Library Search Results - NonTarget Hits with Details

Acq. Method Path



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

240501 scan

Analysis File Name 240502 data.uaf

Acq. Method File

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

File Name7.DPath NameD:\MassHunter\GCMS\1\data\RBEL\240501 scanSample Name7Sample TypeSample

 Acq. Date-Time
 5/1/2024 10:41:42 PM
 Acq. Operator

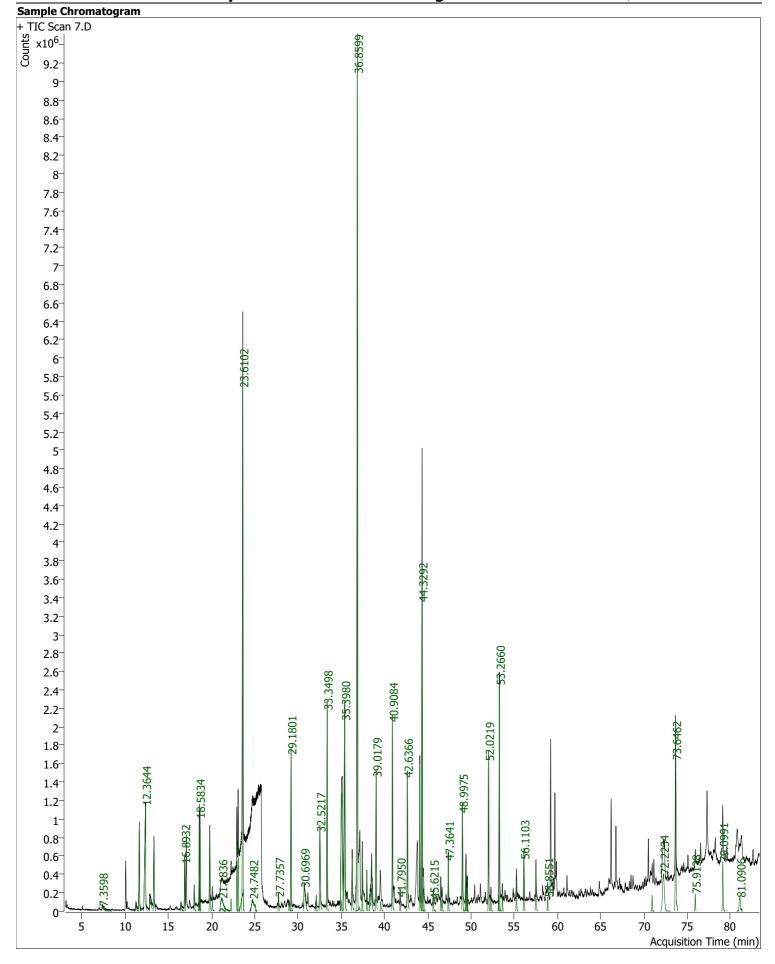
 Instrument Name
 GCMSD
 Dil.
 1

CAS# **Component RT Compound Name Formula Estimated** Component **Match Factor** Area Conc. 7.3598 1,3-Propanediol 504-63-2 C3H8O2 733667.0 93.8 11.2406 1,2-Propanediol, 3-methoxy-623-39-2 C4H10O3 512224 7 87 4 11.6430 Propane, 1,1-diethoxy-4744-08-5 C7H16O2 4427121.4 78.8 96-48-0 C4H6O2 97.7 12.3644 Butyrolactone 9419176.1 12.8498 Methyltartronic acid 595-98-2 C4H6O5 1420684.3 96.2 1000506-61-7 13.3319 2-(2-methoxyethoxy)propanoic acid, O-acetyl-C8H14O5 3735468.2 78.5 16.4418 3-Ethoxy-1,2-propanediol 1874-62-0 C5H12O3 438353.6 83.3 16.8932 1,3-Dioxolane-4-methanol, 2-ethyl-53951-44-3 C6H12O3 2156153.4 85.1 17,9938 Phenol 108-95-2 C6H6O 1090033.7 95.2 18.5834 1,3-Dioxolane-4-methanol, 2-ethyl-53951-44-3 C6H12O3 4335674.0 91.8 1000431-41-8 18.5866 C6H10O3 1418139.0 75.0 Propyl pyruvate 18.6582 Diisoamyl ether 544-01-4 C10H22O 3545608.6 95.9 18.6600 N-Methyl methacrylamide 3887-02-3 C5H9NO 778664.3 84.1 19.7889 1,3-Dioxolane-4-methanol, 2-ethyl-53951-44-3 C6H12O3 3560914.5 95.1 20.0871 2-Cyclopenten-1-one, 2-hydroxy-3-methyl-80-71-7 C6H8O2 636895.3 93.6 21.1219 1,1-Ethanediol, diacetate 542-10-9 C6H10O4 528277.2 79.1 21.1836 1,3,5-Trioxane 110-88-3 C3H6O3 3395036.0 79.0 22.2456 Phenol, 2-methyl-95-48-7 C7H8O 79.3 557751.0 22.9220 1-Propanol, 2-(2-hydroxypropoxy)-C6H14O3 2201361.7 80.8 106-62-7 98.5 23.0608 1-Octanol 111-87-5 C8H18O 3421964.8 23.6102 Phenol, 2-methoxy-90-05-1 C7H8O2 25482441.8 98.5 23.6806 Pentanoic acid, 4-oxo-123-76-2 C5H8O3 3497611.6 82.8 24.7482 2-Propanone, 1-hydroxy-116-09-6 C3H6O2 2629768.2 86.2 27.7357 Butanoic acid, 2,2-dimethylpropyl ester 23361-69-5 C9H18O2 692828.5 81.1 28.9418 14786-82-4 556431.0 Phenol, 4-methoxy-3-methyl-C8H10O2 81.0 29.1801 2-Methoxy-5-methylphenol 1195-09-1 C8H10O2 6708200.1 99.2 120-80-9 3018861.8 97 N 30.6969 Catechol C6H6O2 32.1063 Ethanone, 1-(2-hydroxy-5-methylphenyl)-1450-72-2 727064.4 C9H10O2 84.1 32.5217 1,2-Benzenediol, 3-methoxy-934-00-9 C7H8O3 4835123.1 98.0 33.3498 Phenol, 4-ethyl-2-methoxy-2785-89-9 C9H12O2 8453789.1 96.7 35.0133 1,2-Benzenediol, 3-methyl-488-17-5 C7H8O2 517815.0 83.9 35.0676 1,2-Benzenediol, 4-methyl-452-86-8 C7H8O2 15047958.6 84.5 35.0941 Butanoic acid, anhydride 106-31-0 C8H14O3 14324524.5 80.3 35.3980 2-Furanmethanol, tetrahydro-97-99-4 C5H10O2 14005441.9 79.3 35.3981 2,3-dihydroxypropyl isobutyrate 1010458-45-6 C7H14O4 13911383.9 79.3 36.2527 2-Furanmethanol, tetrahydro-97-99-4 C5H10O2 3084685.8 83.1 36.8599 44179533.6 Phenol, 2,6-dimethoxy-91-10-1 C8H10O3 99.3 37.1102 Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-703-23-1 C9H10O3 450961.3 84.2 Phenol, 2-methoxy-4-propyl-37,4305 2785-87-7 C10H14O2 2087071.8 94.3 37.9510 1,2,3-Trimethoxybenzene 634-36-6 C9H12O3 1261696.5 91.0 38.4939 97-72-3 83.1 Propanoic acid, 2-methyl-, anhydride C8H14O3 2553371.6 38.4950 1,3-Dioxolane-4-methanol, 2-ethyl-53951-44-3 C6H12O3 4978254.4 75.3 Vanillin 121-33-5 C8H8O3 6352254.2 98.3 39.0179 93.3 39.5409 Ethanone, 1-(3-hydroxyphenyl)-121-71-1 C8H8O2 637625.2 40.9084 3,5-Dimethoxy-4-hydroxytoluene 6638-05-7 C9H12O3 8100697.3 95.0 41.7950 Eugenol 97-53-0 C10H12O2 572563.9 88.6 42.6366 498-02-2 C9H10O3 6653386.1 99.4 4-Ethyl-2,6-dimethoxyphenol 14059-92-8 C10H14O3 99.4 44.0720 6162115.0 15635176.6 44.3292 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-2503-46-0 C10H12O3 94.5 44.3378 Dodecanoic acid, methyl ester 111-82-0 C13H26O2 8132319.8 93 9 44.4676 Homovanillyl alcohol 2380-78-1 1494385.8 C9H12O3 82.9 Pentanoic acid, 4-oxo-, 2-methylpropyl ester 726854.9 45.6215 3757-32-2 C9H16O3 81.6 1047376.6 46.5029 1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-1835-14-9 C10H12O3 93.9 46.6408 Butyrovanillone 64142-23-0 C11H14O3 586960.0 90.0 47.3641 2,6-Dimethoxy-4-propylphenol 6766-82-1 2088867.2 95.7 C11H16O3 48.9975 Benzenepropanol, 4-hydroxy-3-methoxy-2305-13-7 C10H14O3 5238868.1 96.2 134-96-3 94.7 49.3831 Benzaldehyde, 4-hydroxy-3,5-dimethoxy-C9H10O4 2081225.0 7-Methoxy-1-naphthol 1444499.0 91.7 49.4272 67247-13-6 C11H10O2 49.5659 (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol 20675-95-0 C11H14O3 998242.3 80.9 N,N-Diethyl-p-nitroaniline 49.5659 2216-15-1 C10H14N2O2 981974.6 80.3 Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-52.0219 2478-38-8 C10H12O4 6759989.6 98.2 52.2901 .beta.-(4-Hydroxy-3-methoxyphenyl)propionic acid 1135-23-5 C10H12O4 674803.3 85.4 53.1939 1,6-Dimethoxynaphthalene 3900-49-0 C12H12O2 814675.9 81.3 19037-58-2 Syringylacetone C11H14O4 9815952.7 97.5 53.2660

Library Search Results - NonTarget Hits with Details

Agilent	Trusted Ansv
Agneni	Trusted Ans

Component RT Compound Name		CAS#	Formula	Component Area	Match Factor	Estimated Conc.
53.6190	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	727363.8	88.2	
55.2478	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5650-43-1	C11H14O4	1574703.9	94.9	
56.1103	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	2317879.5	82.2	
57.4986	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	1916163.6	93.8	
58.8551	Asarone	2883-98-9	C12H16O3	672494.8	77.8	
70.9343	Methyl dehydroabietate	1235-74-1	C21H30O2	722876.2	82.5	
72.2234	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	5937981.7	82.6	
73.6462	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	8805653.0	93.5	
75.9138	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	839048.2	82.5	
79.0991	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	2965571.2	90.0	
81.0906	Phenol, 4,4'-methylenebis[2,6-dimethoxy-	15640-40-1	C17H20O6	1508662.8	80.4	



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43.0

45.0

2

1.5

0.5

1

7.4 7.6 7.8 8 8.2 8.4

Acquisition Time (min)

0.6

0.4

0.2

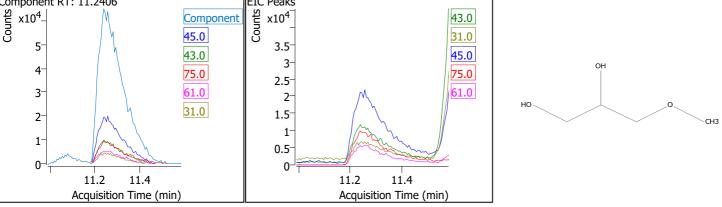
0

7.4 7.6 7.8

8

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.** 623-39-2 11.2406 1,2-Propanediol, 3-methoxy-512224.7 87.4 C4H10O3 Component RT: 11.2406 v10² 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 33.1 0.1 88.0 10 15 20 25 30 35 40 55 60 65 75 80 85 100 105 110 115 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Counts x10²_ 0.9 45.0 0.8 0.7 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 15.0 0.2 33.0 18.0 0.1 88.0 63.0 103.0 71.0 10 15 20 25 30 35 40 50 55 60 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (11.1970-11.3284 min, 23 scans) 7.D St x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 32.0 75.0 0.2 61.0 0.1 88.0 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: 11.2406 **EIC Peaks** x10⁴ Component 43.0



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87.0

57.0

31.0

0.8

0.6

0.4

0.2

11.6

11.7

Acquisition Time (min)

5

4

3

2

1

11.6

11.7

Acquisition Time (min)

11.8

Н3С <

57.0

31.0

--- 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 12.3644 Butyrolactone 97.7 C4H6O2 Component RT: 12.3644 v10² 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 0 25 40 55 75 20 30 35 45 50 60 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 (12.1398-12.5295 min, 66 scans) 7.D st x10² 0.9 0.8 0.7 0.6 0.5 29.0 86.0 0.4^{-} 0.3 56.0 0.2 0.1 10 20 30 40 50 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: 12.3644 Counts Counts x10⁵ 42.0 Component 42.0 41.0 0.9 2.5 41.0 86.0 0.8 0.7 29.0 86.0 2

56.0

0.6

0.5

0.4

0.3

12.2 12.3

12.4

Acquisition Time (min)

12.5

29.0

56.0

1.5

1

12.2

12.3

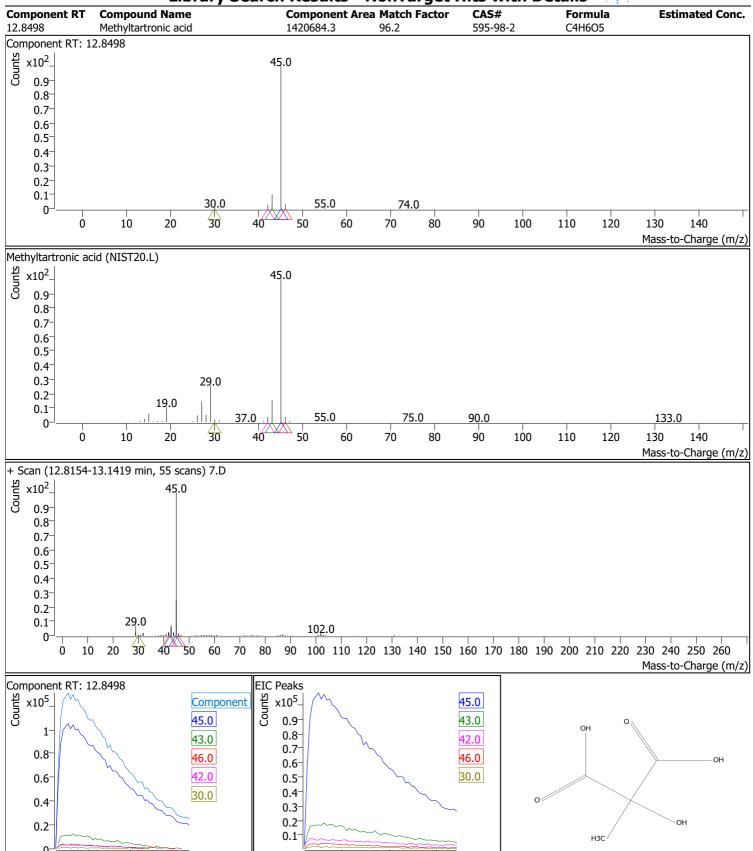
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Acquisition Time (min)

12.5

Library Search Results - NonTarget Hits with Details





12.9

13

Acquisition Time (min)

13.1

12.9

13

Acquisition Time (min)

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13.3

13.4

Acquisition Time (min)

13.5

31.0

нзс

57.0

31.0

3

2

1

13.3

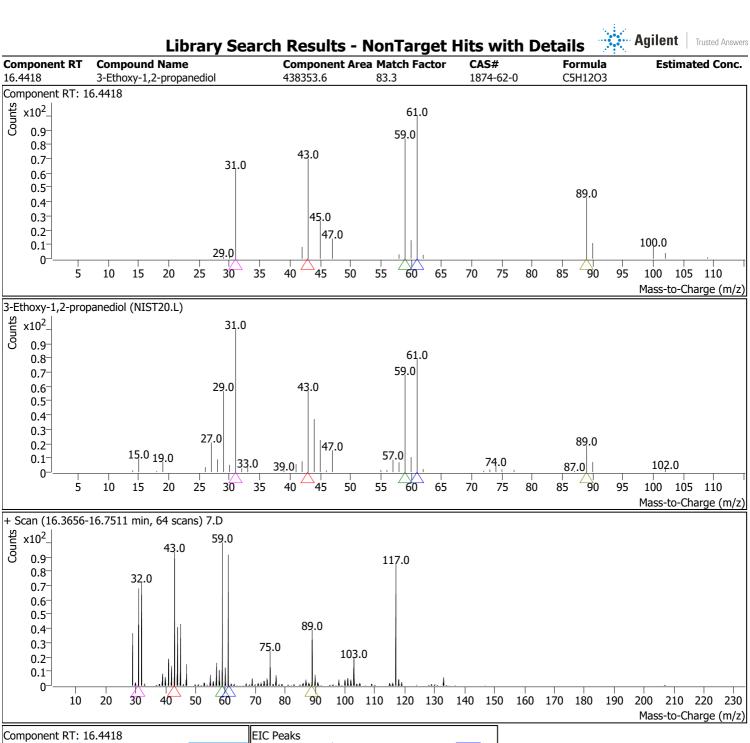
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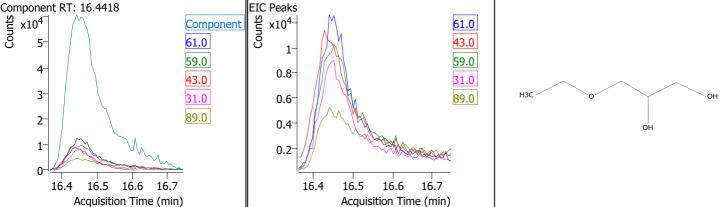
Acquisition Time (min)

13.5

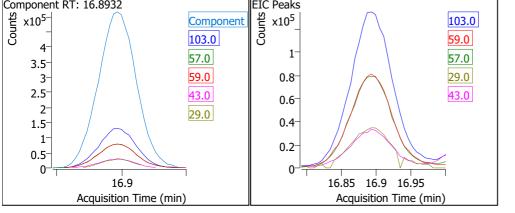
0.6

0.4





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18.1

Acquisition Time (min)

18.2

4

3-

2-

18

40.0

1

0.75

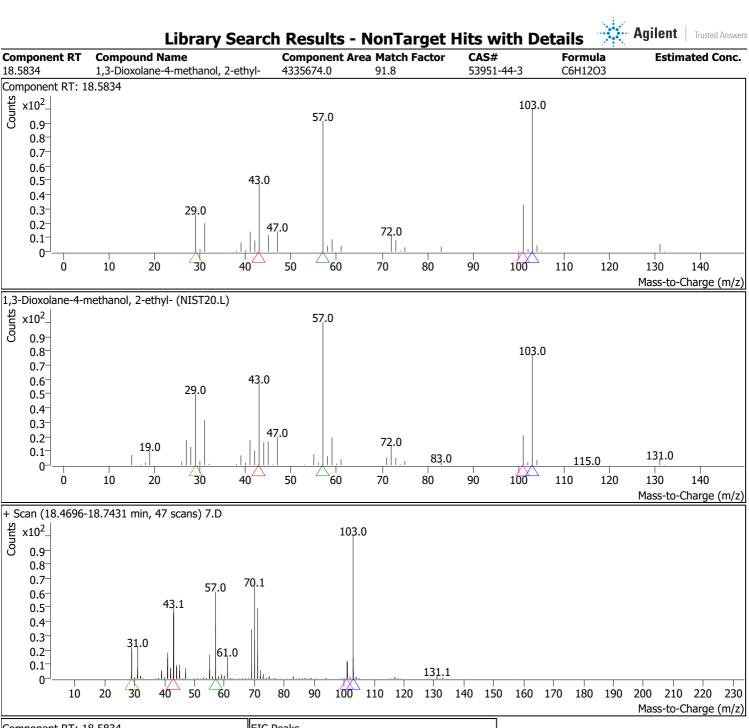
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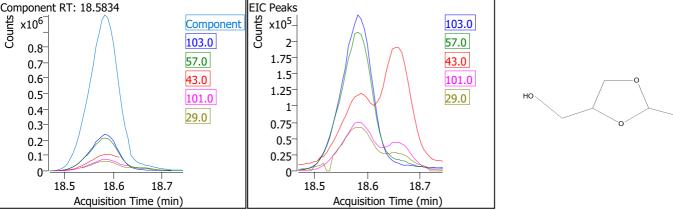
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18

18.1

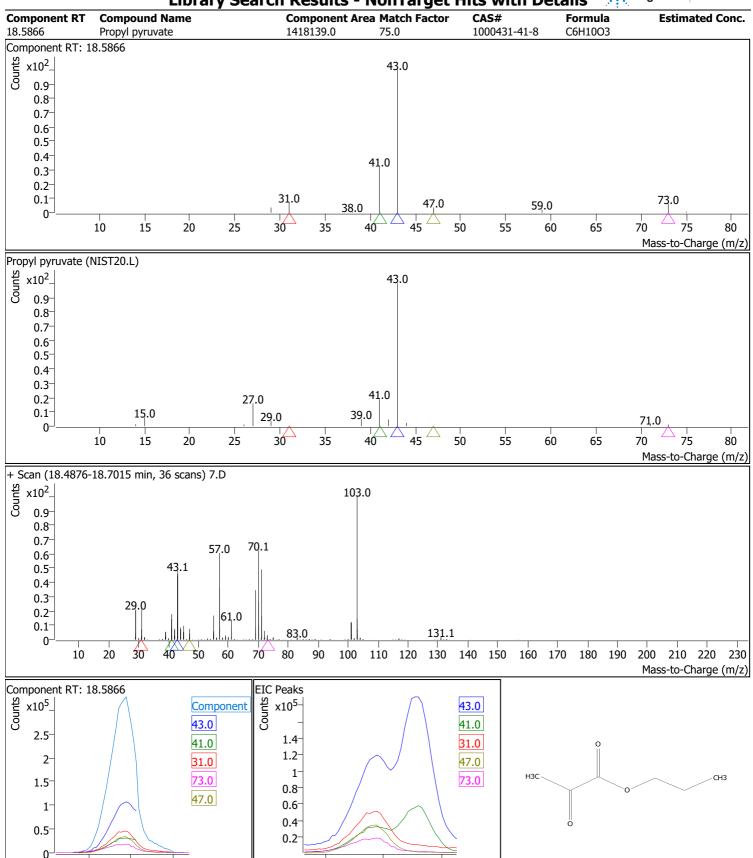
Acquisition Time (min)











18.6

Acquisition Time (min)

18.7

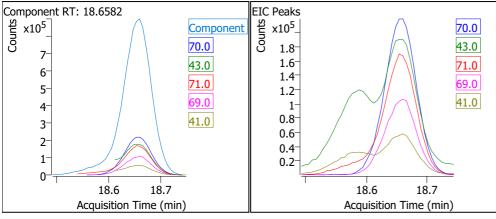
18.5

18.5

18.6

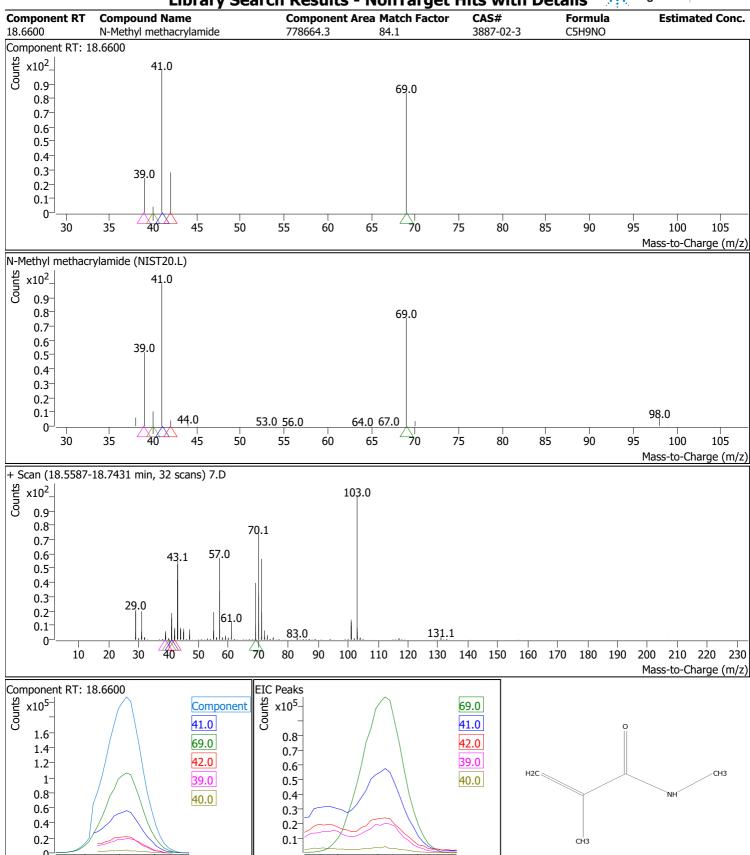
Acquisition Time (min)

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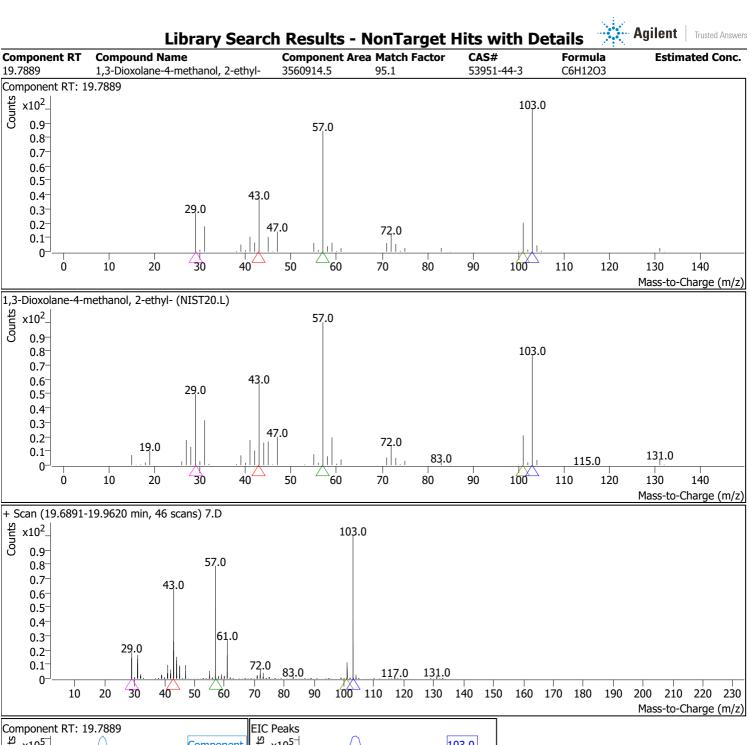
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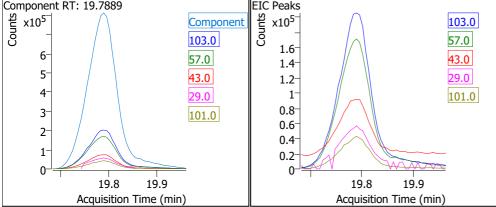
18.65

18.7 Acquisition Time (min)

18.6 18.65 18.7

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.** 80-71-7 20.0871 2-Cyclopenten-1-one, 2-hydroxy-3-636895.3 93.6 C6H8O2 Component RT: 20.0871 x10²_ 112.0 0.9 8.0 0.7 0.6 0.5 0.4 69.0 55.0 0.3 41.0 83.0 39.0 43.0 0.2^{-} 99.0 0.1 0-55 30 35 40 45 50 60 65 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 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (19.9938-20.3307 min, 57 scans) 7.D st x10² 0.8 43.0 0.7 0.6 0.5 0.4 0.3 31.0 112.0 0.2 69.0 103.0 0.1 0 Ó 20 60 80 100 200 220 260 40 120 140 160 180 240 280 300 Mass-to-Charge (m/z) Component RT: 20.0871 **EIC Peaks** Counts Counts x10⁵ $x10^{4}$ 112.0 Component 112.0 55.0 1 2.5 69.0 69.0 0.8 2 55.0 41.0 41.0 83.0 0.6 1.5 нзс 83.0 0.4

20.1

20.2

Acquisition Time (min)

20.3

1

0.5

0.2

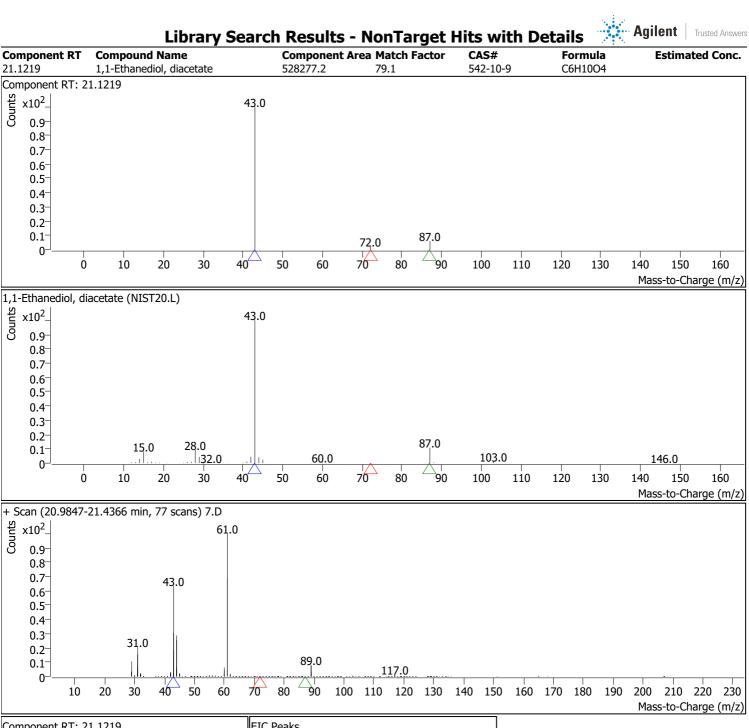
20.1

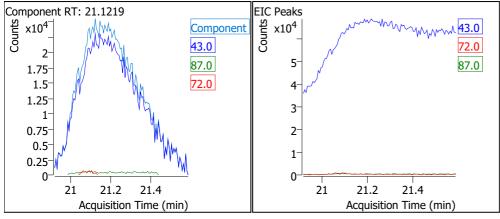
20.2

Acquisition Time (min)

20.3

ОН





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3395036.0 110-88-3 21.1836 1,3,5-Trioxane 79.0 C3H6O3 Component RT: 21.1836 v10² 0.9 61.0 0.8 0.7 43.0 89.0 0.6 0.5 0.4 0.3 31.0 0.2 0.1 29.0 45.0 56.0 0 -90 55 25 30 60 75 10 15 20 35 40 45 50 65 70 80 85 95 100 Mass-to-Charge (m/z) 1,3,5-Trioxane (NIST20.L) Counts x10²_ 0.9 31.0 0.8 61.0 89.0 0.7 0.6 0.5 29.0 0.4 0.3 0.2 0.1 44.0 14.0 56.0 45 90 5 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.8905-22.0966 min, 203 scans) 7.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 117.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.1836 **EIC Peaks** Counts x10⁵ x10⁵ Component 61.0 43.0 0.9 1 43.0 0.8 0.7 0.8 89.0 89.0 0.6 60.0 31.0 0.6 0.5 60.0 0.4

21.5

Acquisition Time (min)

22

0.3

0.1

21

0.4

0.2

21

21.5

Acquisition Time (min)

22

--- 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 22.2456 Phenol, 2-methyl-557751.0 C7H8O Component RT: 22.2456 y x10² 0.9 108.0 0.8 103.0 0.7 0.6 57.0 0.5 0.4 77.0 0.3 90.0 0.2 55.0 39.0 0.1 10 35 50 55 60 75 85 90 95 100 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 0.3 79.0 90.0 0.2 0.1 17.0 58.0 ^{63.0} 68.0 74.0 86.0 | 94.0 100.0 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (22.1726-22.3821 min, 36 scans) 7.D St x10²_ 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 0.1 103.0 117.0 77.0 89.0 10 20 30 40 50 60 70 80 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 22.2456 Counts Counts x10⁴ 108.0 Component 108.0 103.0 1.8 1 107.0 1.6 107.0 1.4 0.8 103.0 57.0 НО 1.2



22.3

Acquisition Time (min)

57.0

77.0

1

0.8

0.6

0

22.2

0.6

0.4

0.2

22.2

22.3

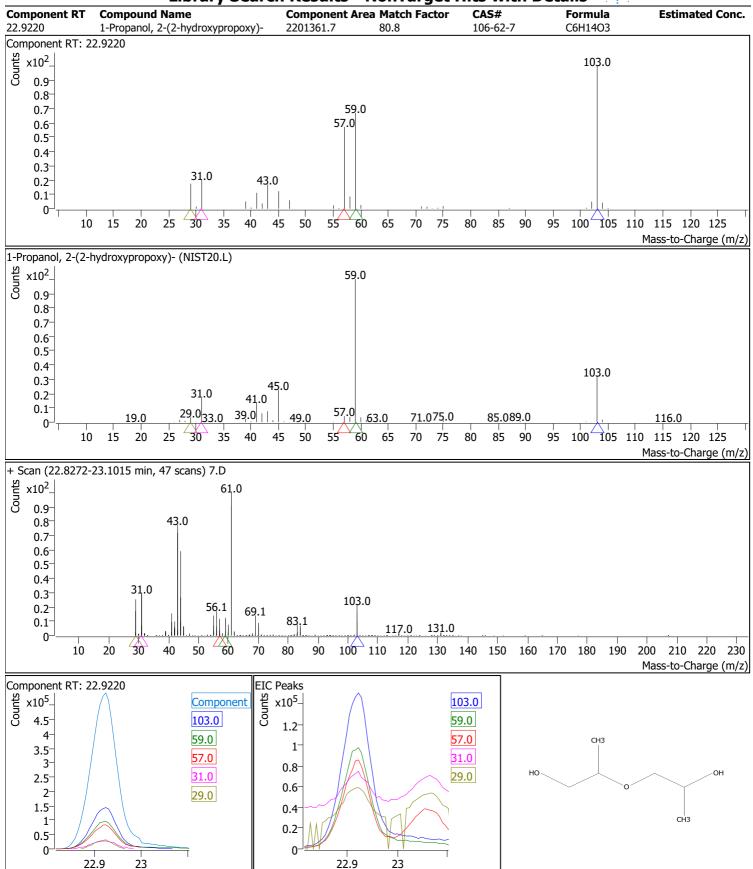
Acquisition Time (min)

77.0

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.** 23.0608 1-Octanol 3421964.8 98.5 111-87-5 C8H18O Component RT: 23.0608 y x10² 0.9 56.0 41.0 0.8 70.1 29.0 0.7 84.1 0.6 0.5 0.4 0.3 0.2 0.1 70 55 100 105 110 115 120 125 130 135 140 45 50 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10²_ 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 (22.9642-23.2454 min, 48 scans) 7.D St x10²_ 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 56.1 69.1 83.1 0.1 103.0 0 10 20 30 40 50 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: 23.0608 Counts Counts x10⁴ 56.0 Component 56.0 55.0 6 55.0 41.0 41.0 70.1 5 4

23.1

Acquisition Time (min)

23.2

70.1

69.1

3

2

1

23

23.1

Acquisition Time (min)

23.2

4

3

2-

23

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 25482441.8 90-05-1 23.6102 Phenol, 2-methoxy-98.5 C7H8O2 Component RT: 23.6102 v10² 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 53.0 0.1 39.0 65.0 80 110 50 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 0.7 81.0 0.6 0.5 0.4 0.3 0.2 53.0 27.0 39.0 0.1 95.0 15.0 110 50 10 20 30 40 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4642-23.7615 min, 51 scans) 7.D St x10²_ 0.9 109.0 124.0 81.0 43.0 0.8 61.0 0.7 0.6 0.5 0.4 0.3 53.0 0.2 31.0 0.1 95.0 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: 23.6102 Counts Counts x10⁶ x10⁶ 109.0 Component 109.0 124.0 4.5 1.2 124.0 81.0 1 3.5 81.0 53.0



23.6

Acquisition Time (min)

23.7

52.0

нзс

0.8

0.6

0.4

0.2

23.5

53.0

52.0

3

2.5

1.5

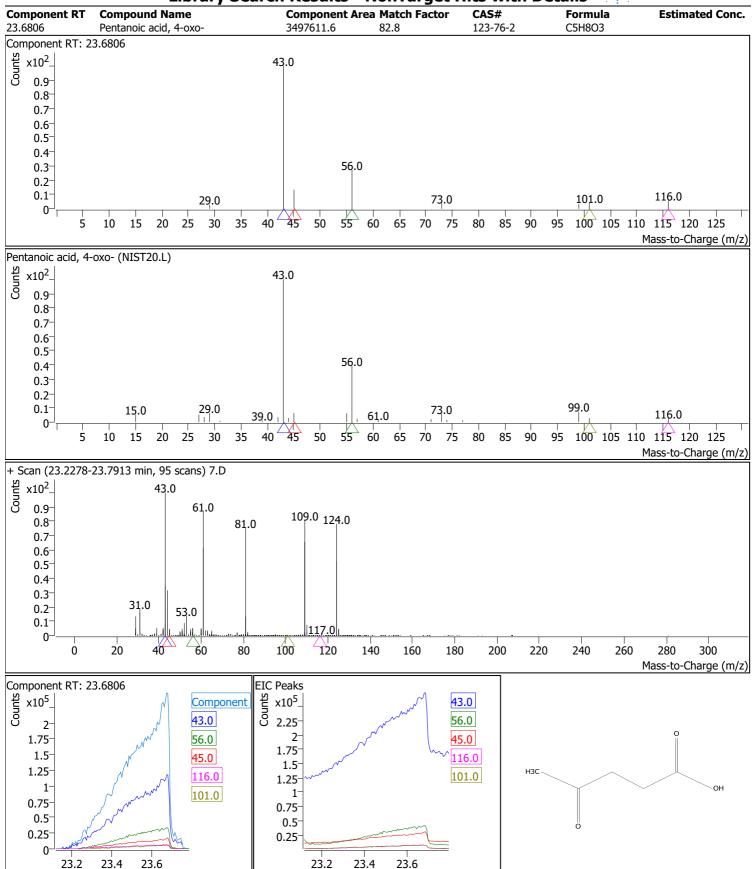
1

23.5

23.6

Acquisition Time (min)





Acquisition Time (min)

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.** 2629768.2 116-09-6 24.7482 2-Propanone, 1-hydroxy-86.2 C3H6O2 Component RT: 24.7482 v10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 74.0 0.2 0.1 56.0 30 $\frac{4}{5}$ 25 55 35 45 65 70 10 15 20 40 50 80 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy- (NIST20.L) Counts x10²_ 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 15.0 29.0 74.0 0.1 27.0 45.0 30 45 65 10 15 20 25 35 40 50 55 60 70 80 Mass-to-Charge (m/z) + Scan (24.4765-25.2421 min, 129 scans) 7.D st x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 103.0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 24.7482 Counts Counts x10⁵⁻ 43.0 Component 31.0 43.0 2.5 1 СНЗ 31.0 74.0 2 0.8 56.0 74.0

24.6 24.8

25

Acquisition Time (min)

110.0

1.5

1

0.5

0-

56.0

110.0

0.6

0.4

0.2

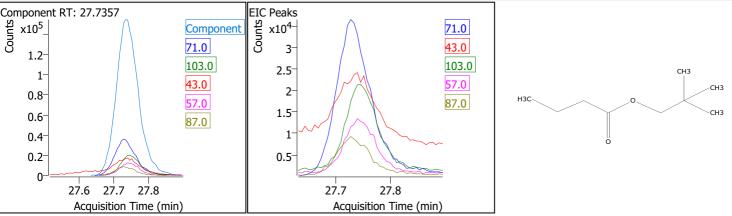
24.6 24.8

25

Acquisition Time (min)

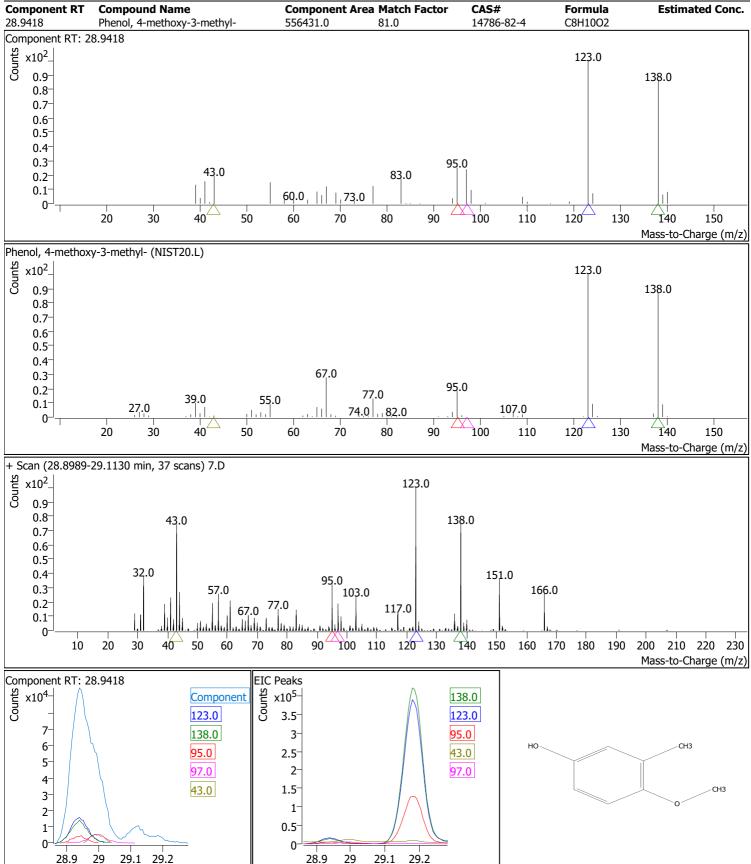
OH

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7357 Butanoic acid, 2,2-dimethylpropyl 692828.5 81.1 23361-69-5 C9H18O2 Component RT: 27.7357 x10²_ 71.0 0.9 8.0 0.7 0.6 103.0 43.0 0.5 0.4 57.0 0.3 87.0 31.0 0.2^{-} 0.1 70 10 20 30 50 60 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L) $x10^{2}$ 71.0 0.9 0.8 0.7 0.6 0.5 0.4 43.0 57.0 0.3 103.0 0.2 87.0 _{93.0} 36.0 0.1 27.0 49.0 130.0 143.0 66.0 0 90 100 10 20 30 40 50 60 70 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6562-27.8619 min, 34 scans) 7.D x10². 71.0 0.9 43.0 0.8 0.7 103.0 0.6 0.5 0.4 57.0 0.3 87.0 31.0 61.0 0.2 0.1 90 100 110 190 200 210 220 10 20 30 40 50 60 70 80 120 130 140 150 160 170 180 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 27.7357 x10⁴ x10⁵ 71.0 Component



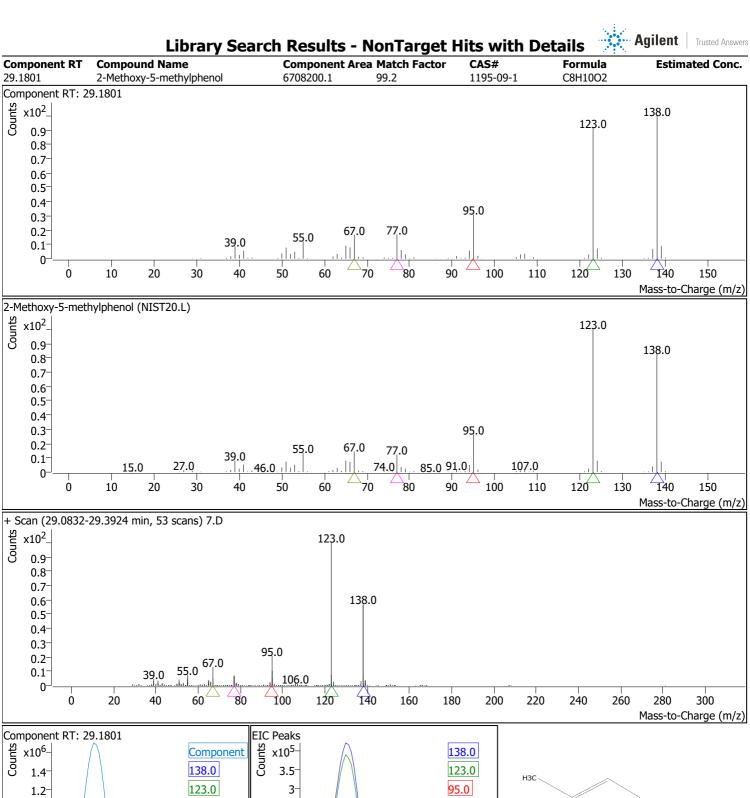


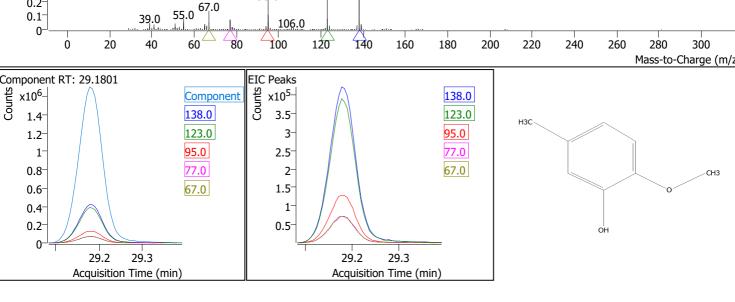




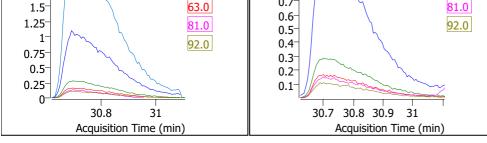
Acquisition Time (min)

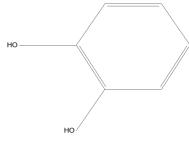
Acquisition Time (min)



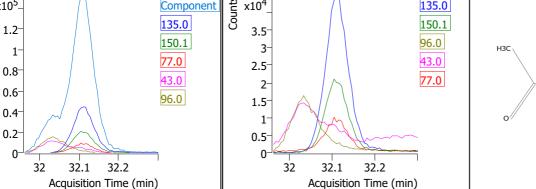


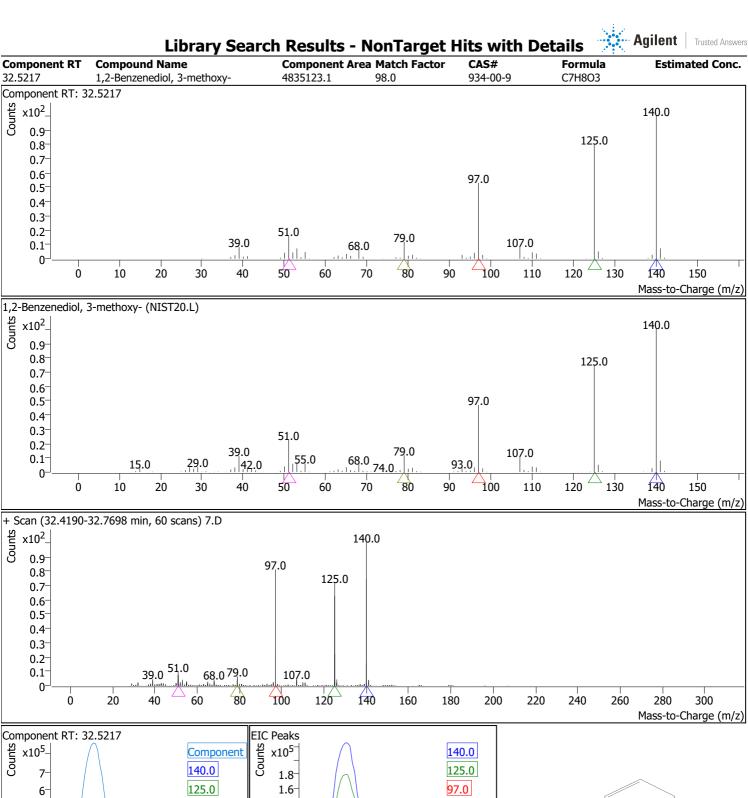
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.6969 Catechol 3018861.8 97.0 C6H6O2 Component RT: 30.6969 y x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 ² 95 10 35 45 50 55 75 80 85 90 100 105 110 115 120 125 60 Mass-to-Charge (m/z) Catechol (NIST20.L) st x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 65 10 15 25 30 35 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.6233-31.0871 min, 79 scans) 7.D st x10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 92.0 103.0 0.1 10 20 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 30.6969 **EIC Peaks** Counts Counts x10⁵ 110.0 Component 110.0 64.0 0.9 2 64.0 0.8 63.0 1.75 0.7

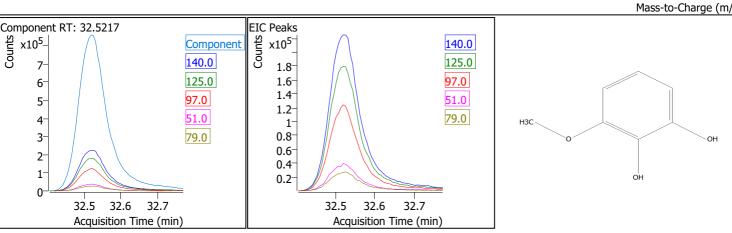


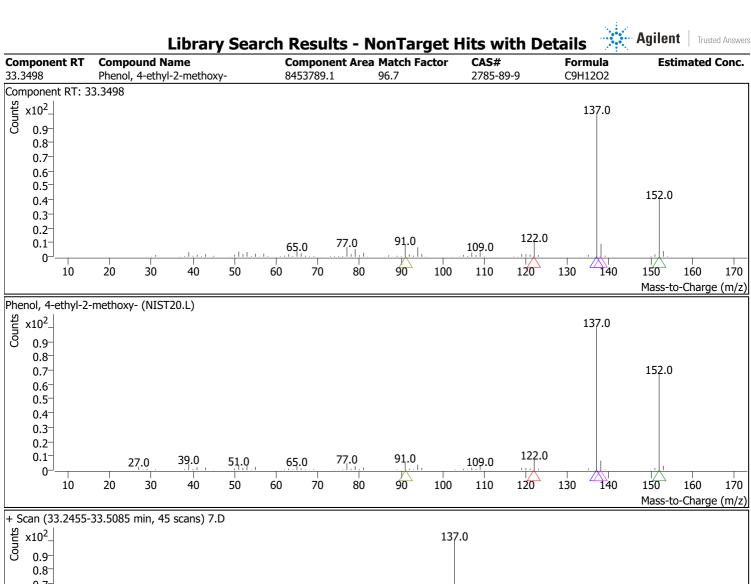


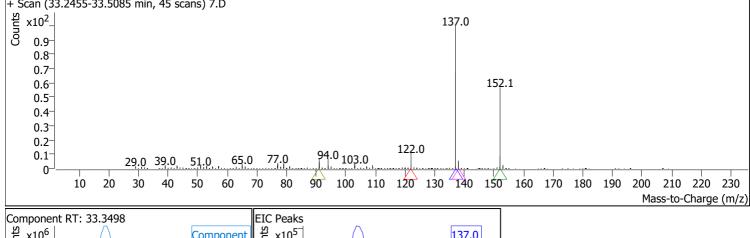
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1450-72-2 32.1063 Ethanone, 1-(2-hydroxy-5-727064.4 C9H10O2 methylphenyl)-Component RT: 32.1063 x10² 135.0 0.9 8.0 0.7 0.6 150.1 0.5 0.4 0.3 77.0 43.0 0.2^{-} 96.0 0.1 68.0 0-150 0 10 20 30 40 50 60 70 80 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 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0265-32.3000 min, 47 scans) 7.D x10². 135.0 0.9 0.8 0.7 0.6 0.5 0.4 43.0 150.0 0.3 77.0 0.2 32.0 96.0 67.0 53.0 0.1 ولناحا يتصبحنا لنستين ومارينا بايتو 150 190 200 210 220 230 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) Component RT: 32.1063 **EIC Peaks** Counts Counts x10⁴ x10⁵. 135.0 Component но 150.1 135.0 1.2 3.5 150.1 96.0 3 **Н3С** 1 77.0 43.0 2.5 0.8

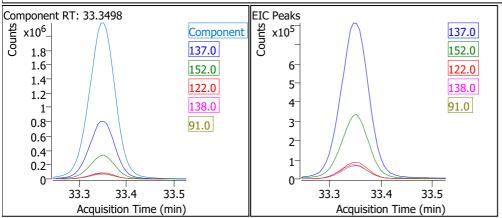


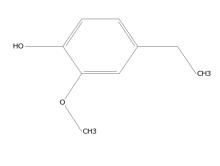


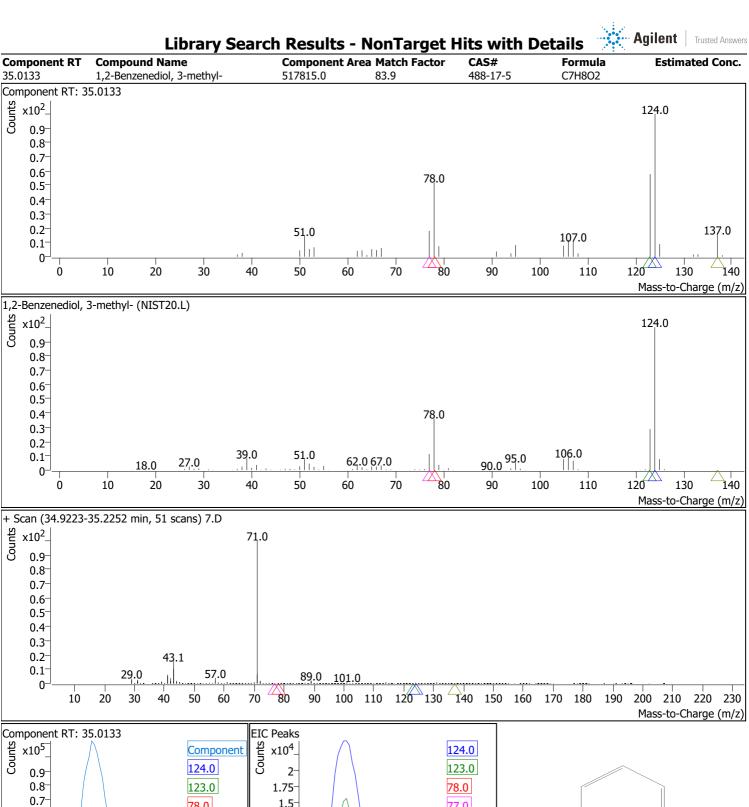


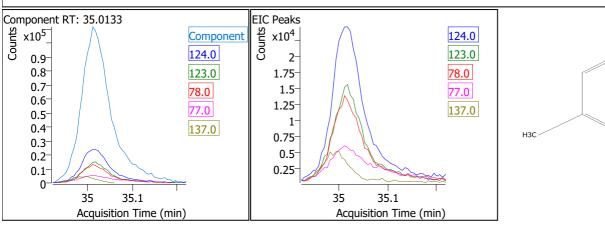












--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 452-86-8 35.0676 1,2-Benzenediol, 4-methyl-15047958.6 C7H8O2 Component RT: 35.0676 v10² 0.9 124.0 0.8 0.7 0.6 0.5 0.4 29.0 0.3 0.2 0.1 ⁴30 10 20 100 110 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 4-methyl- (NIST20.L) Counts x10²_ 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 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (34.9223-35.2253 min, 51 scans) 7.D st x10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 57.0 29.0 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) EIC Peaks Component RT: 35.0676 Counts Counts x10⁶ x10⁴ Component 41.0 124.0 42.0 6 1 29.0 29.0 5 0.8



39.0

124.0

42.0

39.0

41.0

0.6

0.4

0.2

34.9

35

35.1

Acquisition Time (min)

4

3-

2

34.9

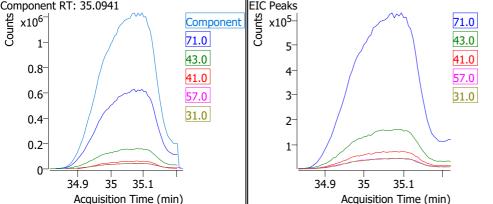
35

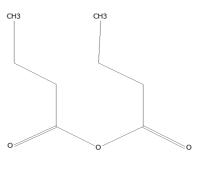
35.1

Acquisition Time (min)

-СН3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.0941 Butanoic acid, anhydride 14324524.5 80.3 C8H14O3 Component RT: 35.0941 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 57.0 0.1 31.0 45.0 85 10 15 20 25 30 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) Butanoic acid, anhydride (NIST20.L) Counts x10²_ 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 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (34.8298-35.2017 min, 63 scans) 7.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 29.0 57.0 89.0 -20 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0941 Counts Counts x10⁶ x10⁵ 71.0 Component CH3 CH3 71.0 43.0 1 5 43.0 41.0 0.8





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 14005441.9 97-99-4 35.3980 2-Furanmethanol, tetrahydro-79.3 C5H10O2 Component RT: 35.3980 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 57.0 0.1 89.0 10 15 25 30 35 40 55 60 65 85 90 100 105 110 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts x10²_ 0.9 71.0 0.8 0.7 0.6 43.0 0.5 0.4 41.0 0.3 0.2 39.0 0.1 15.0 53.0,57.0 61.0 102.0 10 15 20 25 30 35 40 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (35.2017-35.5823 min, 65 scans) 7.D st x10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 43.1 0.2 0.1 57.0 89.0 31.0 131.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 35.3980 **EIC Peaks** Counts Counts x10⁶ 71.0 Component 71.0 43.0 0.8 1.6 43.0 41.0 0.7 1.4

57.0

31.0

41.0

31.0

57.0

0.6

0.5

 0.4^{-}

0.3

0.2

0.1

35.3

35.4

Acquisition Time (min)

35.5

1.2

1

0.8

0.6

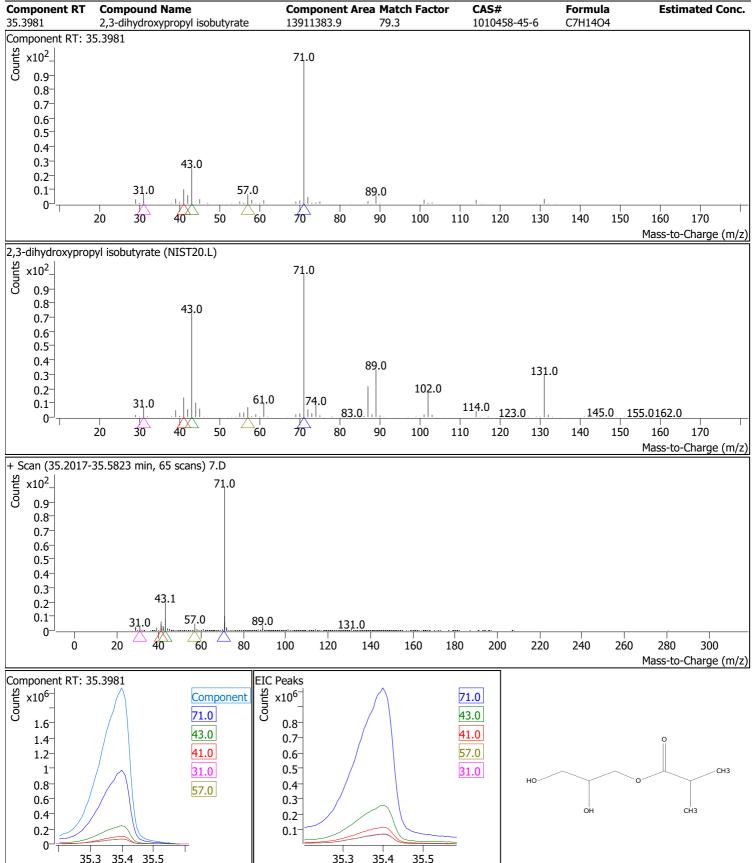
0.4

0.2

35.3 35.4 35.5

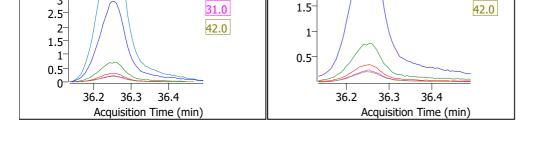
Library Search Results - NonTarget Hits with Details



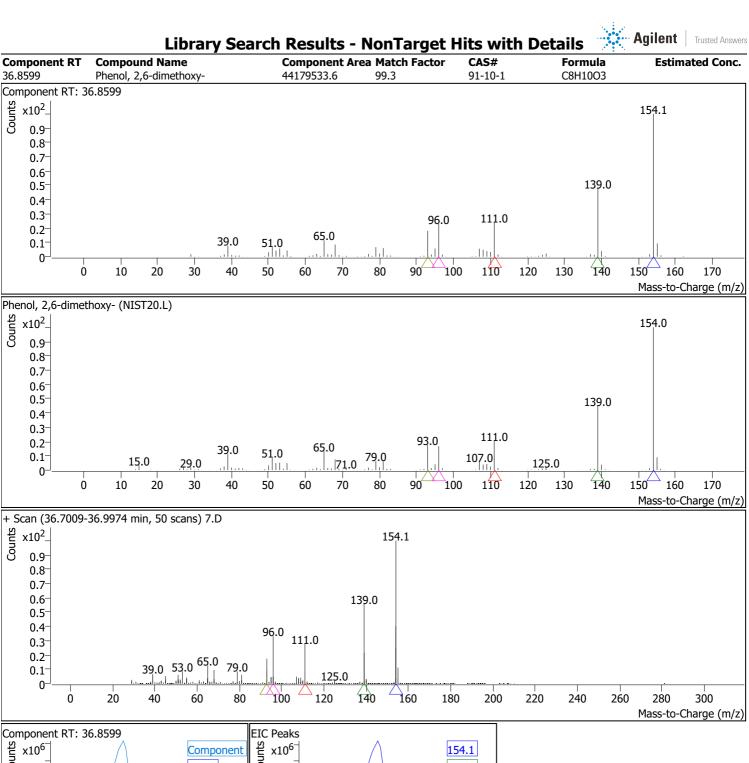


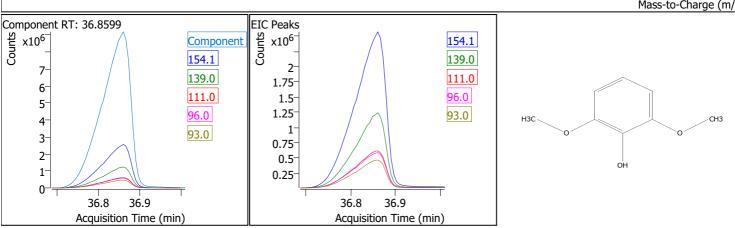
Acquisition Time (min)

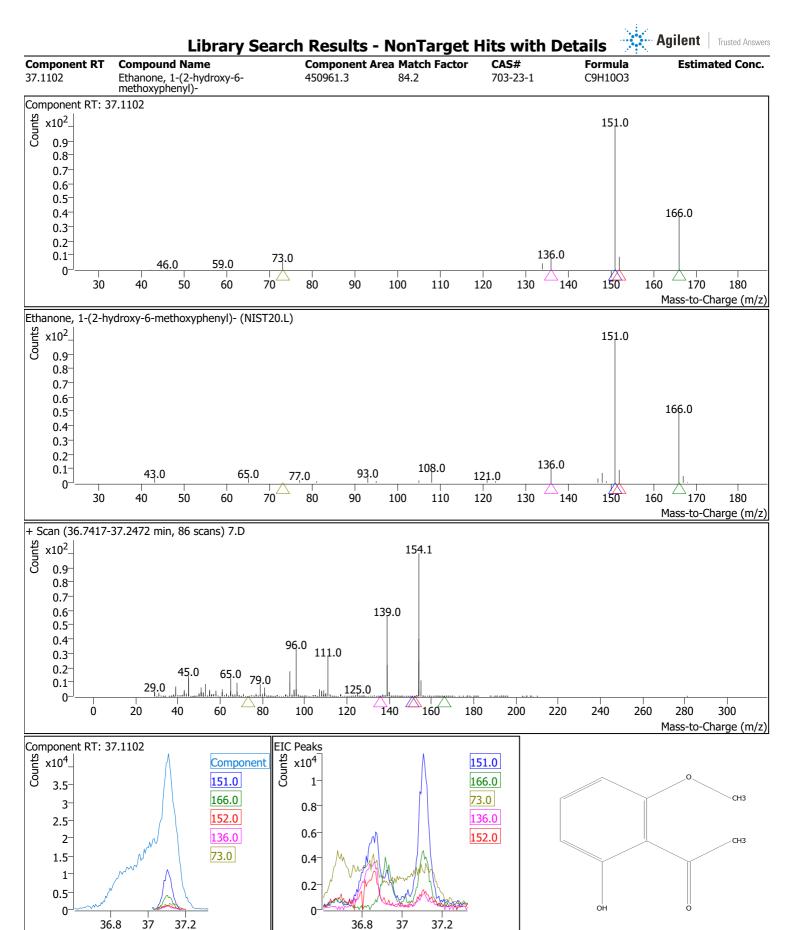
-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.2527 2-Furanmethanol, tetrahydro-3084685.8 83.1 C5H10O2 Component RT: 36.2527 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 57.0 100 105 110 10 15 25 30 35 55 60 65 85 90 95 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts x10²_ 0.9 71.0 0.8 0.7 0.6 43.0 0.5 0.4 41.0 0.3 0.2 39.0 0.1 15.0 53.0,57.0 61.0 67.0 102.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.1352-36.4920 min, 61 scans) 7.D st x10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 43.0 0.2 0.1 31.0 57.0 131.0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 36.2527 Counts x10⁵ x10⁵ 71.0 Component 71.0 43.0 2.5 4.5 43.0 41.0 2 3.5 31.0 41.0



3-

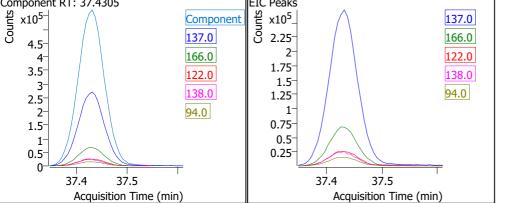






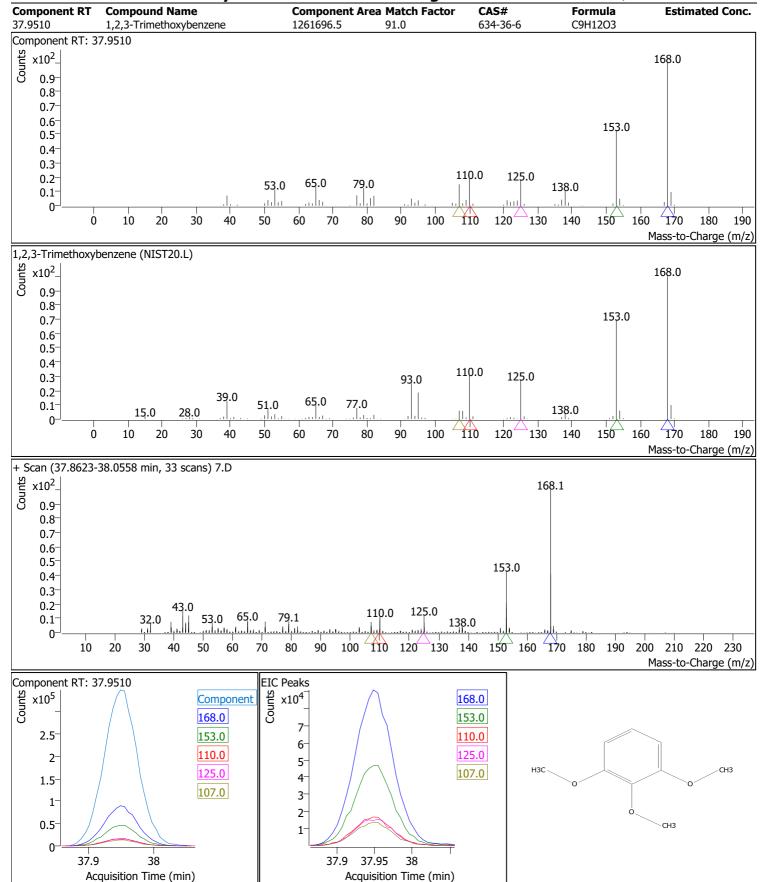
Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4305 Phenol, 2-methoxy-4-propyl-2087071.8 C10H14O2 Component RT: 37.4305 v10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 94.0 77.0 43.0 51.0 65.0 160 - 170 50 10 20 30 60 70 80 90 100 110 120 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10²_ 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 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 Mass-to-Charge (m/z) + Scan (37.3429-37.6099 min, 45 scans) 7.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 166.1 0.3 71.0 103.0 0.2 43.0 122.0 29.0 57.0 0.1 77.0 154.0 10 20 30 40 50 60 70 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 80 Mass-to-Charge (m/z) Component RT: 37.4305 EIC Peaks Counts studo 2.25 2.25 137.0 Component 137.0 166.0 4.5 166.0 122.0



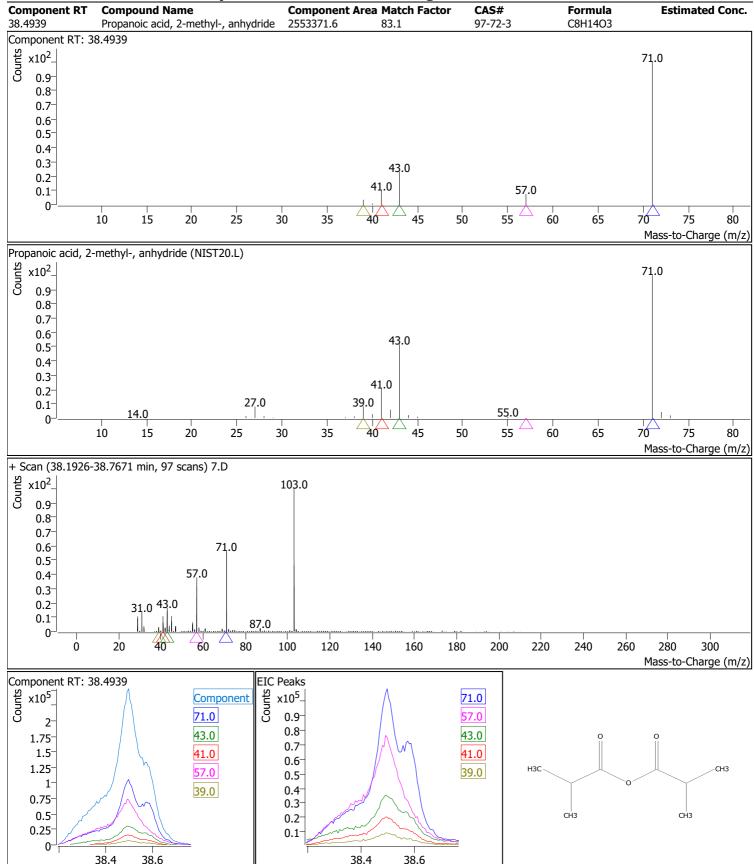






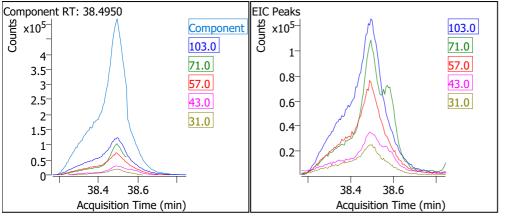


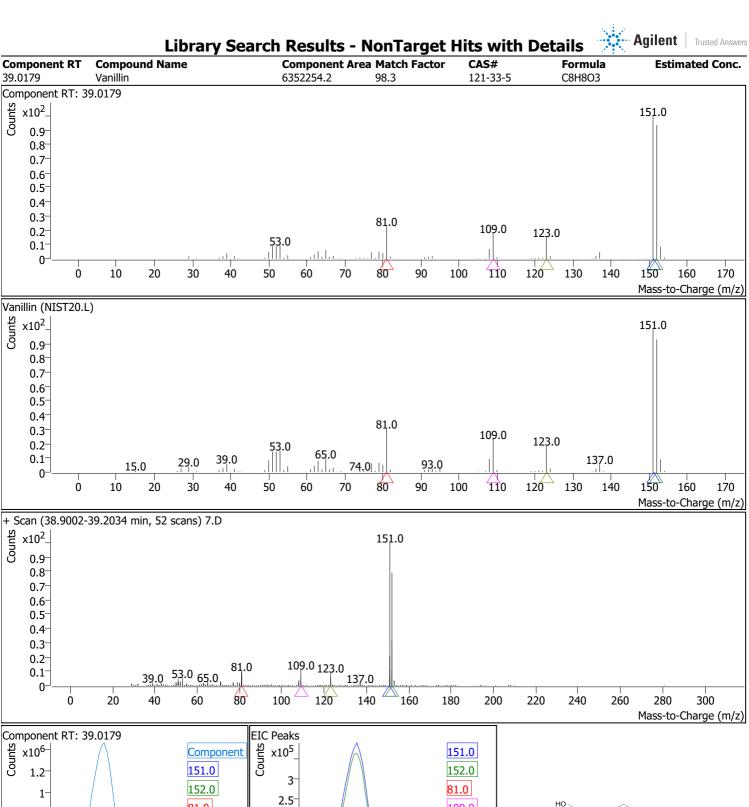


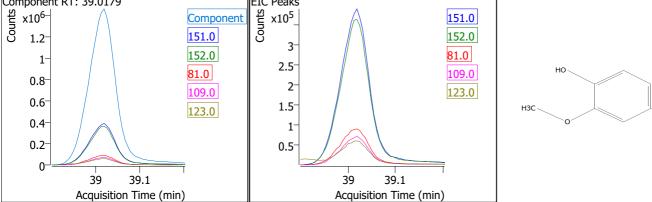


Acquisition Time (min)

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4978254.4 53951-44-3 38.4950 1,3-Dioxolane-4-methanol, 2-ethyl-75.3 C6H12O3 Component RT: 38.4950 v10² 0.9 103.0 0.8 0.7 71.0 57.0 0.6 0.5 0.4 0.3 43.0 0.2 31.0 0.1 70 30 40 100 120 130 140 Ó 10 20 50 60 80 90 110 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 70 0 10 20 30 40 50 60 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (38.1926-38.7671 min, 97 scans) 7.D st x10² 0.9 103.0 0.8 0.7 71.0 0.6 0.5 57.0 0.4 0.3 31.0 43.0 0.2 0.1 87.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 38.4950 x10⁵ 103.0 Component

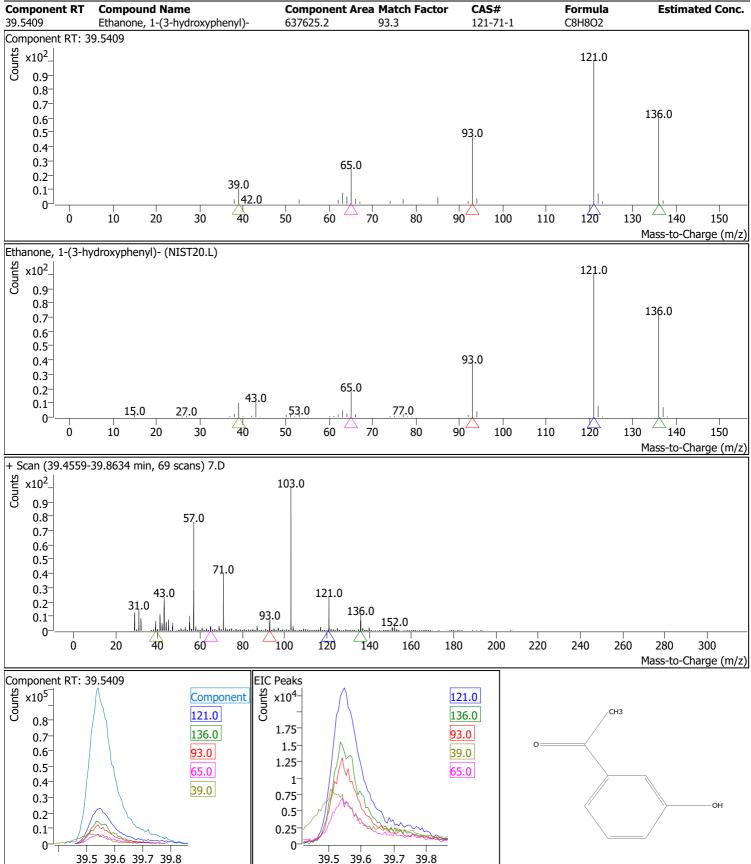








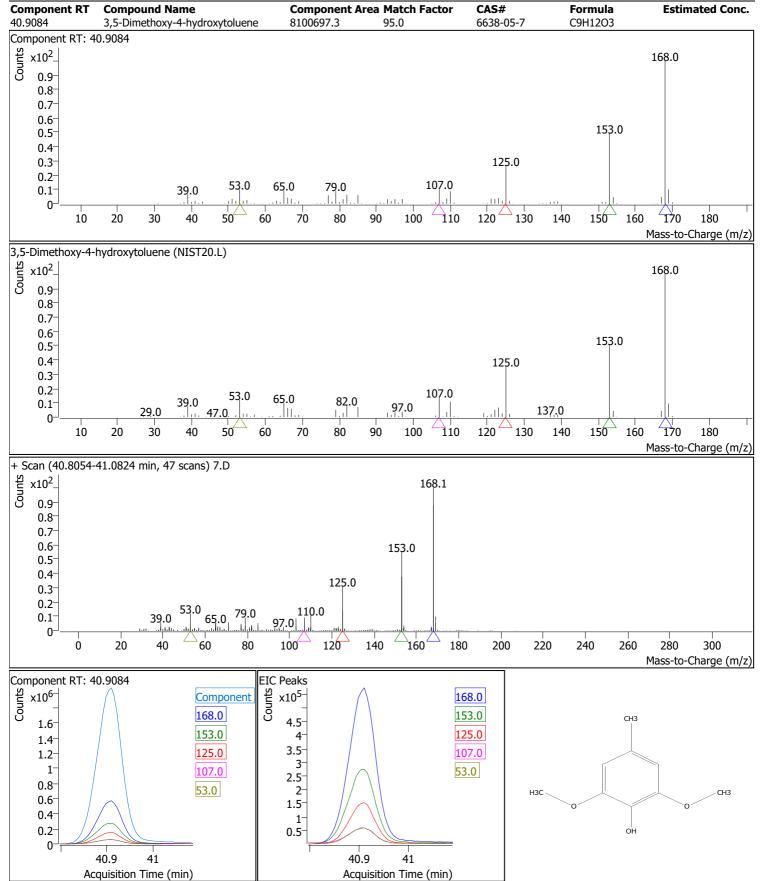




Acquisition Time (min)







--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 41.7950 Eugenol 572563.9 88.6 97-53-0 C10H12O2 Component RT: 41.7950 v10² 0.9 164.0 149.0 0.8 0.7^{-} 0.6 0.5 0.4 137.0 91.0 103.0 121.0 0.3 77.0 0.2 131.0 0.1 150 90 140 10 20 30 40 50 60 70 80 100 110 120 130 170 180 Mass-to-Charge (m/z) Eugenol (NIST20.L) st x10²_ 0.9-164.0 0.8 0.7 0.6 0.5 0.4 149.0 0.3 131.0 0.2 77.0 103.0 91.0 55.0 121.0 0.1 39.0 65.0 27.0 115.0 74.0 ı 150 10 20 30 40 50 60 70 80 90 100 110 120 130 140 170 180 Mass-to-Charge (m/z) + Scan (41.7007-41.9267 min, 39 scans) 7.D st x10² 0.9 71.0 0.8 164.1 0.7 43.0 0.6 0.5 149.0 103.0 0.4^{-} 0.3 32.0 137.0 0.2 77.0 91.1 121.0 57.1 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: 41.7950 **EIC Peaks** Counts x10⁵ x10⁴ 164.0 Component 164.0 149.0 1.2 2.25 149.0 103.0 1 1.75 137.0 137.0



41.8

Acquisition Time (min)

91.0

41.9

1.5

1.25

0.75⁻

0.25

1-

103.0

91.0

41.9

0.8

0.6

0.4

0.2

0

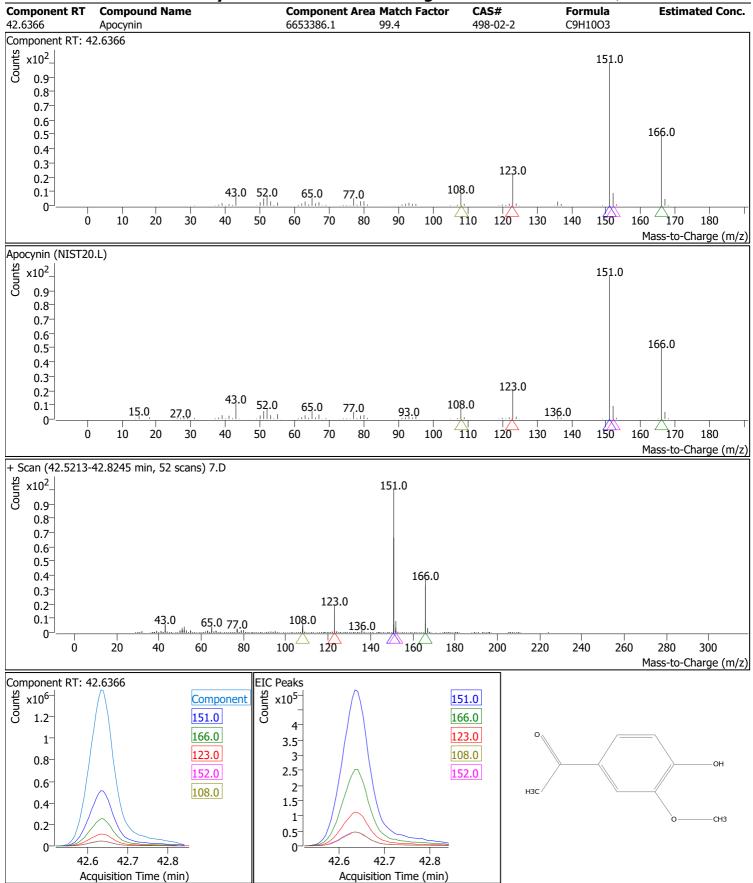
41.8

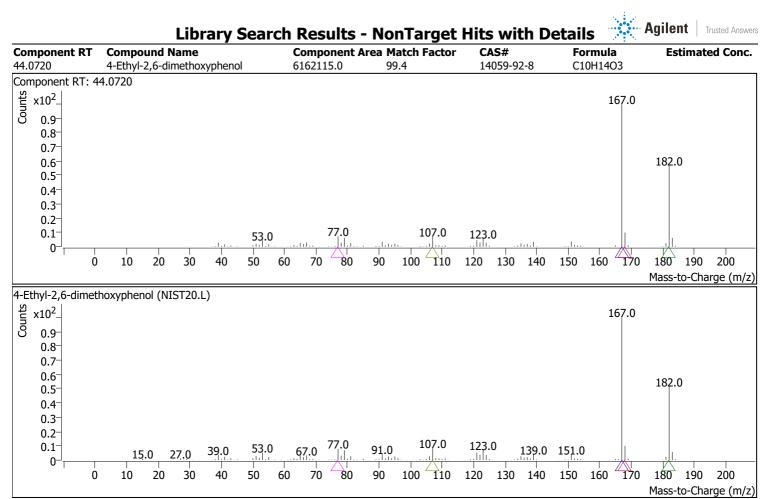
Acquisition Time (min)

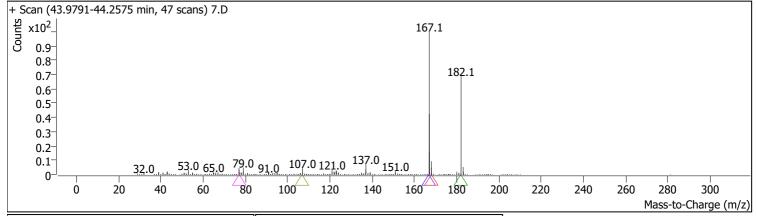
CH2

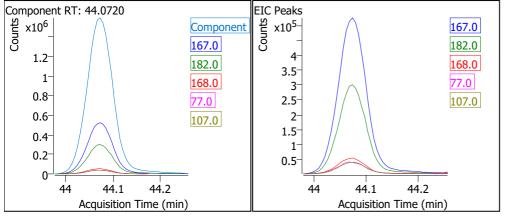


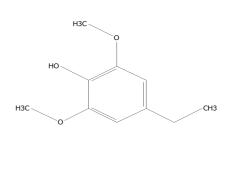












--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-44.3292 15635176.6 94.5 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3292 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 0.2 122.0 43.0 0.1 66.0 77.0 0-120 180 20 30 50 60 70 80 100 110 130 140 150 160 170 190 200 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 85.0⁹1.0 131.0 147.0 164.0 173.0 0 100 130 180 20 30 50 60 80 110 120 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2100-44.4300 min, 38 scans) 7.D x10². 137.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 0.3 74.0 0.2 180.1 122.0 43.0 55.066.0 0.1 171.1 0 100 140 180 200 Ó 20 40 60 80 120 160 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3292 **EIC Peaks** Counts Counts x10⁶ x10⁶_ 137.0 Component 180.1 137.0 1.2 2.5 180.1 122.0 1 2 138.0 122.0 0.8



94.0

138.0

94.0

0.6

0.4

0.2

44.3

44.4

Acquisition Time (min)

44.5

1.5

1

0.5

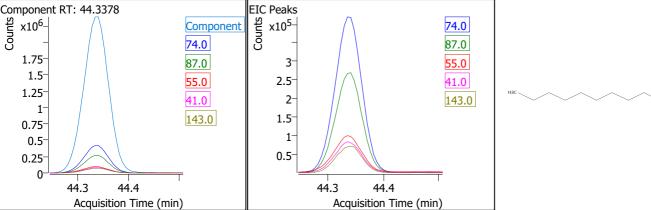
44.3

44.4

Acquisition Time (min)

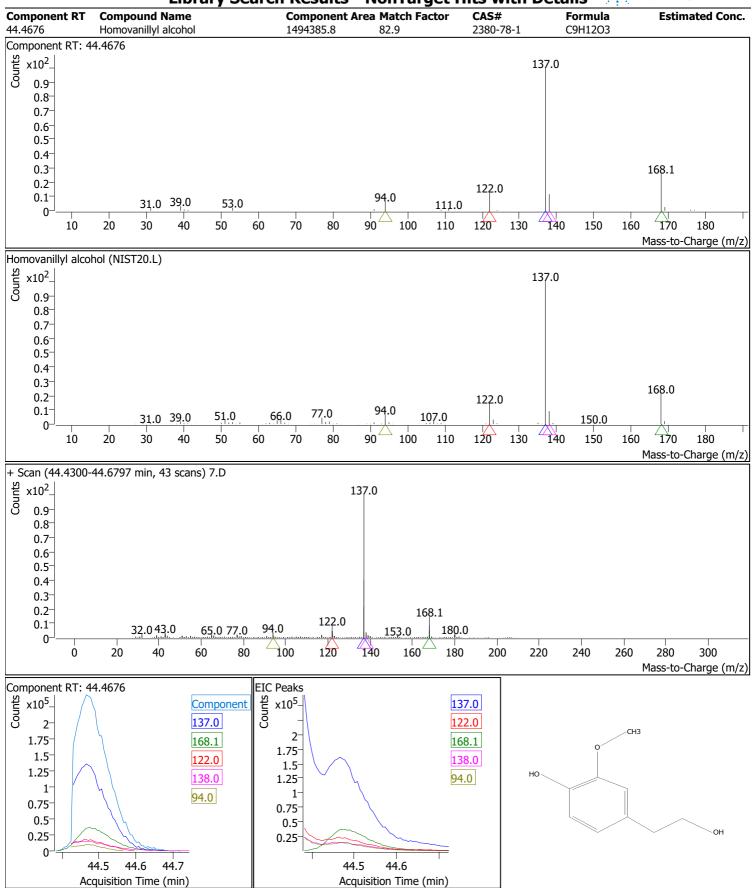
44.5

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3378 Dodecanoic acid, methyl ester 8132319.8 93.9 111-82-0 C13H26O2 Component RT: 44.3378 Counts $x10^{2}$ 74.0 0.9 0.8 0.7^{-} 87.0 0.6 0.5 0.4 0.3 55.0 41.0 143.0 0.2 171.0 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10²_ 0.9 74.0 0.8 87.0 0.7 0.6 0.5 0.4 0.3 55.0 43.0 0.2 69.0 101.0 115.0 0.1 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 -10 10 20 30 40 50 60 70 80 Mass-to-Charge (m/z) + Scan (44.2456-44.5073 min, 45 scans) 7.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 180.1 122.0 0.1 20 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z)









--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Pentanoic acid, 4-oxo-, 2-methylpropyl 726854.9 3757-32-2 45.6215 81.6 C9H16O3 Component RT: 45.6215 x10²_ 99.0 0.9 8.0 0.7 0.6 43.0 0.5 0.4 0.3 0.2^{-} 71.0 117.0 130.0 57.0 0.1 31.0 70 100 130 10 20 30 40 50 60 80 90 110 120 140 150 160 170 Mass-to-Charge (m/z) Pentanoic acid, 4-oxo-, 2-methylpropyl ester (NIST20.L) St x10² 99.0 43.0 0.8 0.7 0.6 0.5 0.4 57.0 0.3 74.0 0.2 27.0 117.0 0.1 15.0 130.0 157.0 0 40 100 130 10 20 30 50 60 70 80 90 110 120 140 150 160 170 Mass-to-Charge (m/z) + Scan (45.5062-45.9462 min, 75 scans) 7.D st x10² 99.0 0.8 0.7 0.6 43.0 0.5 0.4 0.3 117.0 0.2 32.0 181.1 196.1 0.1 0 Ó 20 40 100 200 260 280 60 80 120 140 160 180 220 240 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 45.6215 Counts Counts 99.0 x10⁴ x10⁵. Component 43.0 99.0 1 4 43.0 117.0 3.5 0.8 71.0 71.0 3

45.7 45.8

Acquisition Time (min)

130.0

117.0

130.0

45.6 45.7 45.8 45.9

Acquisition Time (min)

0.6

0.4

0.2

2.5

1.5⁻

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.** 1-Propanone, 1-(4-hydroxy-3-1835-14-9 46.5029 1047376.6 93.9 C10H12O3 methoxyphenyl)-Component RT: 46.5029 Counts x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 123.0 108.0 0.1 52.0 65.0 77.0 0-110 150 180 10 20 30 40 50 60 70 80 90 100 120 130 140 160 170 190 200 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 39.0 29.0 136.0 164.0 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 (46.4359-46.6423 min, 35 scans) 7.D x10². 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 180.1 0.2 32.043.0 0.1 65.0 77.0 91.0 0 40 100 120 180 200 260 Ó 20 60 80 140 160 220 240 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 46.5029 Counts Counts x10⁵. x10⁵-151.0 Component СНЗ 180.0 2 151.0 0.9 1.75 0.8 180.0 123.0 0.7 1.5 123.0 152.0 0.6 1.25

46.5

Acquisition Time (min)

152.0

108.0

46.6

1

0.75

0.5

46.5

Acquisition Time (min)

0.25

0.5

0.4

0.3

0.2

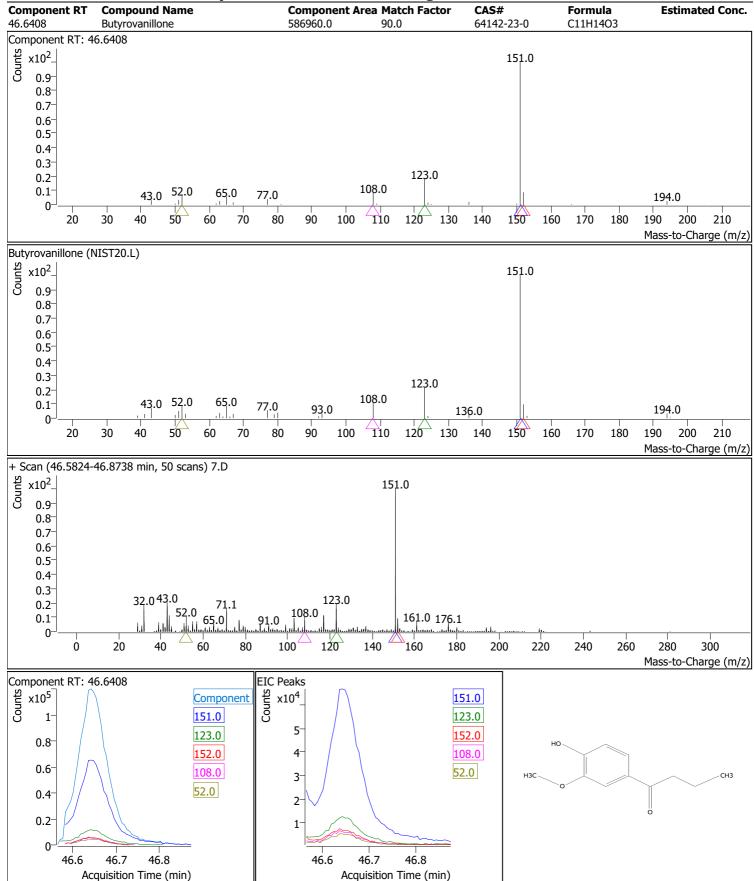
0.1

108.0

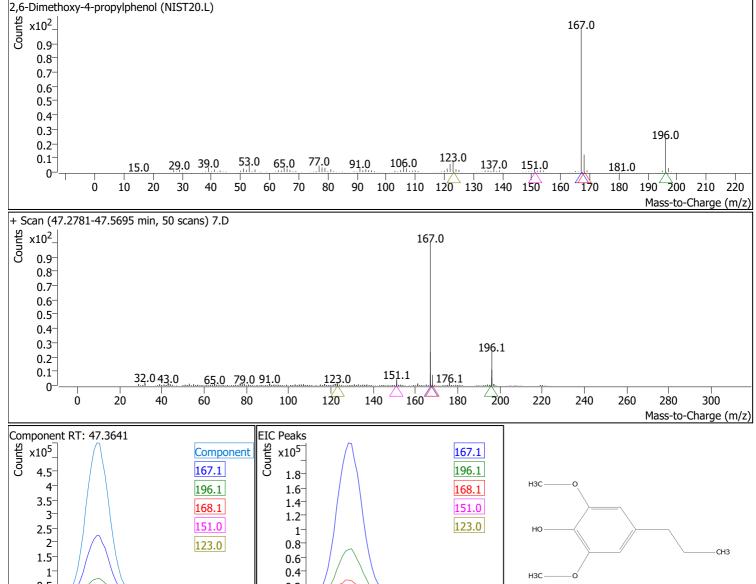
нзс







--- 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 47.3641 2,6-Dimethoxy-4-propylphenol 2088867.2 95.7 C11H16O3 Component RT: 47.3641 y x10² 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 53.0 190 200 120 130 140 150 160 170 10 20 60 70 100 110 Mass-to-Charge (m/z) 2,6-Dimethoxy-4-propylphenol (NIST20.L) Counts x10²_ 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 (47.2781-47.5695 min, 50 scans) 7.D



--- 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 48.9975 Benzenepropanol, 4-hydroxy-3-5238868.1 96.2 C10H14O3 methoxy-Component RT: 48.9975 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 182.1 0.4 0.3 0.2^{-} 122.0 77.0 91.0 107.0 0.1 0-140 180 10 20 30 40 50 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 (48.8836-49.2138 min, 56 scans) 7.D x10². 137.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 182.1 0.3 0.2 51.0 65.0 77.0 91.0 107.0 122.0 0.1 149.0 164.0 0 40 80 100 **4**140 180 260 0 20 60 120 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 48.9975 **EIC Peaks** Counts Counts x10⁶x10⁵ 137.0 Component 182.1 137.0 2.5 0.8 182.1 138.0 0.7 2 122.0 138.0 0.6 1.5 122.0 77.0 0.5

49

49.1

Acquisition Time (min)

49.2

0.4

0.3

0.1

49

49.1

Acquisition Time (min)

49.2

77.0

1

0.5

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.3831 Benzaldehyde, 4-hydroxy-3,5-2081225.0 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3831 x10²_ 182.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 111.0 96.0 167.1 139.0 0.1 159.0 0-160 170 0 10 20 30 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) Benzaldehyde, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts $x10^{2}$ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 111.0 0.2 167.0 93.0 139.0 65.0 39.0 51.0 79.0 0.1 29.0 153.0 15.0 123.0 0 160 170 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2893-49.5911 min, 51 scans) 7.D st x10² 0.9 182.0 131.0 174.0 0.8 0.7 0.6 194.1 0.5 0.4 0.3 0.2 159.0 51.0 65.0 77.0 91.0 32.0 0.1 111.0 139.0 <u>ماناتامانىيىساناتاك</u> 0 60 100 180 0 20 40 80 120 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3831 **EIC Peaks** Counts Counts x10⁵ x10⁵ 182.1 Component o 181.0 182.1 0.8 3 181.0 111.0 0.7 2.5 111.0 96.0 0.6 2 96.0 0.5 167.1



49.4

49.5

Acquisition Time (min)

0.4

0.3

0.2

0.1

167.1

1.5

0.5

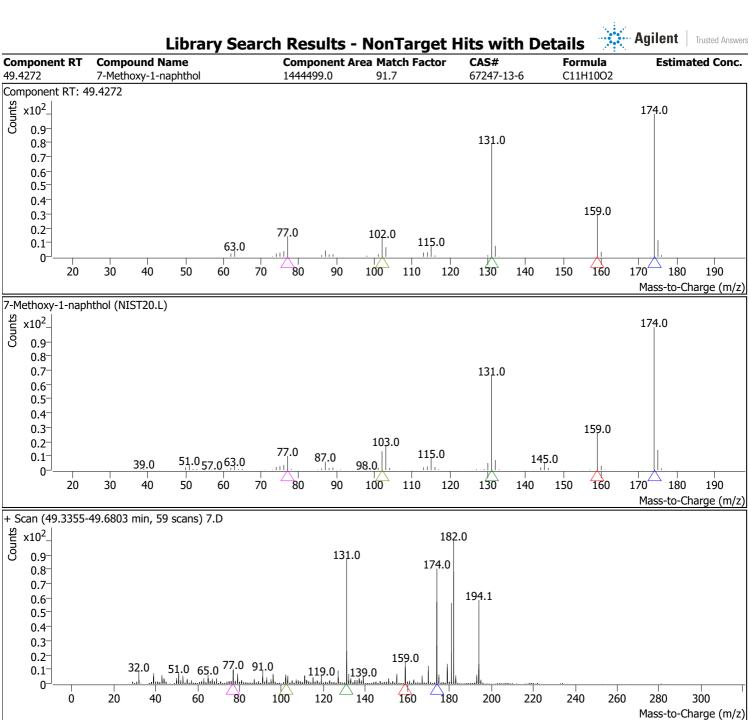
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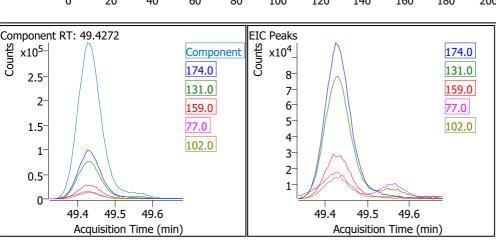
49.4

49.5

Acquisition Time (min)

ОΉ





··· 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 49.5659 (E)-2,6-Dimethoxy-4-(prop-1-en-1-998242.3 80.9 C11H14O3 yl)phenol Component RT: 49.5659 x10². 194.0 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 91.0 0.2^{-} 77.0 119.0 133.0 151.0 163.0 0.1 0-10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 200 210 220 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 27.0 85.0 0 90 180 20 40 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4782-49.7457 min, 46 scans) 7.D x10². 194.1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 179.1 0.2 65.0 77.0 32.043.0 151.0 170.0 0.1 0 120 180 200 260 Ó 20 40 60 80 100 140 160 220 240 280 300 Mass-to-Charge (m/z) Component RT: 49.5659 **EIC Peaks** Counts Counts x10⁴ x10⁵ 194.0 Component 179.0 194.0 5 2 **Н3С** 179.0 91.0 1.75 4 91.0 193.0 1.5 1.25 193.0 3-119.0 НО 1 119.0 2 0.75^{-} 0.5

49.6

Acquisition Time (min)

49.7

49.5

0.25

49.5

49.6

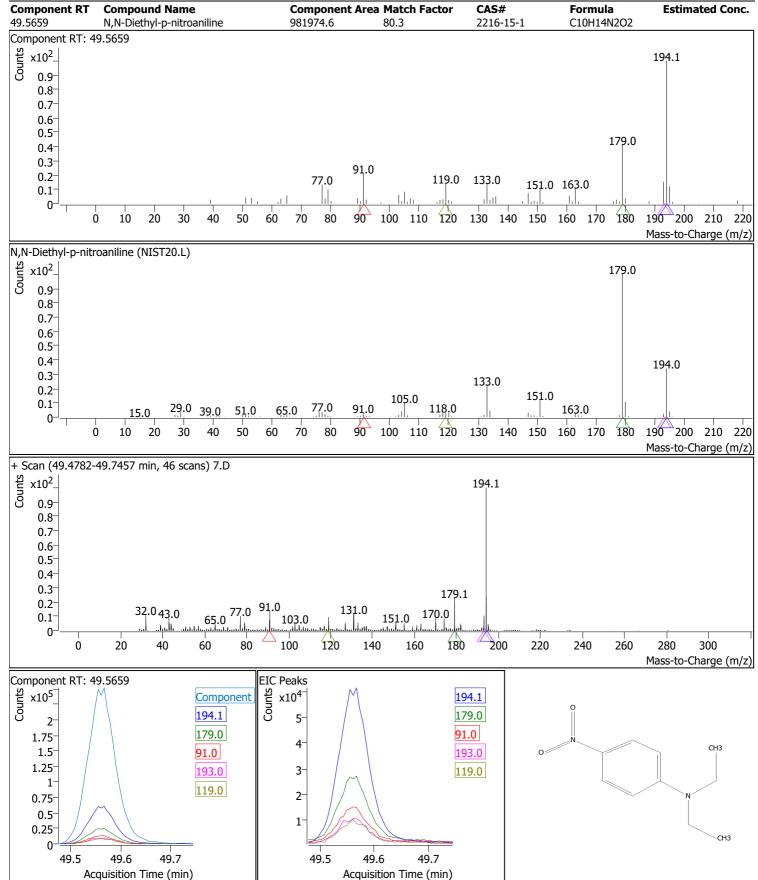
Acquisition Time (min)

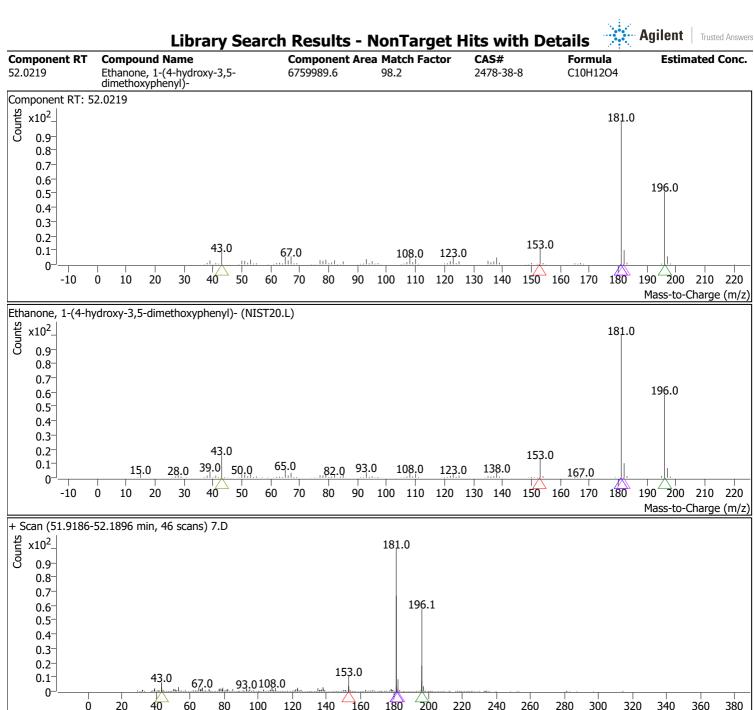
49.7

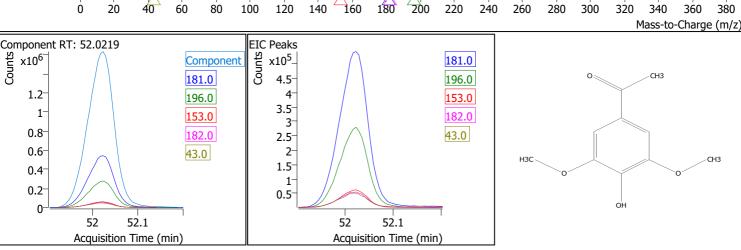
НЗС

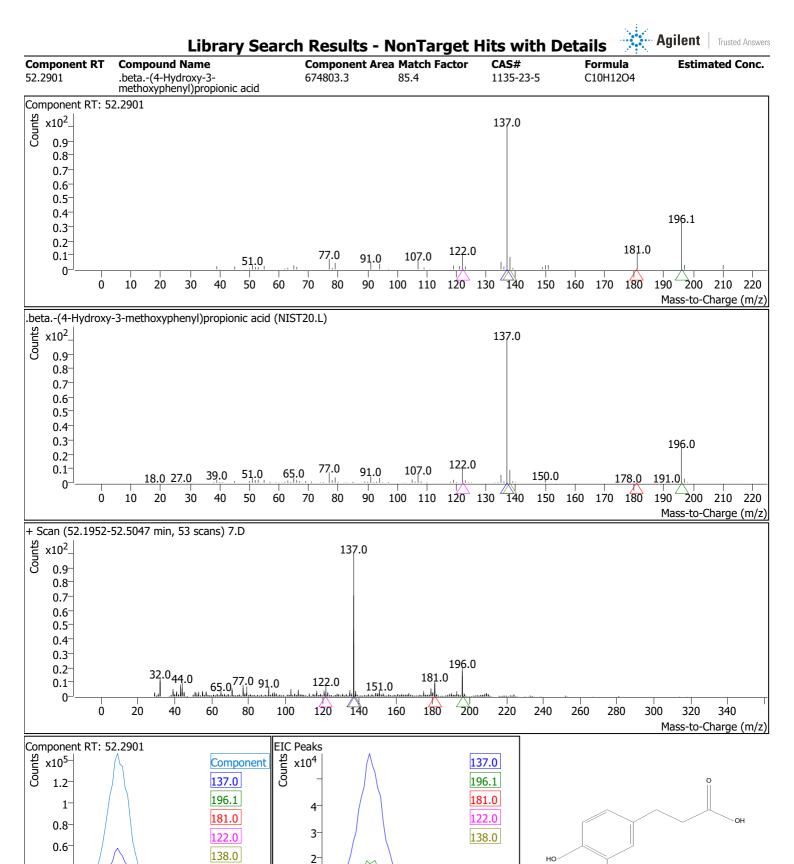












52.3

52.4

Acquisition Time (min)

1

0.4

0.2

52.3

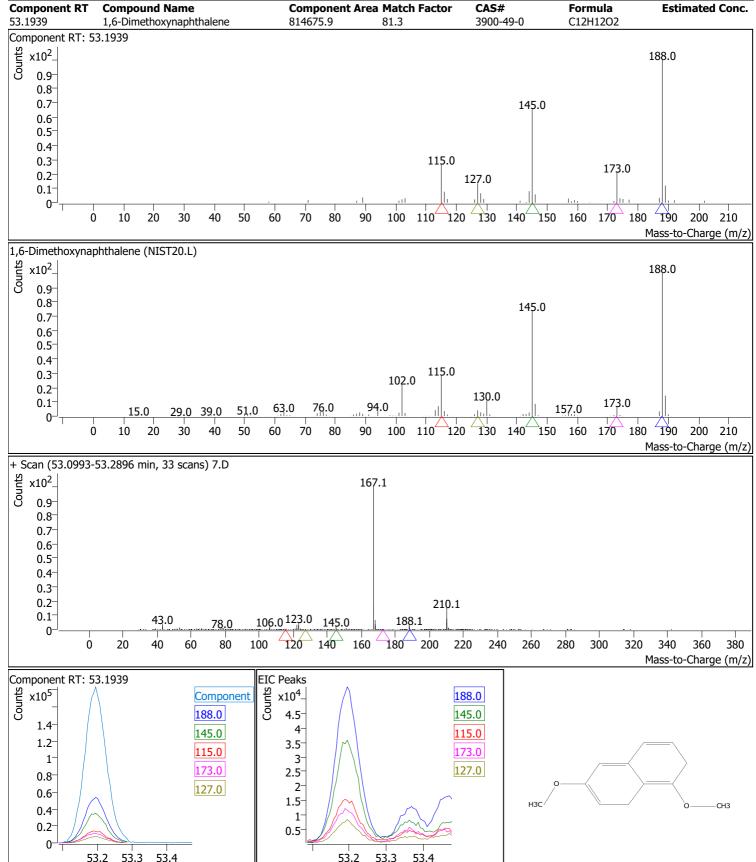
52.4

Acquisition Time (min)

СНЗ



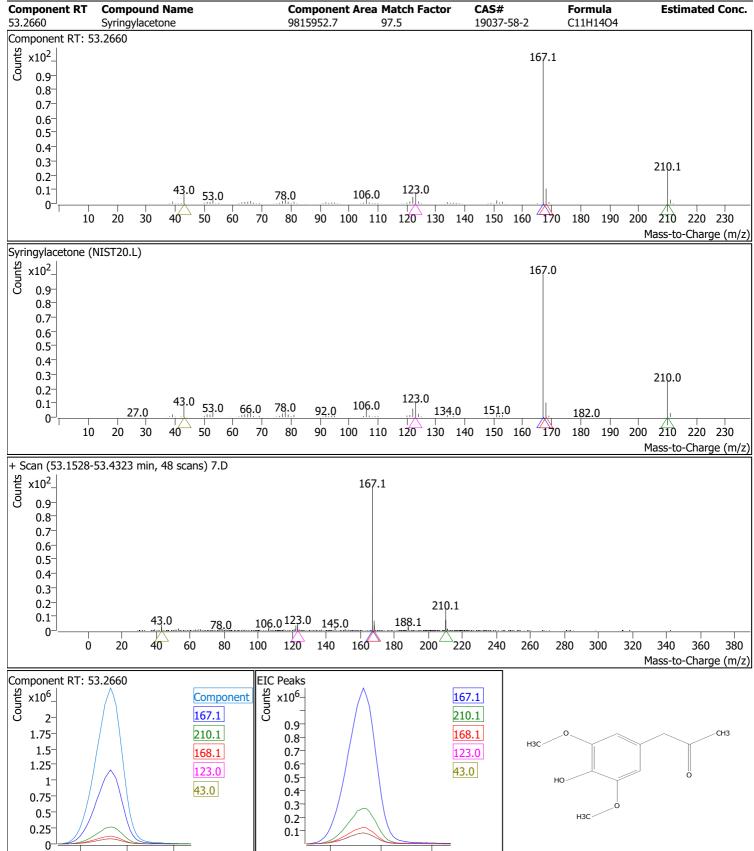




Acquisition Time (min)







53.3

Acquisition Time (min)

53.4

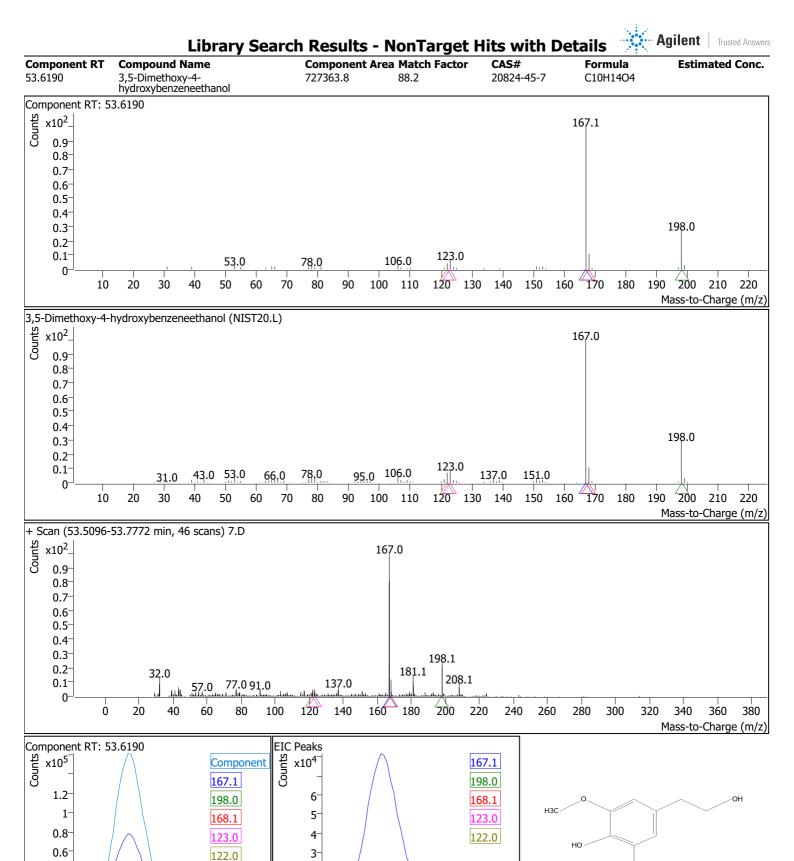
53.2

53.2

53.3

Acquisition Time (min)

53.4



53.6

53.7

Acquisition Time (min)

2-

0

0.4

0.2

53.6

53.7

Acquisition Time (min)

H3C

--- 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-3,5-dimethoxyphenyl)-55.2478 1574703.9 94.9 5650-43-1 C11H14O4 Component RT: 55.2478 x10²_ 181.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 210.0 0.2^{-} 153.0 0.1 67.0 108.0 123.0 138.0 0 150 160 170 180 190 10 20 30 50 60 80 90 100 110 120 130 140 200 Mass-to-Charge (m/z) 1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 181.0 0.9 0.8 0.7 0.6 0.5 0.4 210.0 0.3 0.2 123.0 0.1 108.0 82.0 93.0 138.0 53.0 39.0 29.0 166.0 0 120 130 140 150 160 170 180 190 200 210 220 230 10 20 30 50 60 80 90 100 110 Mass-to-Charge (m/z) + Scan (55.1804-55.3510 min, 29 scans) 7.D x10²_ 181.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 210.1 0.2 $108.0123.0138.0^{\textstyle 153.0}$ 0.1 43.0 67.0 220.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 55.2478 Counts Counts x10⁵ x10⁵_ 181.0 Component 181.0 210.0 2.5 -CH3 210.0 182.0 1 2-182.0 153.0 H3C 0.8

55.3

Acquisition Time (min)

55.4

67.0

153.0

67.0

0.6

0.4

 0.2^{-1}

55.2

1.5

1

55.2

55.3

Acquisition Time (min)

55.4

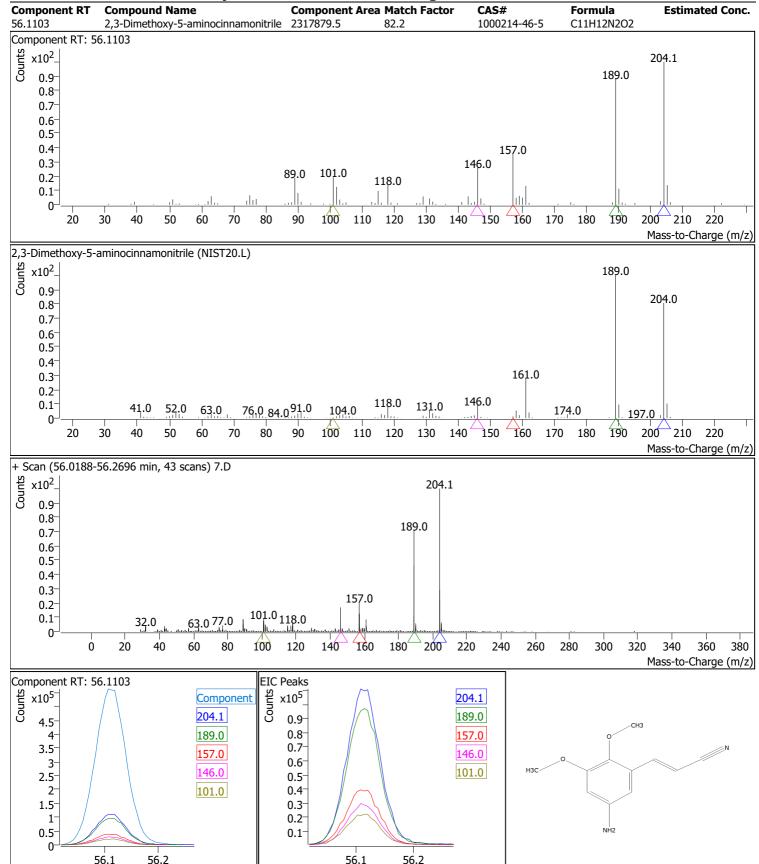
0.5

-OH

-CH3

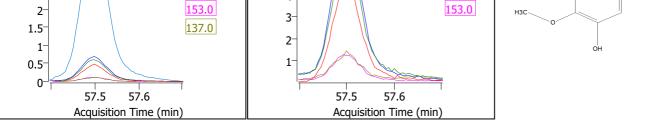






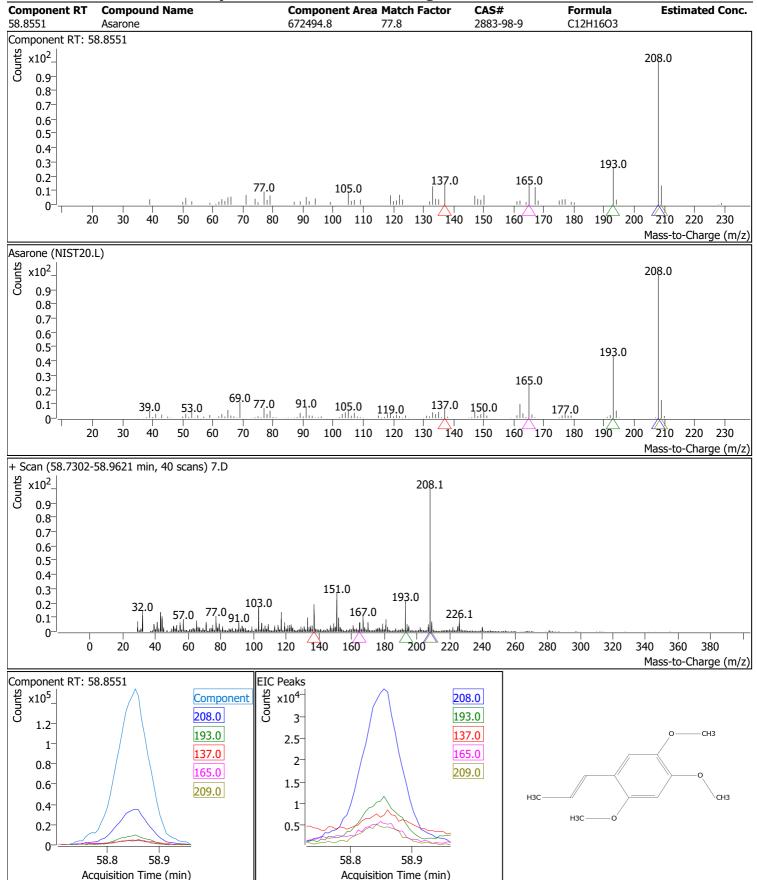
Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol 57.4986 1916163.6 93.8 63543-12-4 C11H16O4 Component RT: 57.4986 x10²_ 168.0 0.9 8.0 0.7 212.0 0.6 0.5 0.4 0.3 153.0 137.0 0.2^{-} 123.0 77.0 107.0 0.1 0-100 110 120 130 140 150 160 170 180 190 200 10 20 30 50 80 90 210 220 230 240 Mass-to-Charge (m/z) 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 212.0 0.6 0.5 0.4 0.3 153.0 0.2 108.0 123.0 137.0 179.0 91.0 77.0 31.039.0 65.0 0.1 85.0 197.0 100 110 120 130 140 150 160 170 180 190 200 10 20 30 60 70 80 90 210 220 230 240 Mass-to-Charge (m/z) + Scan (57.4042-57.7015 min, 51 scans) 7.D x10². 167.0 0.9 0.8 0.7^{-} 212.1 0.6 0.5 0.4 0.3 137.0 103.0 0.2 32.0 153.0 77.0 181.0 202.0 55.0 0.1 0 20 40 60 80 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) Component RT: 57.4986 **EIC Peaks** Counts Counts x10⁴ x10⁵-168.0 Component 167.0 168.0 3.5 167.0 212.0 5 3 137.0 2.5 212.0 4



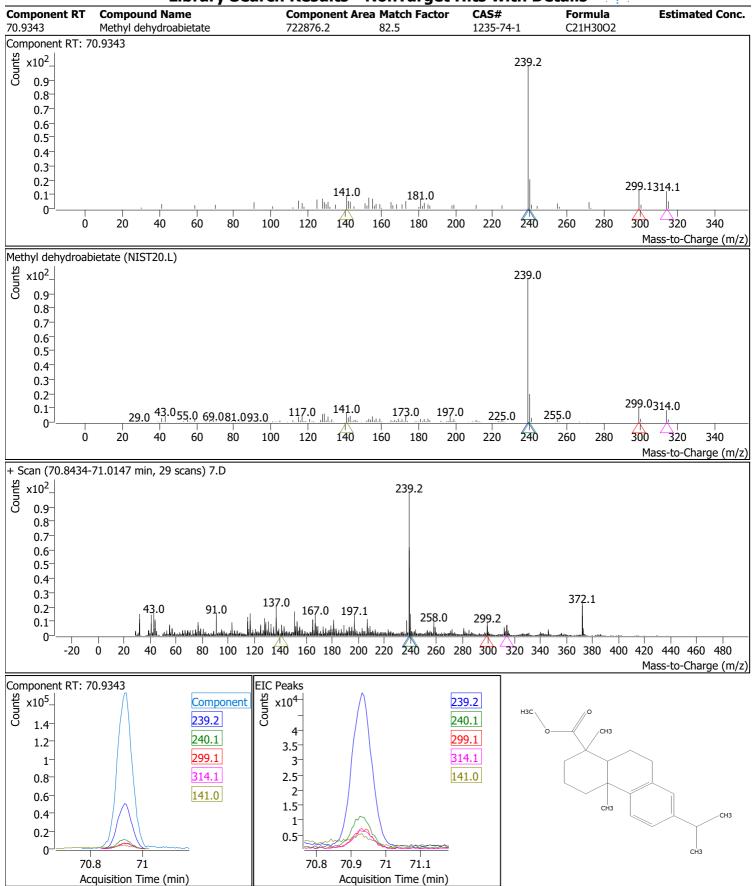






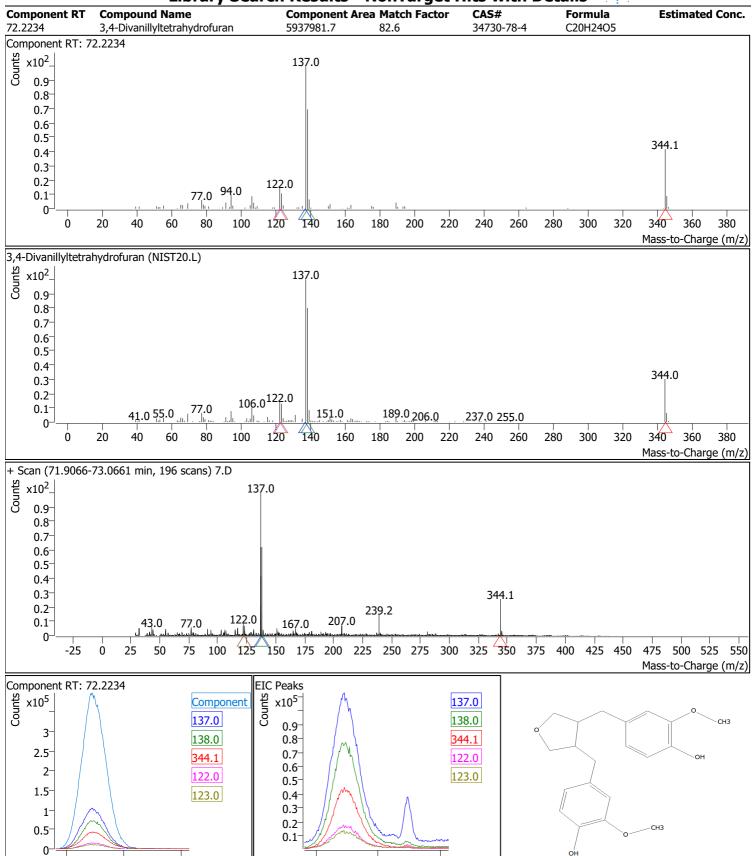












72.5

Acquisition Time (min)

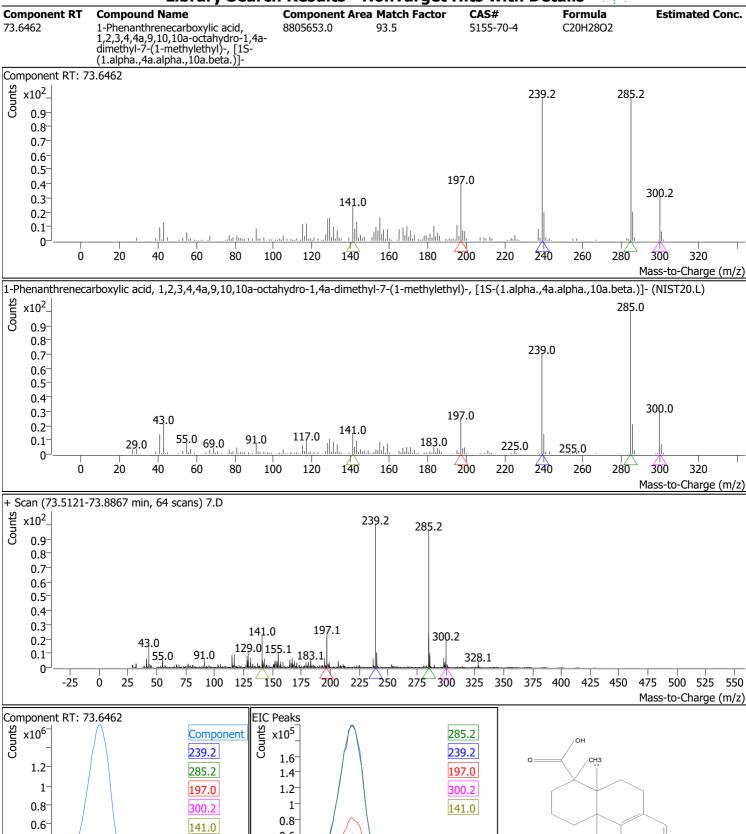
73

72

72.5

Acquisition Time (min)

73



73.7

Acquisition Time (min)

73.6

73.8

0.6

0.4

0.2

0.4

 0.2^{-}

73.6

73.7

Acquisition Time (min)

73.8

СНЗ

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor Component RT Compound Name** CAS# **Formula Estimated Conc.** 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether 75.9138 839048.2 82.5 22318-87-2 C18H22O4 Component RT: 75.9138 x10²_ 151.0 0.9 0.8 0.7° 0.6 0.5 0.4 0.3 0.2 302.1 0.1 65.077.0 91.0 108.0123.0 100 120 300 -20 20 40 140 180 200 220 240 260 280 320 340 Mass-to-Charge (m/z) 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether (NIST20.L) $x10^{2}$ 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2-302.0 <u>15.027.039.051.0</u> 65.077.0 91.0 107.0 0.1 165.0 181.0196.0211.0226.0241.0256.0 220 300 20 140 180 200 240 260 320 340 -20 60 80 100 120 160 280 Mass-to-Charge (m/z) + Scan (75.8310-76.0213 min, 33 scans) 7.D Counts x10²_ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 302.1 137.0 167.0 250 275 300 325 350 375 400 425 450 475 500 525 550 100 200 225 -25 0 25 Mass-to-Charge (m/z) Component RT: 75.9138 EIC Peaks Counts Counts x10⁵ 151.0 Component 151.0 152.0 1 1.4 302.1 91.0 0.8 1.2 302.1 152.0 1 0.6 123.0 91.0 0.8

75.9

Acquisition Time (min)

76

123.0

76

 0.4°

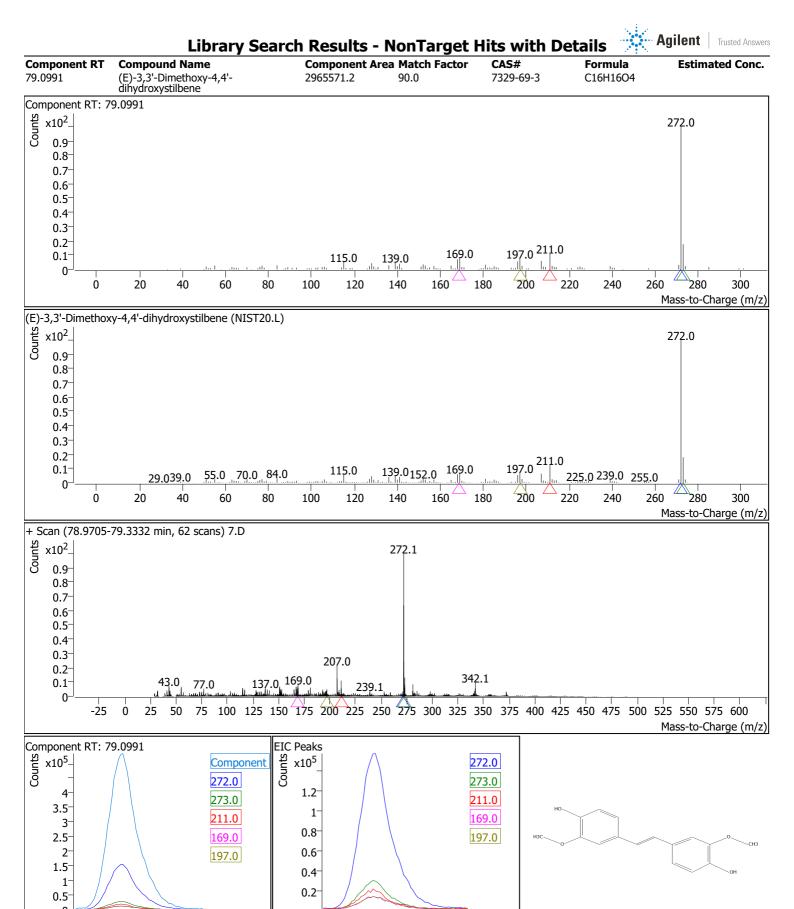
0.2

0.6

0.4

0.2

75.9



79

79.1

79.2

Acquisition Time (min)

79.3

79.1

79.2

Acquisition Time (min)

79.3

