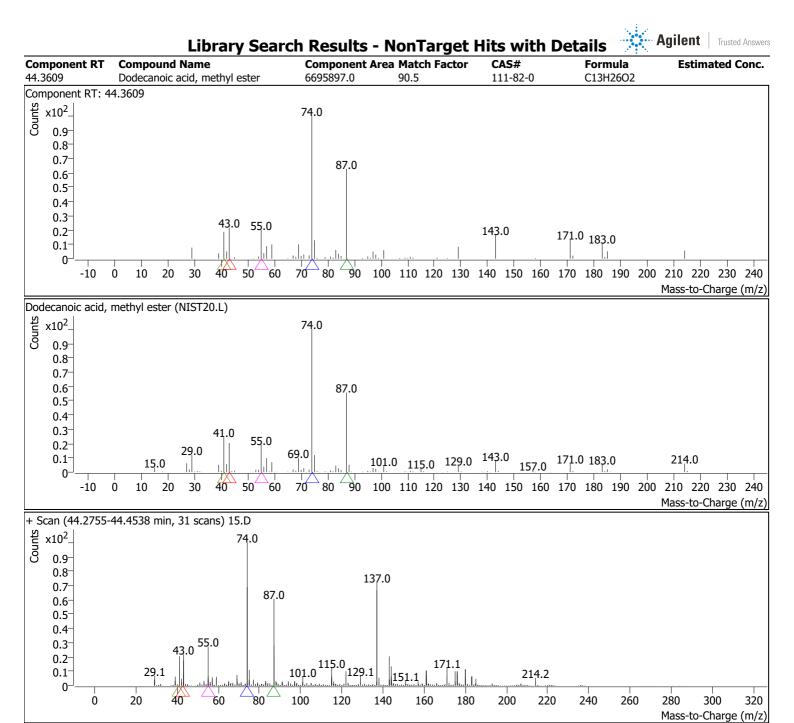
42.3

Acquisition Time (min)

42.4

0.5

СНЗ



44.4

Acquisition Time (min)

74.0

87.0

43.0

55.0

41.0

EIC Peaks

3.5

2.5

1.5

0.5

3

2-

1

Counts x10⁵-

Component 74.0

87.0

43.0

55.0

41.0

Component RT: 44.3609

x10⁶

1.6

1.4

1.2

1

0.8

0.6 0.4

0.2

44.3

44.35

44.4

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 46.1295 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-315462.0 90.5 65996-50-1 C6H5N3O2 Component RT: 46.1295 x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 0.1 121.0 105.0 100 105 110 115 120 125 130 135 140 145 150 155 160 165 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L) st x10² 0.9 151.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 80.0 108.0 0 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) + Scan (46.0490-46.2555 min, 35 scans) 15.D x10². 151.1 0.9 0.8 0.7 0.6 43.0 0.5 0.4 161.0 176.1 0.3 209.0 55.0 131.0 0.2 91.0103.0 0.1 0 120 300 0 20 40 60 80 100 200 220 240 260 280 Mass-to-Charge (m/z) Component RT: 46.1295 **EIC Peaks** Counts Counts x10⁴ x10⁴– 151.0 Component 151.0 152.0 6 6 152.0 105.0 5 5 121.0 121.0 4



46.1 46.15 46.2

Acquisition Time (min)

4

3 2

1

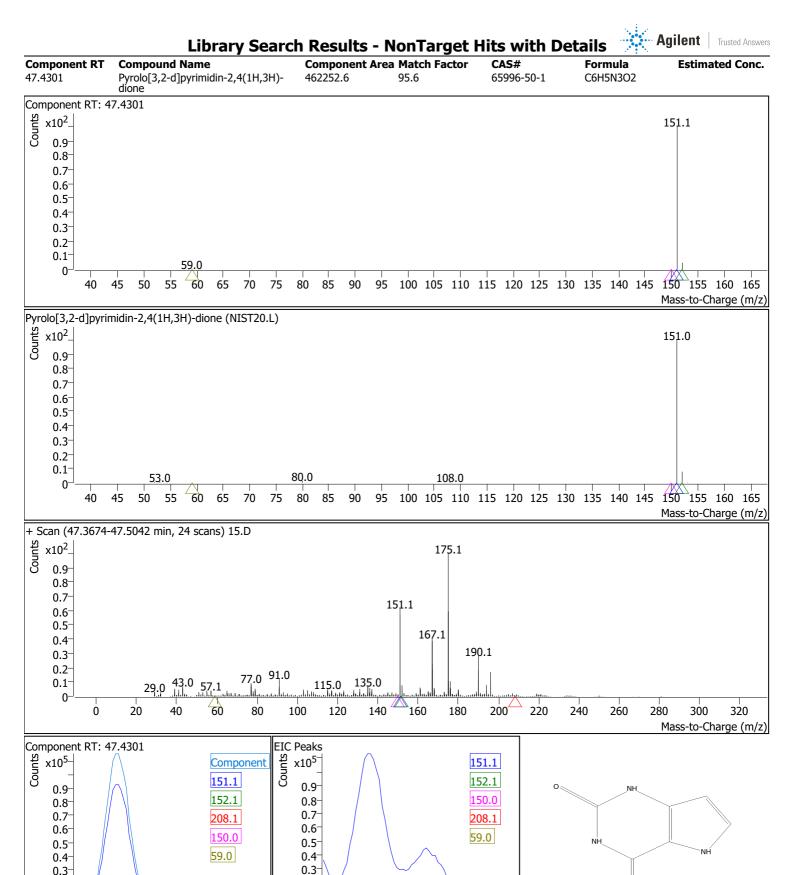
46.1 46.15 46.2

Acquisition Time (min)

105.0

3-

2-



Acquisition Time (min)

47.6

0.2

0.1

47.4

0.3⁻ 0.2⁻

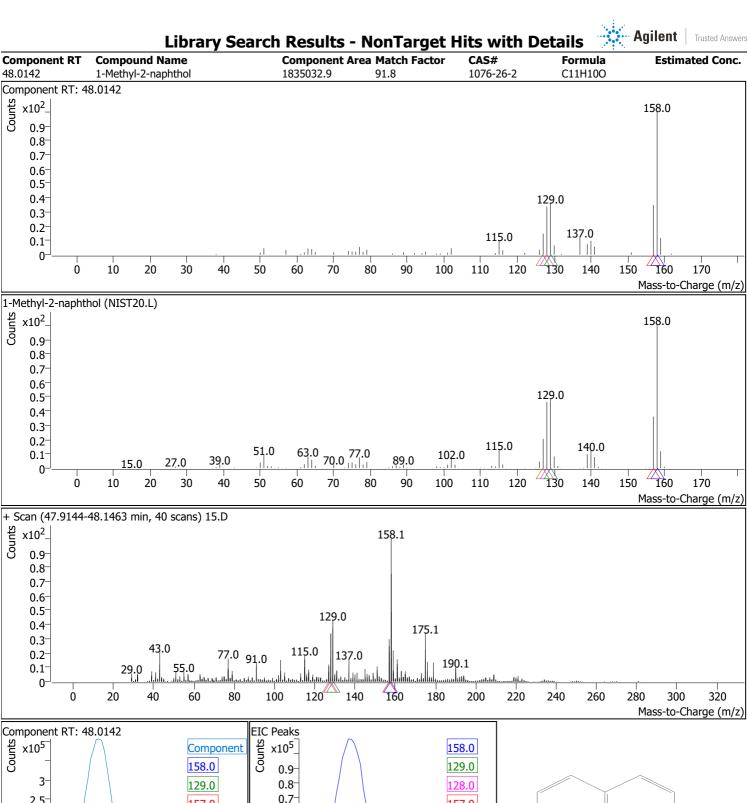
0.1

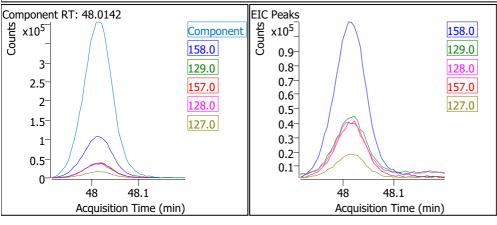
47.4

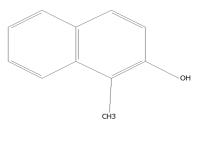
47.5

Acquisition Time (min)

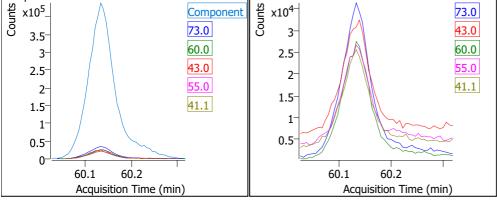
47.6

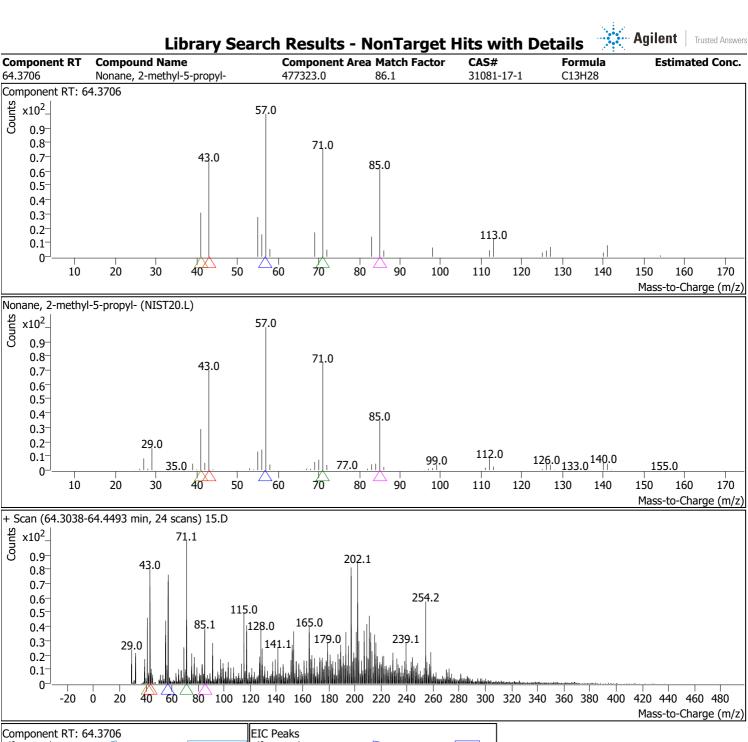


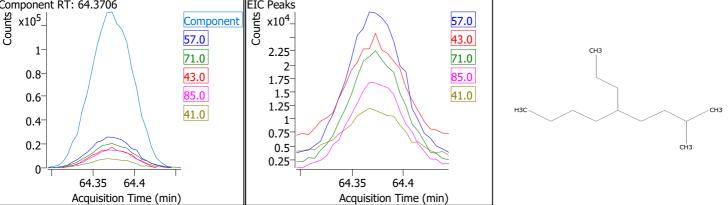




--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 60.1345 n-Hexadecanoic acid 1804063.3 88.5 57-10-3 C16H32O2 Component RT: 60.1345 v10² 0.9 73.0 60.0 0.8 43.0 0.7^{-} 55.0 0.6 129.0 256.1 0.5 0.4 0.3 0.2 0.1 0 20 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) n-Hexadecanoic acid (NIST20.L) st x10² 0.9 43.0 60.0 0.8 0.7 0.6 0.5 29.0 256.0 0.4 129.0 0.3 97.0 213.0 0.2 115.0 157.0 171.0 185.0 0.1 143.0 227.0 199.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) + Scan (60.0384-60.3179 min, 48 scans) 15.D St x10² 0.9 73.0 0.8 115.0 0.7 0.6 201.1 129.1 0.5 91.0 243.1 0.4^{-} 32.0 103.0 141.0 0.3 0.2 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 -20 Mass-to-Charge (m/z) EIC Peaks Component RT: 60.1345 Counts Counts x10⁴ 73.0 Component 73.0 43.0 3 3.5

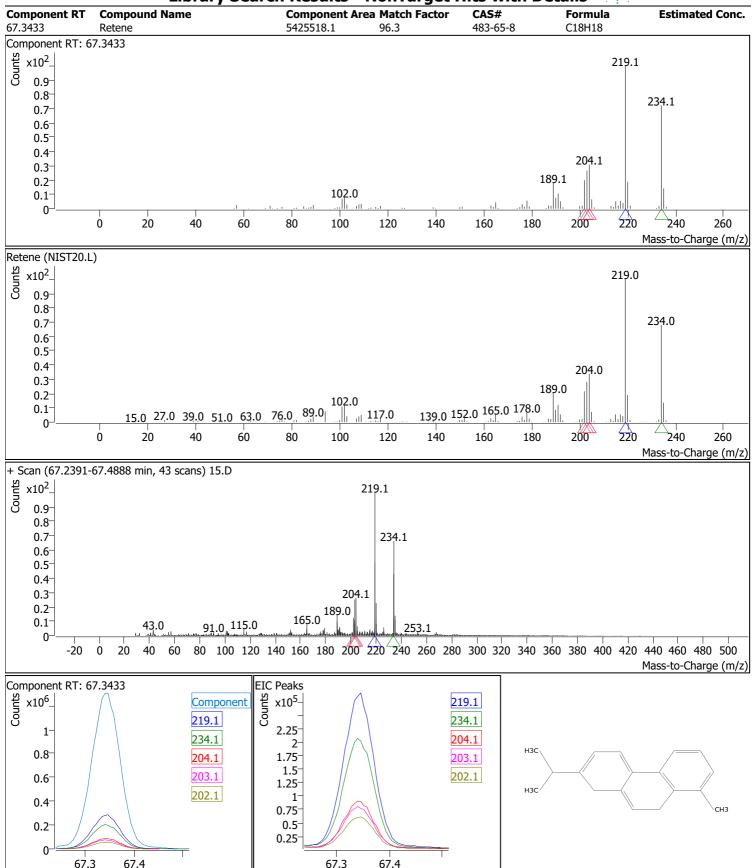








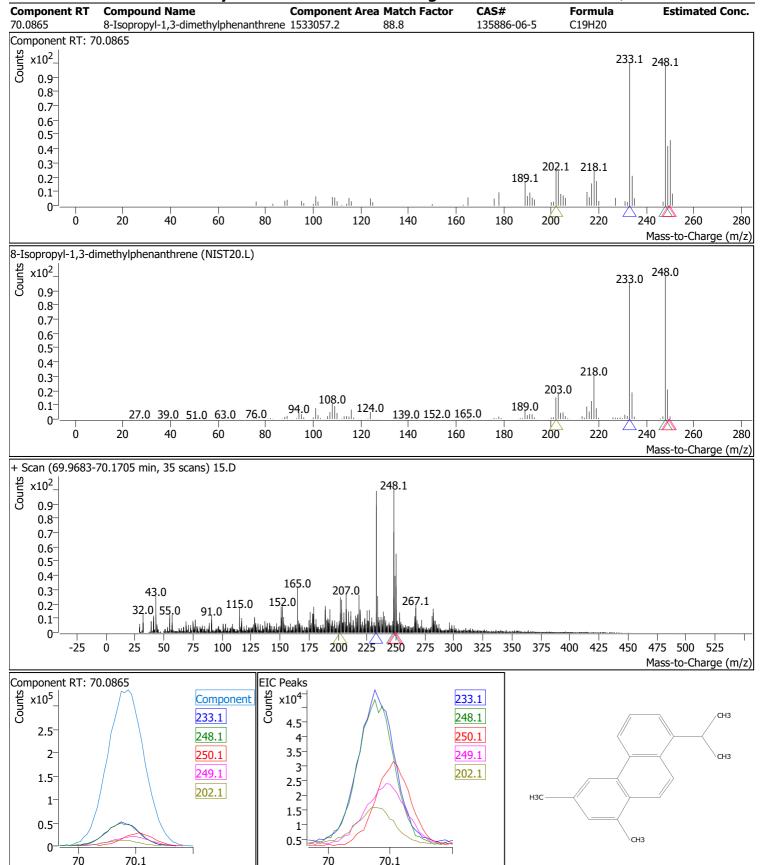




Acquisition Time (min)



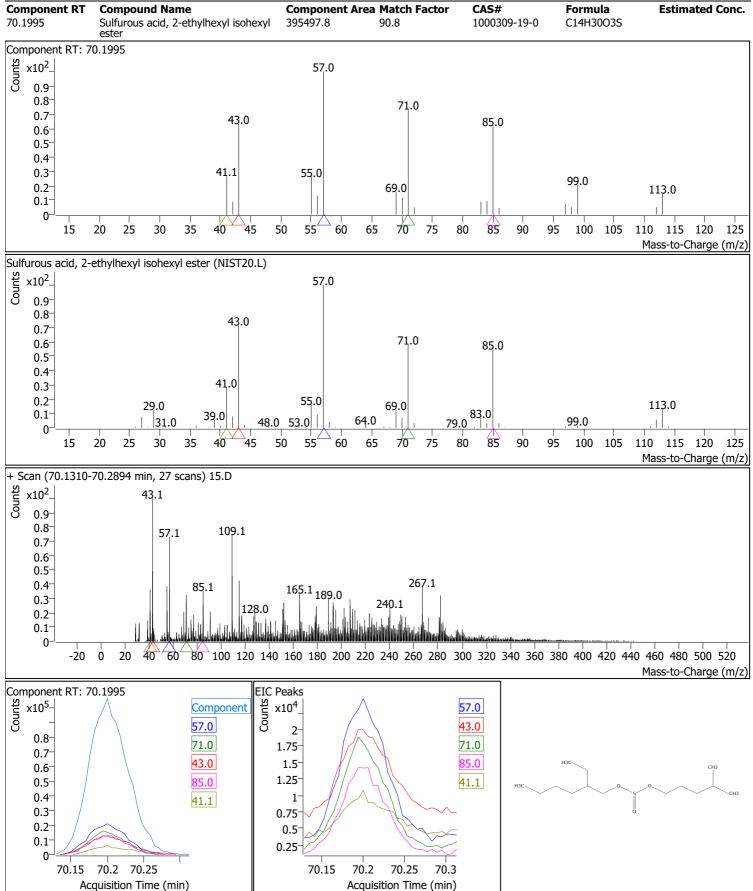




Acquisition Time (min)

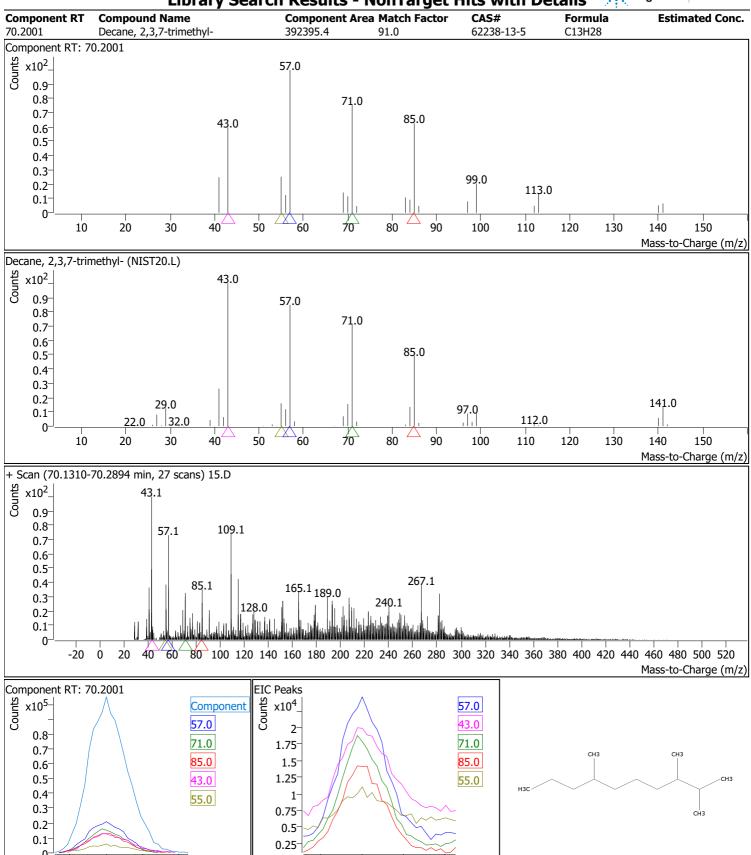
Library Search Results - NonTarget Hits with Details











70.2

70.25

Acquisition Time (min)

70.3

70.15

70.2 70.25

Compound Name Component RT Component Area Match Factor CAS# **Formula Estimated Conc.** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6821 7483069.3 92.4 5155-70-4 C20H28O2 Component RT: 73.6821 $x10^{2}$ 239.1 285.2 0.9 0.8 0.7 0.6 0.5 0.4^{-} 197.1 300.1 0.3 141.0 0.2 155.1 0.1 200 240 280 300 320 0 20 40 60 80 100 120 140 160 180 220 260 Mass-to-Charge (m/z) 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L) Counts x10²_ 285.0 0.9 0.8 239.0 0.7° 0.6 0.5 0.4 300.0 0.3 197.0 43.0 0.2 141.0 55.0 _{69.0} 91.0 183.0 0.1 225.0 255.0 240 280 300 0 20 40 60 80 100 120 140 160 180 200 220 260 320 Mass-to-Charge (m/z) + Scan (73.5657-73.8689 min, 52 scans) 15.D 돌 x10². 239.2 0.9 285.2 0.8 0.7 0.6 0.5 0.4 0.3 197.1 91.0 115.0 141.0 300.2 0.2 43.0 179.0 0.1 253.1 200 225 250 -25 25 50 75 100 150 175 275 300 325 350 375 400 425 450 475 500 525 550 125 Mass-to-Charge (m/z) Component RT: 73.6821 EIC Peaks x10⁶ x10⁵ 285.2 Component 239.1 239.1 1.2 1.6 СНЗ 285.2 197.1 1 1.4 197.1 300.1 1.2 0.8 300.1 1 141.0 0.6 0.8 141.0

73.7

73.8

Acquisition Time (min)

0.6

0.4

0.2

73.6

0.4

0.2

73.6

73.7

73.8

Acquisition Time (min)

СНЗ

