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



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

240502 data.uaf **Analysis File Name** 

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

5.D **File Name Path Name** D:\MassHunter\GCMS\1\data\RBEL\240501 scan **Sample Name** 5 **Sample Type** Sample Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

Acq. Date-Time 5/1/2024 7:40:05 PM **Instrument Name** GCMSD Dil. 1

Component R	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
5.0400	2-Furanol, tetrahydro-	5371-52-8	C4H8O2	434675.2	91.7	
7.3446	1,3-Propanediol	504-63-2	C3H8O2	742506.0	84.2	
11.2395	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	566611.8	84.9	
11.6391	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	5579504.6	79.0	
12.3398	Oxalic acid, diallyl ester	1000309-22-9	C8H10O4	2333502.9	80.0	
12.3673	Butyrolactone	96-48-0	C4H6O2	7213911.2	76.4	
12.3674	Butanoic acid, 4-hydroxy-	591-81-1	C4H8O3	9243303.8	96.5	
12.8226	Methyltartronic acid	595-98-2			96.1	
	•		C4H6O5	1462117.7		
13.3374	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	4386222.5	79.0	
16.4415	3-Ethoxy-1,2-propanediol	1874-62-0	C5H12O3	467083.0	87.5	
16.8824	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	1316027.2	83.9	
17.9787	Phenol	108-95-2	C6H6O	1530797.3	96.1	
18.5679	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2816238.3	93.8	
18.6534	Diisoamyl ether	544-01-4	C10H22O	3161009.8	97.0	
19.7716	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2330943.0	93.8	
20.0706	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	526051.2	92.6	
21.1623	1,3,5-Trioxane	110-88-3	C3H6O3	1444208.3	76.3	
22.2439	Carbamic acid, methyl-, 3-methylphenyl ester	1129-41-5	C9H11NO2	552078.3	88.1	
22.4524	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	477961.9	92.0	
22.9084	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	1476338.7	78.8	
23.0562	1-Octanol	111-87-5	C8H18O	3055456.6	98.1	
23.6017	Phenol, 2-methoxy-	90-05-1	C7H8O2	24824933.3	98.6	
25.0343	Glycerin	56-81-5	C3H8O3	7063177.2	78.8	
27.7231	4-Isopropoxy-2-butanone	32541-58-5	C7H14O2	645289.9	81.8	
27.7259	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	828843.6	82.3	
29.1719	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	4852827.8	99.2	
30.6831	Catechol	120-80-9	C6H6O2	4125098.9	96.3	
32.1005	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	516864.7	91.1	
32.5118	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	4987793.7	97.8	
33.3426	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	6670140.0	95.1	
34.1387	Furan, tetrahydro-2-(methoxymethyl)-	19354-27-9	C6H12O2	454360.7	76.8	
35.0178	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	509748.5	93.9	
35.0184	1,2-Benzenediol, 3-methyl-	488-17-5	C7H8O2	506482.9	89.8	
35.0881	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	15928096.7	82.2	
35.3878	Butanoic acid, anhydride	106-31-0	C8H14O3	16283653.9	80.7	
36.2414	Furan, tetrahydro-2-(methoxymethyl)-	19354-27-9	C6H12O2	3488709.8	82.1	
36.8506	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	43473399.0	98.9	
37.4240	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	1324225.1	93.6	
37.9427	1,2,3-Trimethoxybenzene	634-36-6	C9H12O3	1213567.6	90.5	
38.6230	2H-2,4a-Methanonaphthalene, 1,3,4,5,6,7-	1135-66-6	C15H24	724156.1	79.4	
	hexahydro-1,1,5,5-tetramethyl-, (2S)-					
39.0190	Vanillin	121-33-5	C8H8O3	10745201.9	98.7	
39.5267	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	652842.6	95.2	
40.8961	2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]-	1000131-52-4	C8H11NO2	1465508.6	81.4	
40.8992	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	6973221.2	94.5	
41.7884	Phenol, 2-methoxy-4-(2-propenyl)-, acetate	93-28-7	C12H14O3	515705.0	85.6	
42.6303	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	6100-74-9	C9H10O3	8293589.4	98.9	
42.6312	Apocynin	498-02-2	C9H10O3	8294303.3	99.1	
44.0667	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	5806144.7	98.5	
44.3276	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	16734060.1	91.2	
44.3340	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6278172.1	86.9	
44.4669	Homovanillyl alcohol	2380-78-1	C9H12O3	1869606.3	87.6	
44.9708	3,4-Dimethoxyphenylacetone	776-99-8	C11H14O3	447408.7	78.7	
45.5971	Morpholine, 4-methyl-	109-02-4	C5H11NO	458139.7	75.8	
45.6016	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	1035409.0	83.1	
45.9969	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	445194.6	79.5	
46.4911	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	920678.4	92.8	
46.6325	Butyrovanillone	64142-23-0	C11H14O3	1069133.3	92.2	
47.3550	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	1630239.2	93.0	
48.3799	Benzeneacetic acid, .alpha.,4-dihydroxy-3-methoxy-, methyl ester	2911-74-2	C10H12O5	450870.6	81.7	
48.9878	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	6476909.6	96.6	
49.3686	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2353548.5	96.0	
49.4192	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	1301703.8	90.9	
49.5546	N,N-Diethyl-p-nitroaniline	2216-15-1	C10H14N2O2	1001616.8	79.5	
	,	Dago 1 of 99			onorated at 11:20 A	M F/2/2024

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

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86.4

88.2

Component	RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
49.5546	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-	1135-24-6	C10H10O4	1007538.9	80.3	
50.6433	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	1081-71-6	C10H10O5	483869.0	76.0	
50.7661	Propanoic acid, 2-methyl-, anhydride	97-72-3	C8H14O3	539065.1	76.0	
52.0121	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	8074305.7	98.1	
52.2778	.beta(4-Hydroxy-3-methoxyphenyl)propionic acid	1135-23-5	C10H12O4	669422.9	87.9	
53.1871	1,6-Dimethoxynaphthalene	3900-49-0	C12H12O2	733649.2	79.1	
53.2577	Syringylacetone	19037-58-2	C11H14O4	11180306.5	97.4	
53.6053	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	603178.3	82.5	
55.2315	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5650-43-1	C11H14O4	1486376.3	92.3	
56.1063	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	2428025.9	83.8	
57.4879	Dihydrosyringenin	20736-25-8	C11H16O4	2155124.3	90.1	
57.4879	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	2150845.1	89.6	
58.8348	Isoelemicin	487-12-7	C12H16O3	625759.8	78.5	
58.8351	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-	487-11-6	C12H16O3	641149.0	79.8	
66.3352	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C20H38O2	1251163.7	89.2	
67.3064	2-Isopropyl-10-methylphenanthrene	66552-97-4	C18H18	472185.8	83.5	
70.9283	Methyl dehydroabietate	1235-74-1	C21H30O2	1302884.7	90.1	
72.1956	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6662065.5	86.7	
73.6620	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	13565441.1	92.9	
75.9073	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	873882.8	81.0	

65996-50-1

7329-69-3

C6H5N3O2

C16H16O4

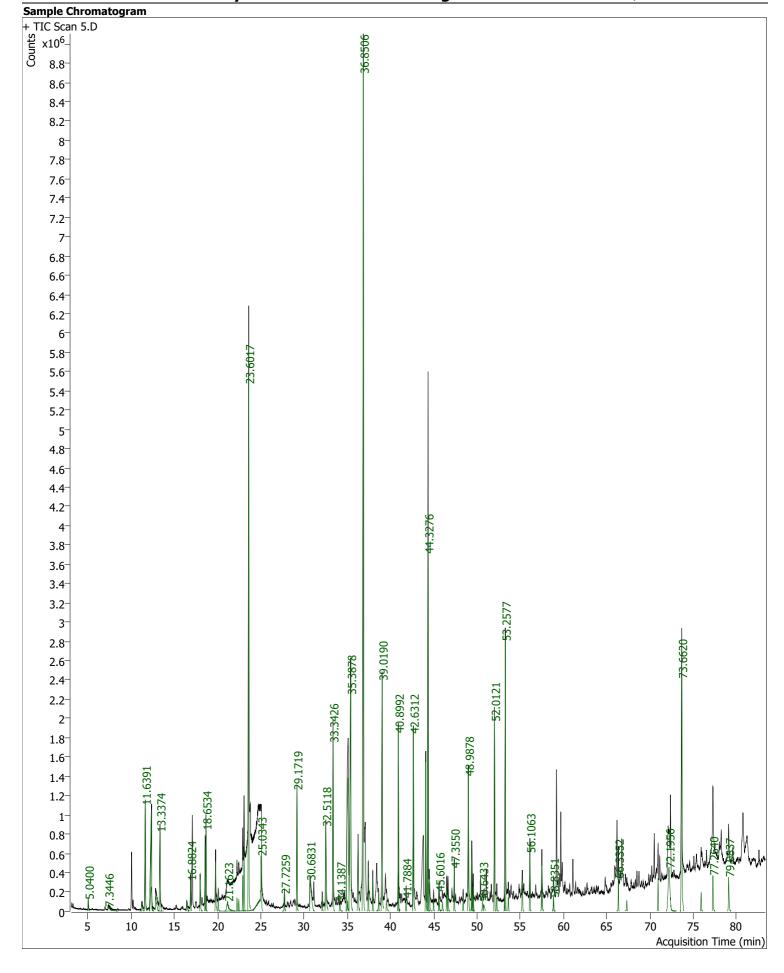
1751843.7

1931479.7

77.2640

79.0837

Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene



#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5.0400 2-Furanol, tetrahydro-434675.2 5371-52-8 C4H8O2 Component RT: 5.0400 v10<sup>2</sup> 0.9 42.1 0.8 0.7 0.6 0.5 0.4 57.0 0.3 39.0 31.0 0.2 87.0 29.0 0.1 0 30 85 20 25 35 40 55 65 70 75 80 90 95 Mass-to-Charge (m/z) 2-Furanol, tetrahydro- (NIST20.L) st x10<sup>2</sup> 0.9 42.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 27.0 57.0 39.0 0.2 71.0 47.0 84.0 87.0 0.1 55.0 25.0 50.0 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (4.9623-5.2218 min, 44 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 29.0 57.0 0.3 0.2 71.0 87.0 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 5.0400 EIC Peaks Counts Counts x10<sup>5</sup> x10<sup>4</sup> 42.1 Component 42.1 41.1 1 41.1 57.0 2.5 0.8 39.0 57.0



5.05

5.1 5.15 5.2

Acquisition Time (min)

31.0

2-

1-

1.5

0.5

39.0

31.0

5.2

0.6

0.4

0.2

5.1

#### --- 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 7.3446 1,3-Propanediol 742506.0 C3H8O2 Component RT: 7.3446 v10<sup>2</sup> 0.9 58.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 0.2 45.0 0.1 40.0 61.0 15 60 75 5 10 20 25 30 35 40 55 65 70 80 85 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10<sup>2</sup>\_ 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 68.0 73.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (7.3029-8.5219 min, 206 scans) 5.D St x10<sup>2</sup> 0.9 58.0 0.8 0.7 0.6 0.5 44.0 $0.4^{-}$ 0.3 0.2 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: 7.3446 EIC Peaks Counts st x10<sup>4</sup>. x10<sup>4</sup> Component 57.0 58.0 58.0 3.5 0.9 57.0 31.0 0.8 3 0.7 45.0 31.0 2.5 0.6 45.0 46.0 2 0.5

46.0

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1

7.4 7.6 7.8 8 8.2 8.4

Acquisition Time (min)

0.4

0.3

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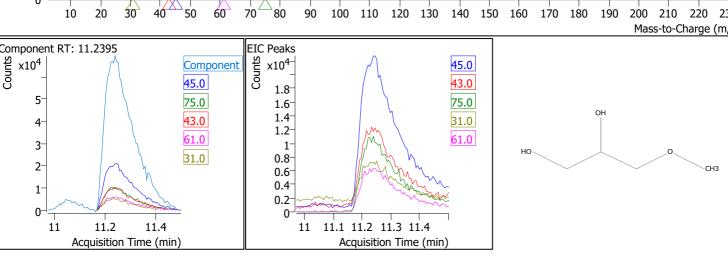
7.4 7.6 7.8

8

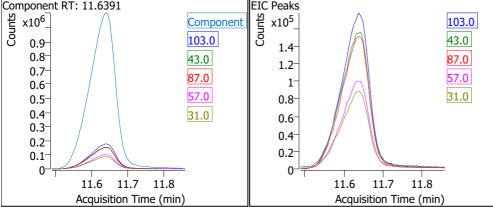
Acquisition Time (min)

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.** 623-39-2 11.2395 1,2-Propanediol, 3-methoxy-566611.8 C4H10O3 Component RT: 11.2395 v10<sup>2</sup> 0.9 45.0 0.8 $0.7^{-}$ 0.6 75.0 43.0 0.5 0.4 61.0 0.3 31.0 0.2 33.0 0.1 75 85 10 15 20 25 30 35 40 45 50 55 60 65 90 95 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) st x10<sup>2</sup>\_ 0.9-45.0 0.8 0.7 0.6 43.0 0.5 0.4 75.0 0.3 31.0 61.0 0.2 33.0 0.1 27.0 47.0 88.0 19.0 57.0 63.0 75 5 10 15 20 25 30 35 40 45 50 55 60 65 70 80 85 90 95 Mass-to-Charge (m/z) + Scan (11.1746-11.4235 min, 42 scans) 5.D St x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 75.0 $0.4^{-}$ 0.3 31.0 61.0 0.2 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: 11.2395 EIC Peaks



### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5579504.6 4744-08-5 11.6391 Propane, 1,1-diethoxy-79.0 C7H16O2 Component RT: 11.6391 v10<sup>2</sup> 0.9 103.0 43.0 87.0 0.8 0.7 57.0 0.6 31.0 0.5 0.4 0.3 0.2 117.0 0.1 0 40<sup>2</sup> 30 70 130 10 20 50 60 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 131.0 130 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.4902-11.8576 min, 62 scans) 5.D St x10<sup>2</sup> 0.9 103.0 0.8 87.0 43.0 0.7 0.6 31.0 57.0 0.5 $0.4^{-}$ 0.3 0.2 117.0 0.1 69.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 11.6391 Counts 0.9x10<sup>5</sup> 103.0 Component 103.0 43.0 0.9 1.4

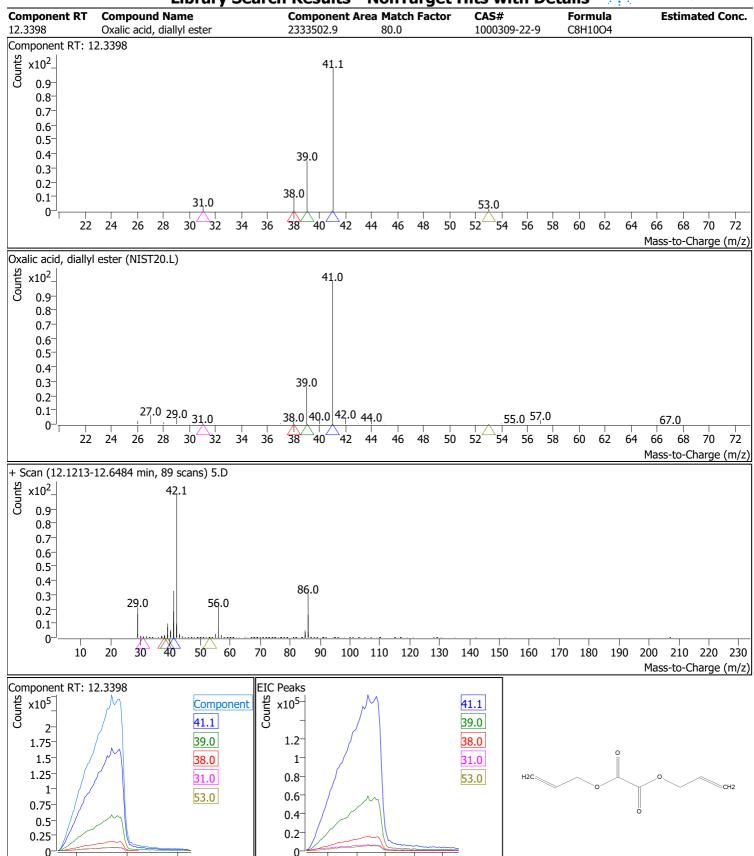


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# **Library Search Results - NonTarget Hits with Details**





12.2 12.3 12.4 12.5 12.6

Acquisition Time (min)

12.2

12.4 Acquisition Time (min)

12.6

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 96-48-0 12.3673 Butyrolactone 7213911.2 76.4 C4H6O2 Component RT: 12.3673 v10<sup>2</sup> 0.9 86.0 0.8 0.7 42.1 0.6 0.5 0.4 56.0 29.0 0.3 0.2 0.1 40.0 40 25 30 55 20 35 50 60 65 70 75 80 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) Counts x10<sup>2</sup>\_ 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 0-85 20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (12.1268-12.5176 min, 66 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 0.4 86.0 0.3 29.0 56.0 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 12.3673 Counts Counts x10<sup>5</sup> 42.1 Component 86.0 86.0 2.5 6 42.1 29.0 2-5 56.0 56.0

12.3

12.4

Acquisition Time (min)

85.0

1.5

1

0.5

12.2

29.0

85.0

4

3

2

1

12.2

12.3 12.4

# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 12.3674 Butanoic acid, 4-hydroxy-9243303.8 96.5 591-81-1 C4H8O3 Component RT: 12.3674 $x10^{2}$ 42.0 0.9 0.8 $0.7^{-}$ 0.6 41.0 0.5 86.0 0.4 56.0 0.3 0.2 85.0 55.0 57.0 0.1 38.0 86 50 52 54 56 60 62 64 66 68 70 72 74 76 78 80 82 Mass-to-Charge (m/z) Butanoic acid, 4-hydroxy- (NIST20.L) st x10<sup>2</sup> 0.9 0.8 0.7 0.6 41.0 0.5 0.4 86.0 56.0 0.3 0.2 40.0 85.0 0.1 87.0 60 62 64 66 68 70 72 74 76 78 80 82 84 86 88 90 92 46 48 50 52 54 56 58 Mass-to-Charge (m/z) + Scan (12.1268-12.5176 min, 66 scans) 5.D St x10<sup>2</sup> 0.9 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 86.0 0.3 29.0 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 60 Mass-to-Charge (m/z) Component RT: 12.3674 EIC Peaks Counts Counts x10<sup>5</sup> 42.0 Component 42.0 41.0 2.5 0.8 41.0 86.0 0.7 2 ОН 29.0 0.6 86.0

12.2 12.3 12.4 12.5 12.6

Acquisition Time (min)

56.0

1.5

1

0.5

29.0

56.0

12.6

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0.4

0.3

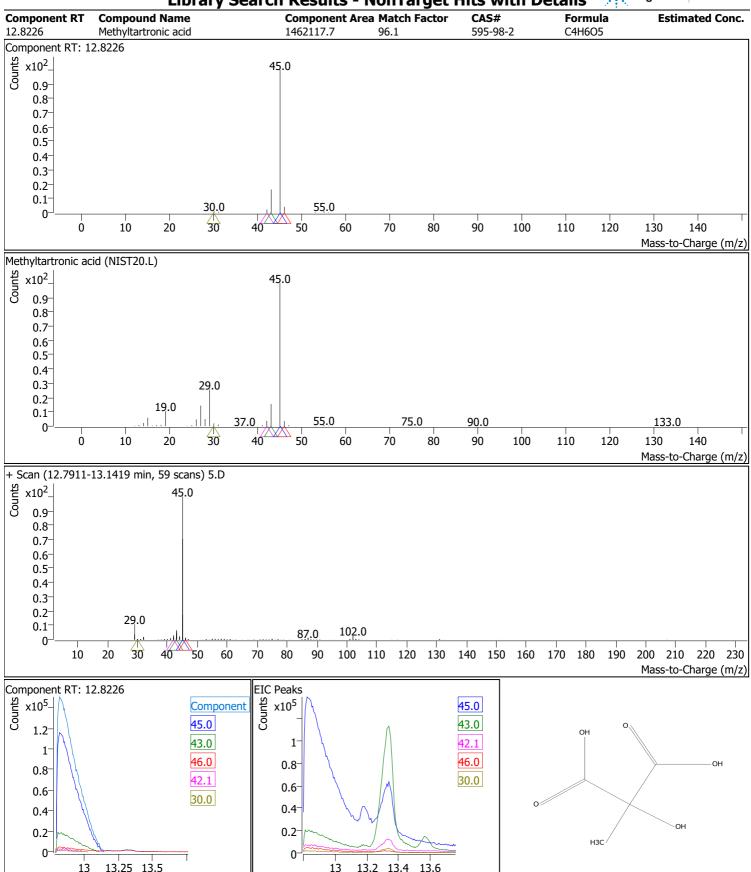
0.1

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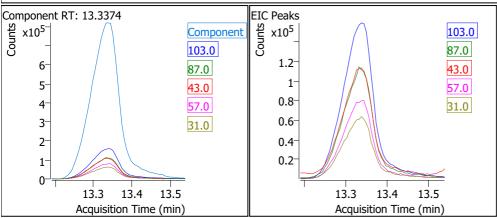
# **Library Search Results - NonTarget Hits with Details**





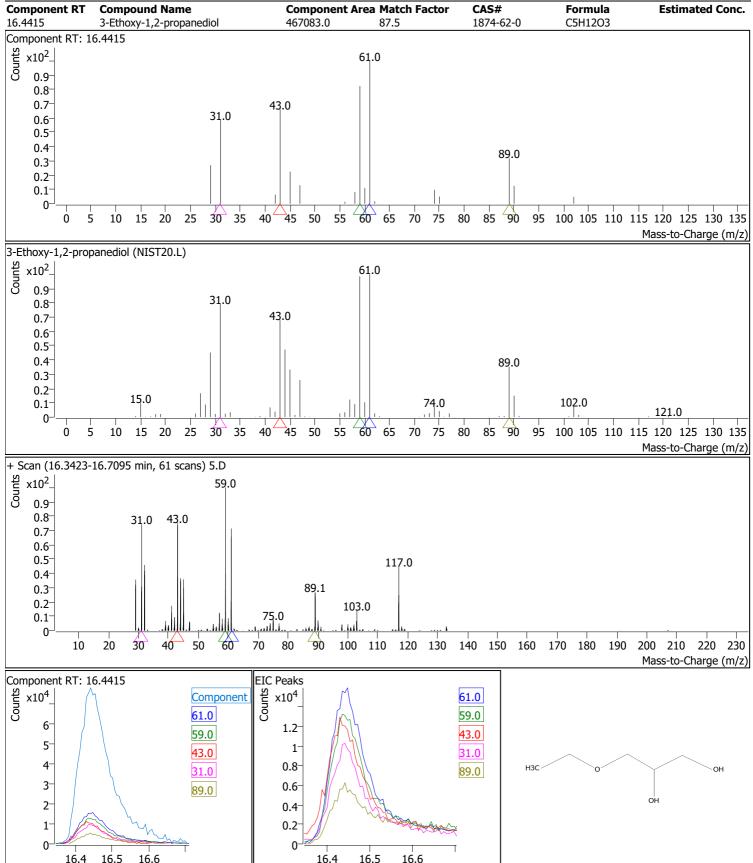
Acquisition Time (min)

### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 13.3374 Propane, 1,1-diethoxy-4386222.5 79.0 C7H16O2 Component RT: 13.3374 v10<sup>2</sup> 0.9 103.0 0.8 87.0 0.7 43.0 0.6 57.0 0.5 31.0 0.4 0.3 0.2 0.1 0 30 40 70 120 130 10 20 50 60 100 110 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 70.0 131.0 130 10 20 30 40 50 60 70 80 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (13.2014-13.5403 min, 58 scans) 5.D St x10<sup>2</sup> 0.9 103.0 43.0 87.0 0.8 0.7 57.0 0.6 29.0 0.5 $0.4^{-}$ 0.3 0.2 117.0 0.1 69.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 13.3374 EIC Peaks Counts Counts x10<sup>5</sup> 103.0 Component 103.0 87.0









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.** 53951-44-3 16.8824 1,3-Dioxolane-4-methanol, 2-ethyl-1316027.2 83.9 C6H12O3 Component RT: 16.8824 v10<sup>2</sup> 0.9 103.0 0.8 0.7 59.0 0.6 0.5 0.4 0.3 29.0 131.0 43.0 0.2 0.1 ×60 100 120 130 Ó 10 20 30 40 50 70 80 90 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 <del>\_\_\_</del>60 130 0 10 20 30 40 50 70 80 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (16.7967-16.9950 min, 34 scans) 5.D St x10<sup>2</sup> 0.9 103.0 0.8 0.7 59.0 0.6 44.0 0.5 $0.4^{-}$ 0.3 29.0 0.2 131.1 117.0 0.1 75.0 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) EIC Peaks Component RT: 16.8824 Counts Counts x10<sup>5</sup> x10<sup>4</sup> 103.0 Component 103.0 59.0 2.5 59.0 57.0 6 2

29.0

131.0



57.0

29.0

131.0

16.9

Acquisition Time (min)

1.5

1

0.5

5

4

3

2

16.85 16.9 16.95

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#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 108-95-2 17.9787 Phenol 1530797.3 96.1 C6H6O Component RT: 17.9787 v10<sup>2</sup> 0.9 94.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 55.0 63.0 50.0 25 40 55 95 20 30 35 45 50 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10<sup>2</sup>\_0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 39.0 0.2 0.1 55.0 47.050.0 63.0 27.0 74.0 40 95 20 25 30 35 45 50 55 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) + Scan (17.9162-18.2496 min, 57 scans) 5.D St x10<sup>2</sup> 0.9 94.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 66.0 39.0 0.1 117.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 17.9787 **EIC Peaks** Counts Counts x10<sup>5</sup> 94.0 Component 94.0 66.0 2.5 66.0 1 65.0 2 39.0 65.0 0.8

18.1

Acquisition Time (min)

18.2

40.0

39.0

40.0

18.1

Acquisition Time (min)

18.2

0.6

0.4

0.2

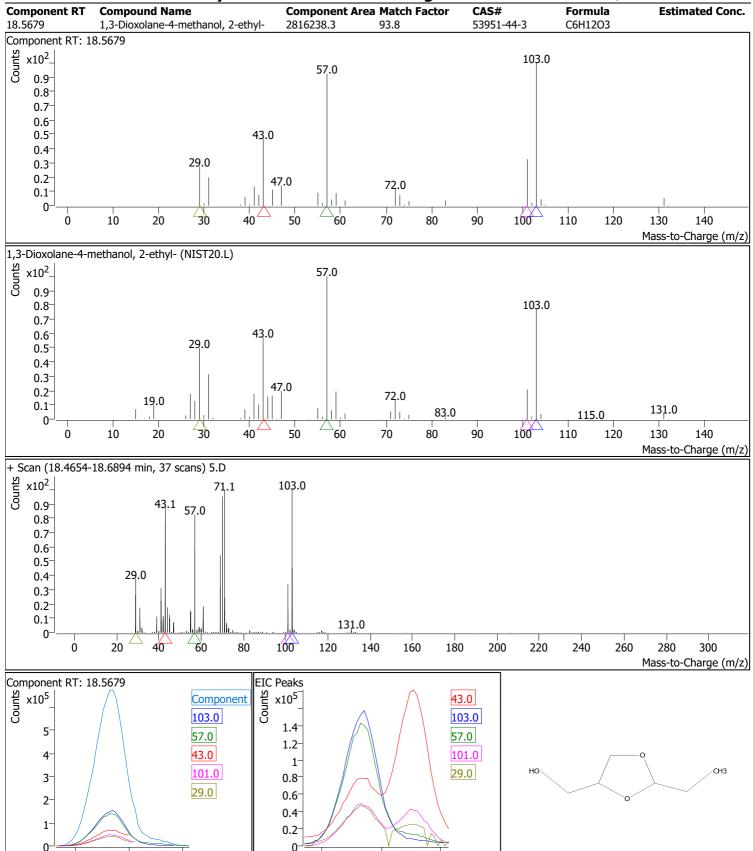
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1

0.5







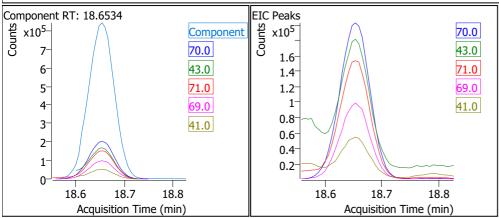
18.6 Acquisition Time (min)

18.5

18.5

18.6

#### Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 544-01-4 18.6534 Diisoamyl ether 3161009.8 97.0 C10H22O Component RT: 18.6534 v10<sup>2</sup> 0.9 70.0 43.0 0.8 0.7 0.6 0.5 0.4 0.3 41.0 55.0 101.0 0.2 39.0 45.0 0.1 100 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 105 110 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 43.0 70.0 0.8 0.7 0.6 0.5 0.4 41.0 0.3 55.0 0.2 101.0 29.0 39.0 45.0 0.1 31.0 53.0 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (18.5647-18.7544 min, 32 scans) 5.D St x10<sup>2</sup> 0.9 43.1 0.8 0.7 0.6 0.5 57.0 103.0 $0.4^{-}$ 0.3 29.0 61.0 0.2 0.1 131.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 18.6534 **EIC Peaks** Counts St x10<sup>5</sup>x10<sup>5</sup> 70.0 Component 70.0 43.0 1.6 6 43.0 71.0 1.4



# --- 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 19.7716 1,3-Dioxolane-4-methanol, 2-ethyl-2330943.0 93.8 C6H12O3 Component RT: 19.7716 v10<sup>2</sup> 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 72.0 0.1 <del>2</del>30 40 100 120 130 Ó 10 20 50 70 80 90 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 <del>2</del>30 0 10 20 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (19.6777-19.9918 min, 53 scans) 5.D St x10<sup>2</sup> 0.9 103.0 0.8 0.7 0.6 43.0 0.5 $0.4^{-}$ 31.0 0.3 0.2 72.0 0.1 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: 19.7716 Counts Counts x10<sup>5</sup> 103.0 Component 103.0 57.0 1 57.0 43.0 3.5



29.0

101.0

43.0

101.0

29.0

3<sup>-</sup> 2.5

2

1.5<sup>-</sup>

0.5

19.7

19.8

19.9

Acquisition Time (min)

0.8

0.6

0.4

 $0.2^{-1}$ 

19.7

19.8

19.9

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 80-71-7 20.0706 2-Cyclopenten-1-one, 2-hydroxy-3-526051.2 92.6 C6H8O2 methyl-Component RT: 20.0706 x10<sup>2</sup>. 112.0 0.9 8.0 0.7 0.6 0.5 0.4 69.1 55.0 0.3 83.1 41.1 $0.2^{-}$ 99.0 0.1 0-<del>7</del>0 55 30 35 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 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (19.9799-20.3129 min, 57 scans) 5.D x10<sup>2</sup> 43.0 0.8 0.7 0.6 0.5 0.4 0.3 112.1 31.0 0.2 55.0 103.0 69.0 83.0 0.1 117.0 0 70 190 200 210 220 230 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 20.0706 **EIC Peaks** Counts Counts x10<sup>4</sup>x10<sup>5</sup> 112.0 Component 112.0 69.1 0.9 2.5 69.1 55.0 0.8 0.7 2-55.0 41.1 0.6 83.1 83.1 1.5 нзс 0.5

41.1

1

0.5

0

20

20.1

20.2

Acquisition Time (min)

0.4

0.3<sup>-</sup> 0.2<sup>-</sup>

0.1

20

20.1

20.2

Acquisition Time (min)

ОН

### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 110-88-3 21.1623 1,3,5-Trioxane 1444208.3 76.3 C3H6O3 Component RT: 21.1623 v10<sup>2</sup> 0.9 89.0 0.8 61.0 0.7 0.6 0.5 0.4 43.0 0.3 29.0 0.2 0.1 0 <del>3</del>0 <del>9</del>0 75 10 15 20 25 40 50 55 65 80 85 95 100 Mass-to-Charge (m/z) 1,3,5-Trioxane (NIST20.L) Counts x10<sup>2</sup>\_ 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 0-<del>3</del>0 <del>2</del>0 10 15 20 25 35 40 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (21.0289-21.2286 min, 34 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 31.0 89.0 0.1 117.0 60 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.1623 **EIC Peaks** Counts Counts x10<sup>4</sup>. x10<sup>5</sup>-Component 89.0 43.0 8 0.8 7 61.0 89.0 0.7 6 43.0 29.0 0.6 5 60.0 0.5 4



21.5

Acquisition Time (min)

0.4

0.3

0.2

0.1

21

29.0

3

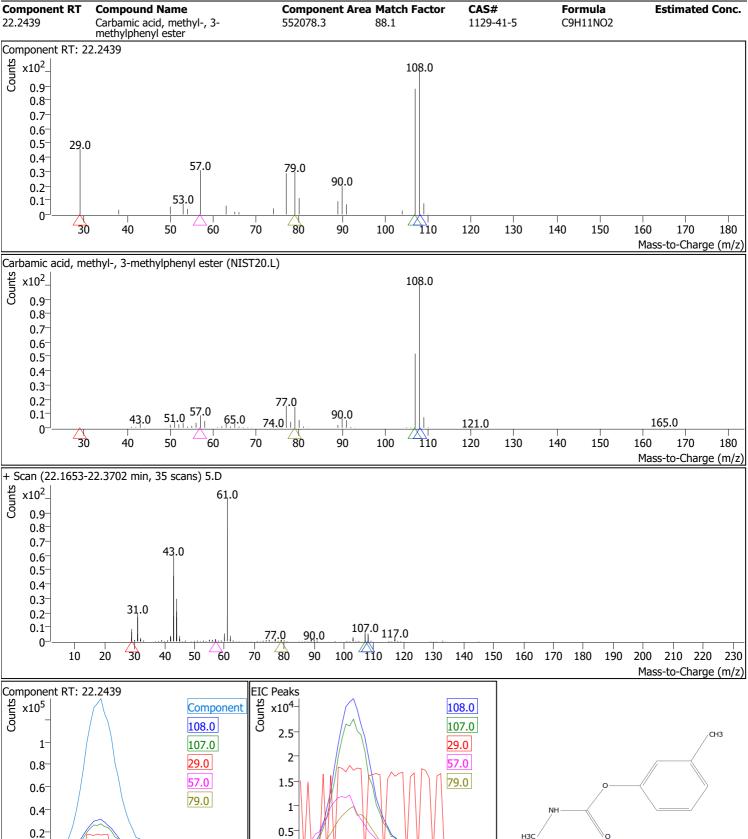
2

1

21

21.5





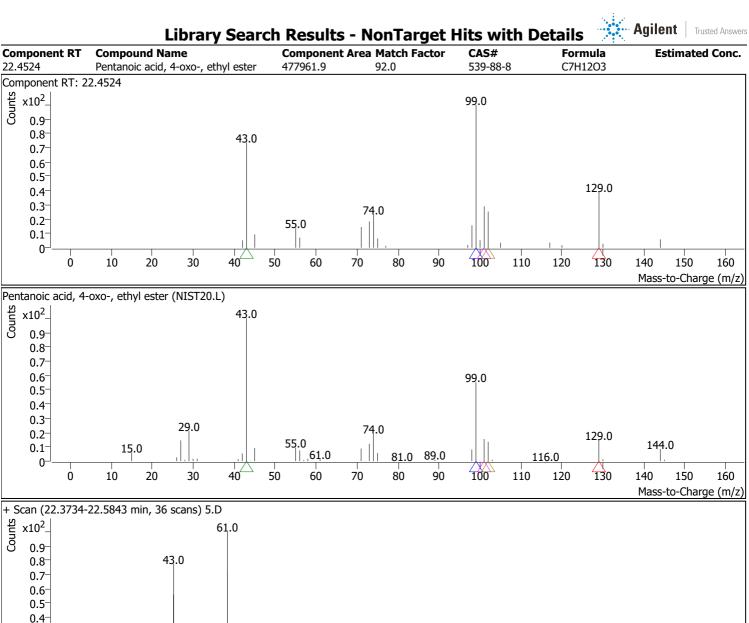
22.3

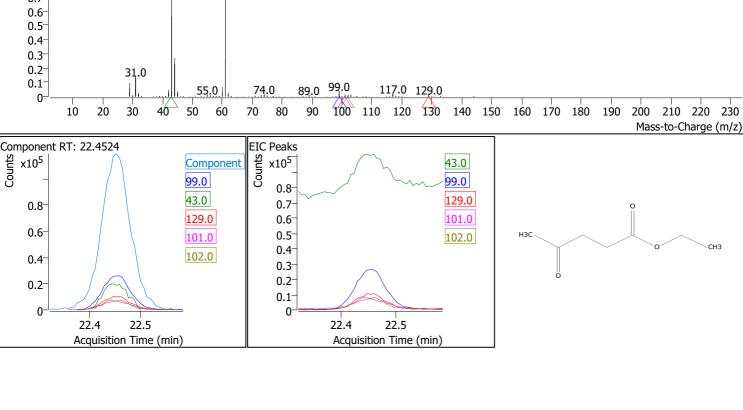
Acquisition Time (min)

22.2

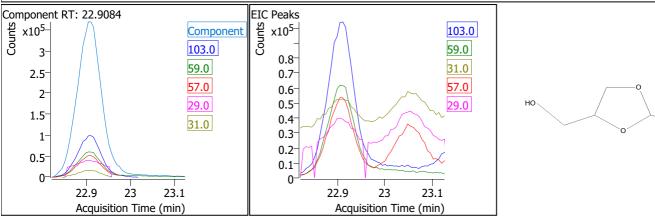
22.2

22.3





# -- 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 22.9084 1,3-Dioxolane-4-methanol, 2-ethyl-1476338.7 78.8 C6H12O3 Component RT: 22.9084 v10<sup>2</sup> 0.9 103.0 0.8 $0.7^{-}$ 59.0 0.6 29.0 0.5 0.4 0.3 43.0 0.2 131.0 0.1 70 100 120 Ó 10 20 30 40 50 80 90 110 130 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 <del>\_\_\_</del>60 0 10 20 30 40 50 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (22.8183-23.1254 min, 52 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 43.0 0.6 0.5 $0.4^{-}$ 0.3 31.0 0.2 70.1 84.1 103.0 0.1 117.0 0 60 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 22.9084 **EIC Peaks** x10<sup>5</sup> 103.0 Component



# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0562 1-Octanol 3055456.6 98.1 111-87-5 C8H18O Component RT: 23.0562 v10<sup>2</sup> 0.9 56.0 41.0 70.0 0.8 84.0 0.7 0.6 0.5 0.4 0.3 0.2 0.1 70 55 100 105 110 115 120 125 130 135 140 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 55 20 25 30 35 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9589-23.2443 min, 49 scans) 5.D St x10<sup>2</sup>\_ 0.9 61.0 0.8 0.7 43.0 0.6 0.5 $0.4^{-}$ 0.3 31.0 0.2 56.1 70.1 0.1 84.1 103.0 117.0 10 20 30 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: 23.0562 **EIC Peaks** Counts x10<sup>5</sup> Counts x10<sup>4</sup> 56.0 Component 56.0 55.0 5 55.0 41.0 6 70.0 41.0 5

23.1

Acquisition Time (min)

23.2

69.0

70.0

69.0

3

2

1

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.** 90-05-1 23.6017 Phenol, 2-methoxy-24824933.3 98.6 C7H8O2 Component RT: 23.6017 v10<sup>2</sup> 0.9 109.0 124.0 0.8 0.7 0.6 81.0 0.5 0.4 0.3 0.2 53.0 65.0 0.1 39.0 80 110 10 20 30 40 50 70 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) St x10<sup>2</sup>\_ 0.9 109.0 124.0 0.8 0.7 0.6 0.5 81.0 0.4 0.3 0.2 53.0 27.0 39.0 0.1 65.0 18.0 77.0 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4583-23.7854 min, 56 scans) 5.D st x10<sup>2</sup> 0.9 109.0 0.8 124.0 43.0 0.7 81.0 0.6 61.0 0.5 0.4 0.3 0.2 53.0 31.0 0.1 95.0 117.0 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: 23.6017 Counts x10<sup>6</sup> x10<sup>6</sup> 109.0 Component 109.0 124.0 1.2 4 124.0 81.0 3.5 1-81.0 53.0

125.0

нзс



53.0

125.0

0.8

0.6

0.4

0.2

23.5

23.6

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23.7

Acquisition Time (min)

3

2

1-

23.5

23.6

23.7

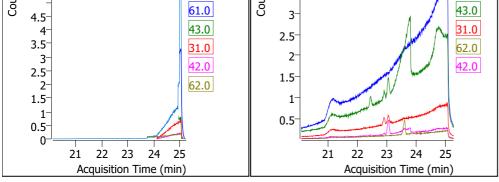
Acquisition Time (min)

2.5

1.5

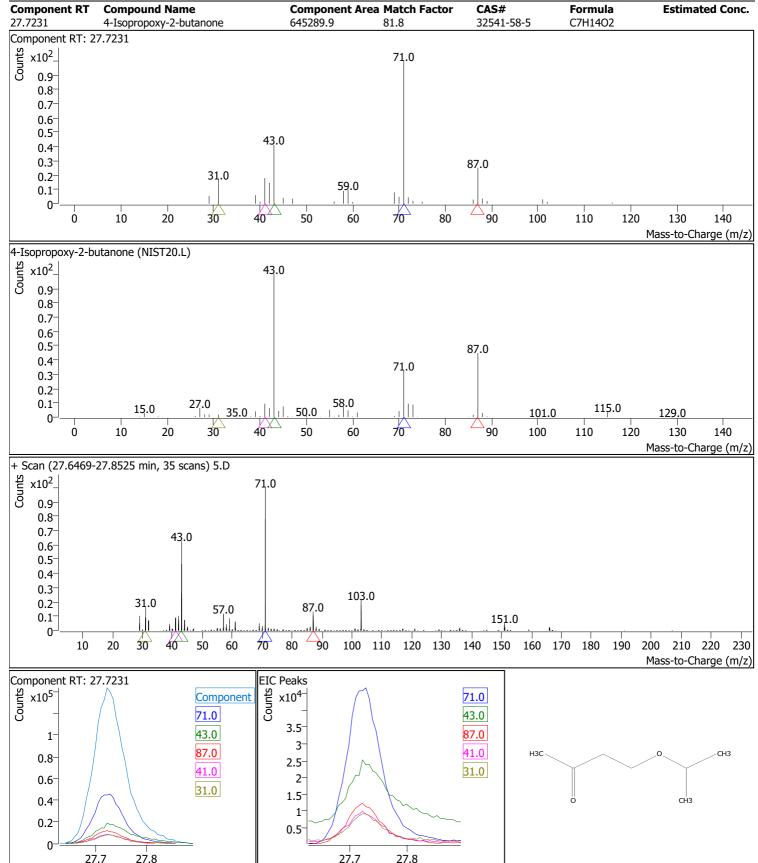
0.5

# --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 25.0343 Glycerin 7063177.2 78.8 56-81-5 C3H8O3 Component RT: 25.0343 v10<sup>2</sup> 0.9 61.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 31.0 0.2 0.1 45.0 33.0 0 5 25 75 10 15 20 30 55 70 80 Mass-to-Charge (m/z) Glycerin (NIST20.L) x10<sup>2</sup>\_ 0.9 61.0 43.0 0.8 0.7 0.6 0.5 31.0 0.4 0.3 15.0 0.2 27.0 0.1 19.0 55.0 58.0 74.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 Mass-to-Charge (m/z) + Scan (24.9448-25.0734 min, 22 scans) 5.D st x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 31.0 0.2 0.1 103.0 117.0 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) EIC Peaks Component RT: 25.0343 Counts Counts x10<sup>5</sup>\_ 61.0 Component 61.0 43.0 3 4.5 43.0 31.0 2.5



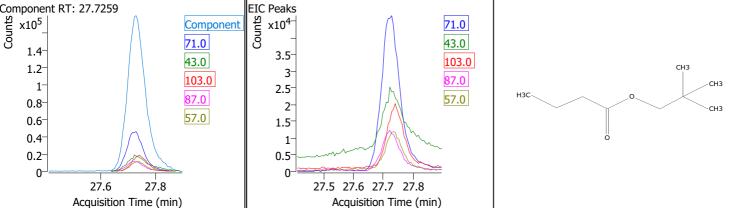


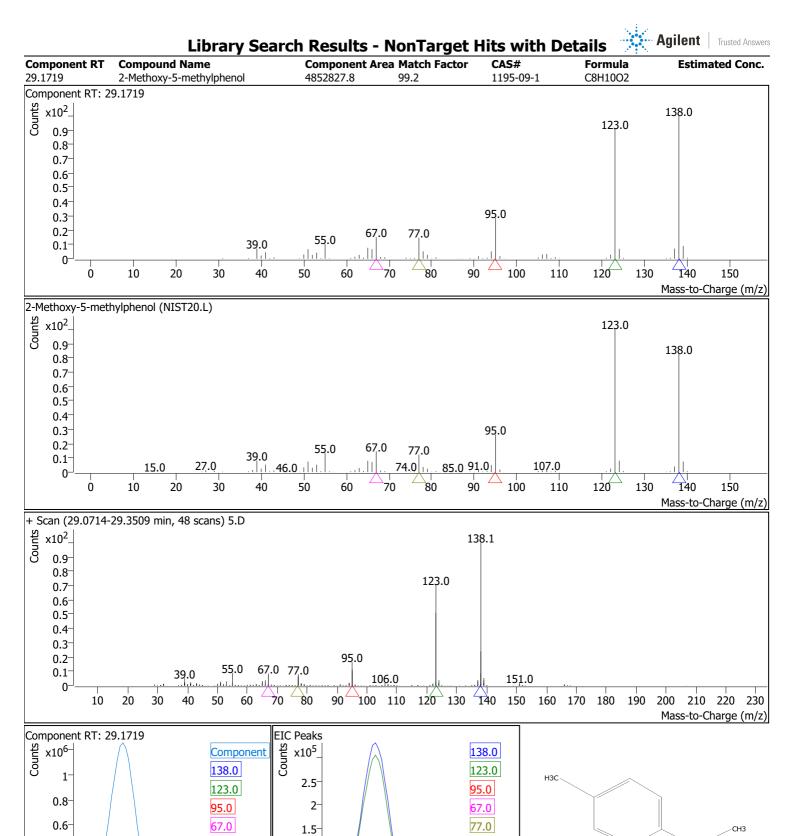




Acquisition Time (min)

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 82.3 27.7259 Butanoic acid, 2,2-dimethylpropyl 828843.6 23361-69-5 C9H18O2 Component RT: 27.7259 x10<sup>2</sup>\_ 71.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 103.0 0.3 87.0 57.0 31.0 $0.2^{-}$ 0.1 0-70 10 20 30 50 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 <sub>93.0</sub> 36.0 0.1 27.0 49.0 130.0 143.0 66.0 0 10 20 30 40 50 60 70 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6481-27.8525 min, 35 scans) 5.D x10<sup>2</sup>. 71.0 0.9 0.8 0.7 43.0 0.6 0.5 0.4 0.3 103.0 31.0 0.2 87.0 57.0 0.1 151.0 190 200 210 220 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 27.7259 **EIC Peaks** Counts Counts x10<sup>4-</sup> x10<sup>5</sup> 71.0 Component 71.0 43.0





29.2

Acquisition Time (min)

29.3

77.0

1-

0.5

0.4

0.2

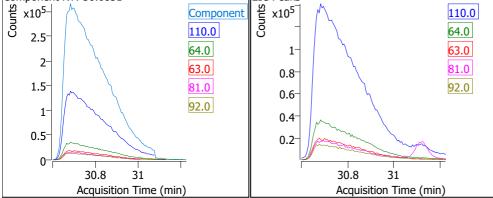
29.1

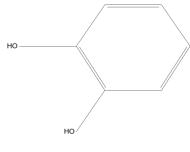
29.2

Acquisition Time (min)

29.3

# ··· 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 30.6831 Catechol 4125098.9 96.3 C6H6O2 Component RT: 30.6831 y x10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 100 105 110 115 120 125 10 50 80 85 Mass-to-Charge (m/z) Catechol (NIST20.L) st x10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 <del>∠</del>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 (30.5995-31.0752 min, 81 scans) 5.D St x10<sup>2</sup>\_ 0.9 110.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 64.0 0.2 92.0 103.0 81.0 0.1 53.0 10 20 40 50 60 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 30.6831 EIC Peaks Counts x10<sup>5</sup>\_ x10<sup>5</sup> 110.0 Component 110.0 64.0 2.5 64.0 63.0 1-2





#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1450-72-2 32.1005 Ethanone, 1-(2-hydroxy-5-516864.7 91.1 C9H10O2 methylphenyl)-Component RT: 32.1005 x10<sup>2</sup>\_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 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 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0283-32.2097 min, 30 scans) 5.D st x10<sup>2</sup> 0.9 135.0 0.8 0.7 0.6 0.5 0.4 150.1 0.3 43.0 0.2 96.0 0.1 150 180 190 200 210 220 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Component RT: 32.1005 **EIC Peaks** Counts Counts $x10^{4}$ 135.0 x10<sup>5</sup> Component НО 150.0 135.0 4.5 1 150.0 77.0 **Н3С** 77.0 3.5 136.0 0.8 3 136.0 79.0 0.6 2.5

32.05 32.1 32.15 32.2

Acquisition Time (min)

79.0

0.4

0.2

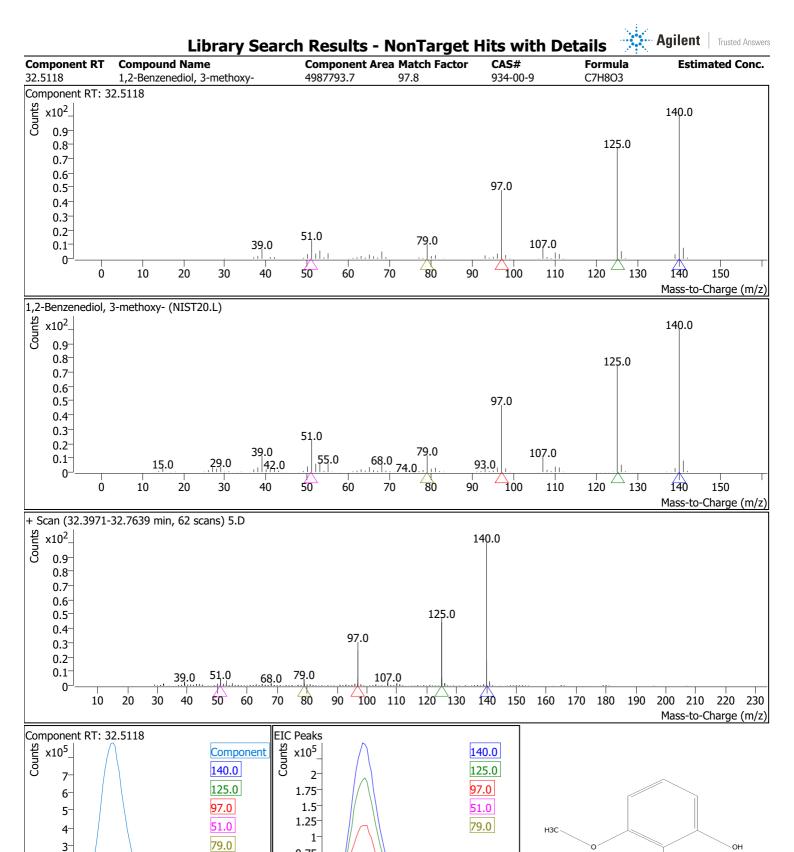
32.1

32.2

Acquisition Time (min)

2

1.5





32.6

Acquisition Time (min)

32.7

0.75

0.5

2

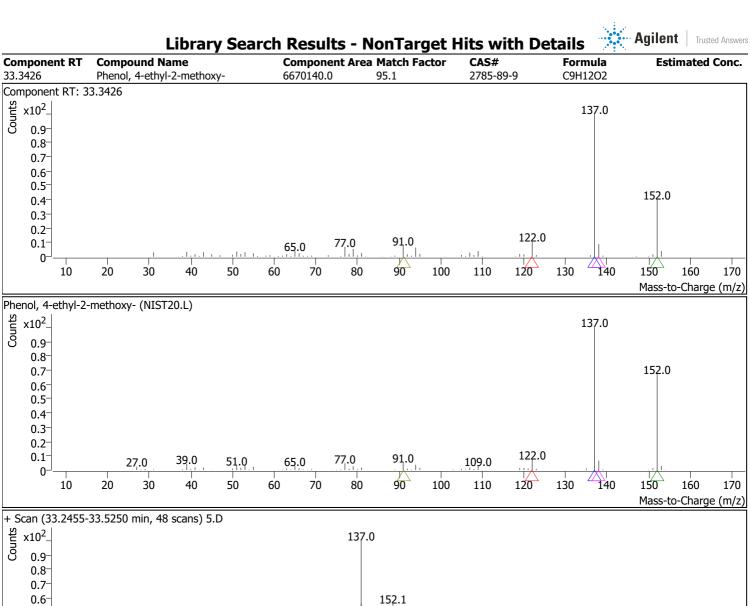
32.5

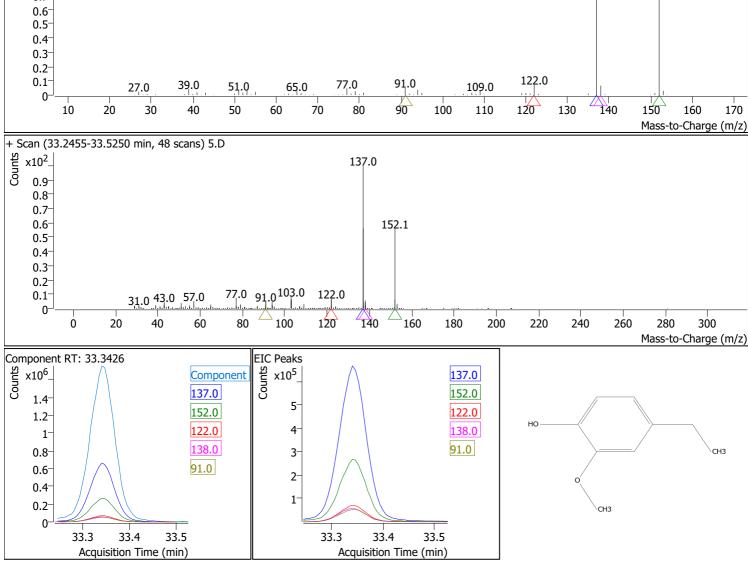
32.6

Acquisition Time (min)

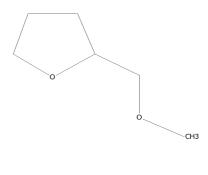
32.7

ОН





# --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 34.1387 Furan, tetrahydro-2-(methoxymethyl)- 454360.7 19354-27-9 C6H12O2 Component RT: 34.1387 v10<sup>2</sup> 0.9 71.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 43.0 0.2 58.0 87.0 0.1 101.0 29.0 40 <sup>∠</sup> 30 75 85 100 105 110 115 120 125 Mass-to-Charge (m/z) Furan, tetrahydro-2-(methoxymethyl)- (NIST20.L) st x10<sup>2</sup>\_ 0.9-71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 0.1 58.0 15.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (34.0963-34.2353 min, 23 scans) 5.D st x10<sup>2</sup> 0.9 71.0 0.8 $0.7^{-}$ 0.6 43.0 0.5 $0.4^{-}$ 57.0 0.3 87.0 0.2 29.0 103.0 115.0 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 34.1387 Counts Counts x10<sup>4</sup> Component 71.0 71.0 43.0 0.8 43.0 3 87.0 0.7



# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 452-86-8 35.0178 1,2-Benzenediol, 4-methyl-509748.5 93.9 C7H8O2 Component RT: 35.0178 v10<sup>2</sup> 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 0.2 51.0 106.0 0.1 38.0 10 20 30 40 50 60 70 90 100 110 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 4-methyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 124.0 0.8 78.0 0.7 0.6 0.5 0.4 0.3 51.0 0.2 107.0 39.0 62.0 67.0 95.0 55.0 0.1 27.0 74.0 19.0 10 20 30 40 50 60 70 80 90 100 110 130 140 Mass-to-Charge (m/z) + Scan (34.9223-35.2255 min, 52 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 43.1 0.2 0.1 29.0 57.0 89.0101.0 80 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0178 Counts Counts x10<sup>4</sup>-124.0 Component 124.0 123.0 0.8 1.8 78.0 123.0 0.7 1.6 78.0 1.4 77.0 0.6



35.1

Acquisition Time (min)

35.2

106.0

1.2

0.8

 $0.6^{-}$ 

 $0.4^{\circ}$ 

0.2

1

77.0

106.0

0.5

0.4

0.3-

0.2

0.1

35

35.1

Acquisition Time (min)

35.2

-СН3

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 35.0184 506482.9 488-17-5 C7H8O2 1,2-Benzenediol, 3-methyl-89.8 Component RT: 35.0184 v10<sup>2</sup> 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 0.2 51.0 106.0 137.0 0.1 38.0 10 20 30 40 50 60 70 90 100 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 3-methyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 124.0 0.8 0.7 0.6 0.5 0.4 78.0 0.3 0.2 106.0 39.0 51.0 0.1 62.0 67.0 27.0 18.0 10 20 30 40 50 60 70 80 90 100 110 130 140 Mass-to-Charge (m/z) + Scan (34.9223-35.2255 min, 52 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 0.4 0.3 43.1 0.2 0.1 29.0 57.0 89.0101.0 80 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0184 Counts Counts x10<sup>4</sup>-124.0 Component 124.0 123.0 8 1.8 78.0 123.0 7 1.6 6 78.0 1.4 77.0

35.1

Acquisition Time (min)

35.2

106.0

НЗС

1.2

0.8

0.6

 $0.4^{\circ}$ 

0.2

1

77.0

106.0

5

4

3

2

1

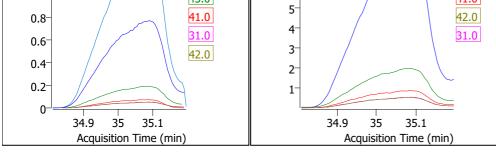
35

35.1

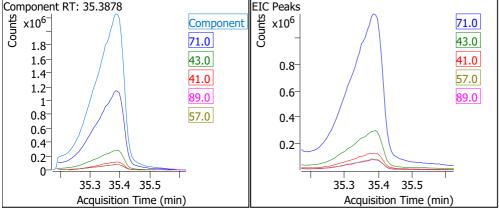
Acquisition Time (min)

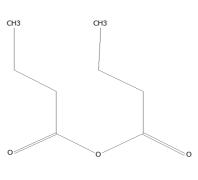
35.2

# -- 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 35.0881 2-Furanmethanol, tetrahydro-15928096.7 C5H10O2 Component RT: 35.0881 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 57.0 10 25 30 35 55 60 65 70 85 90 95 100 105 110 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts x10<sup>2</sup>\_ 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 (34.8132-35.1899 min, 64 scans) 5.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 43.1 0.2 0.1 31.0 57.0 89.0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0881 Counts Counts x10<sup>6</sup> x10<sup>5</sup> 71.0 Component 71.0 43.0 6 1 43.0 41.0 5

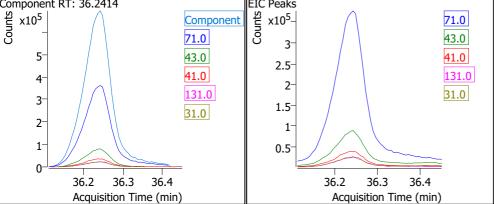


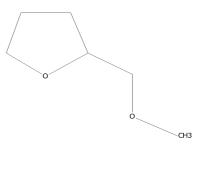
# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.3878 Butanoic acid, anhydride 16283653.9 80.7 C8H14O3 Component RT: 35.3878 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 57.0 89.0 0.1 90 10 15 20 25 30 35 55 65 70 75 95 Mass-to-Charge (m/z) Butanoic acid, anhydride (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 41.0 0.1 55.0 29.0 60.0 85.0 89.0 5 10 15 20 25 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (35.1899-35.6061 min, 71 scans) 5.D st x10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.1 0.2 0.1 29.0 57.0 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) Component RT: 35.3878 **EIC Peaks** Counts V106x10<sup>6</sup> 71.0 Component CH3 CH3 71.0 43.0 1.8 1.6 43.0 41.0 0.8

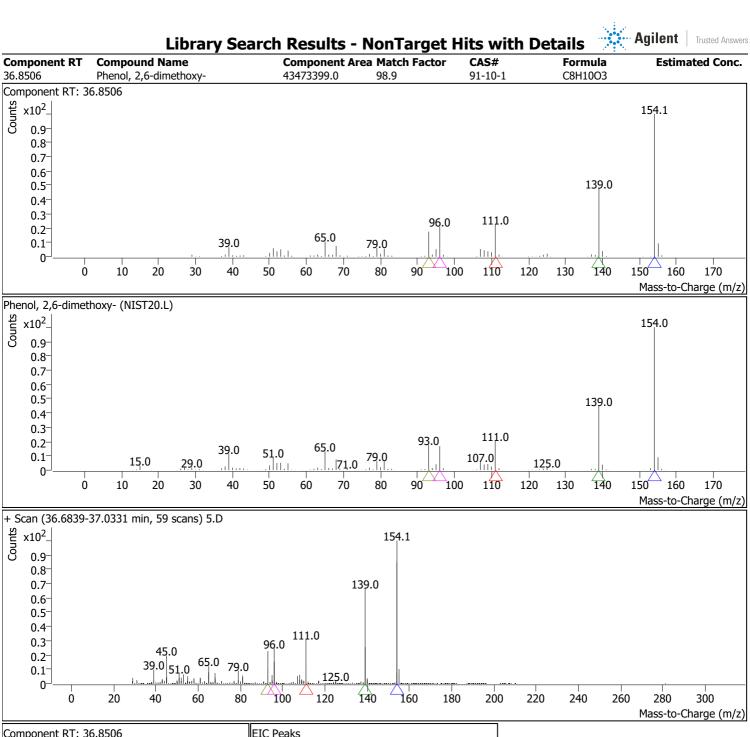


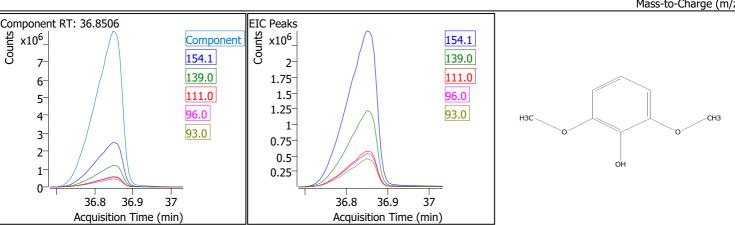


# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.2414 Furan, tetrahydro-2-(methoxymethyl)- 3488709.8 19354-27-9 C6H12O2 Component RT: 36.2414 v10<sup>2</sup> 0.9 71.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 43.0 0.2 0.1 57.0 60 65 95 100 105 110 115 120 125 Mass-to-Charge (m/z) Furan, tetrahydro-2-(methoxymethyl)- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 0.1 58.0 10 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (36.1077-36.4148 min, 52 scans) 5.D st x10<sup>2</sup> 0.9 71.0 0.8 $0.7^{-}$ 0.6 $0.5^{\circ}$ $0.4^{-}$ 0.3 43.1 0.2 0.1 131.0 103.0 10 20 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: 36.2414 Counts x10<sup>5</sup> Counts x10<sup>5</sup>– 71.0 Component 71.0 43.0 3-5 43.0 41.0 2.5

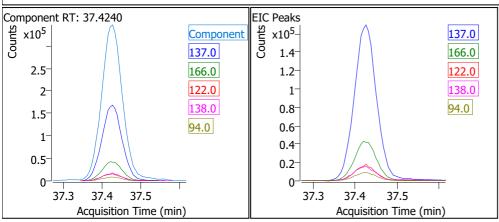






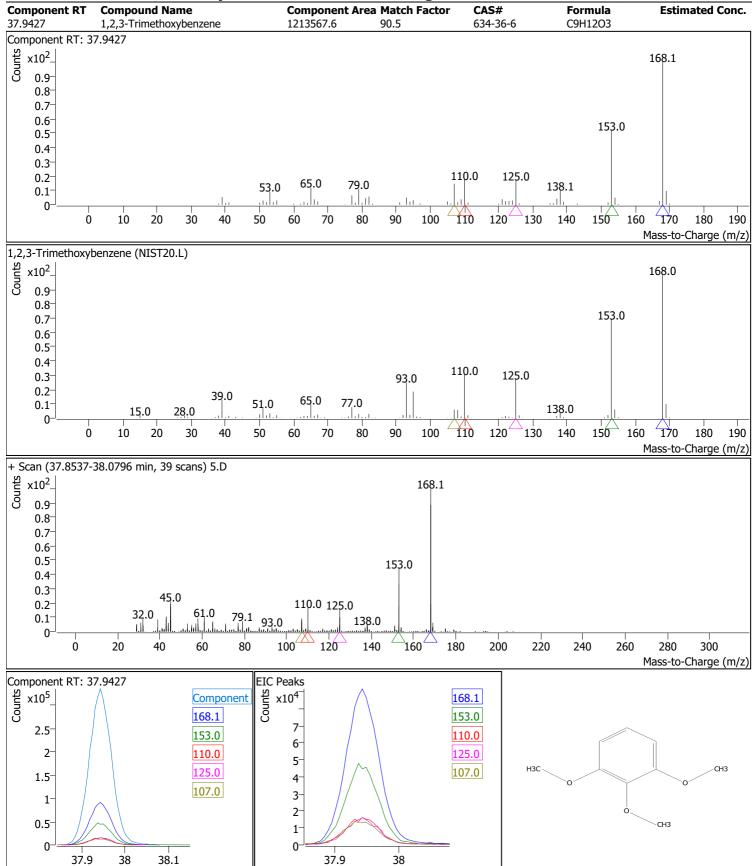


#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4240 Phenol, 2-methoxy-4-propyl-1324225.1 93.6 C10H14O2 Component RT: 37.4240 v10<sup>2</sup> 0.9 137.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 77.0 94.0 29.0 51.0 160 170 50 120 10 20 30 40 60 70 80 100 110 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 Mass-to-Charge (m/z) + Scan (37.3433-37.5623 min, 37 scans) 5.D st x10<sup>2</sup> 0.9 137.1 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 71.0 103.0 166.1 0.2 57.0 43.1 0.1 122.0 94.0 154.0 61.0 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: 37.4240 EIC Peaks Counts x10<sup>5</sup> Counts x10<sup>5</sup>-137.0 Component 137.0 166.0 1.4



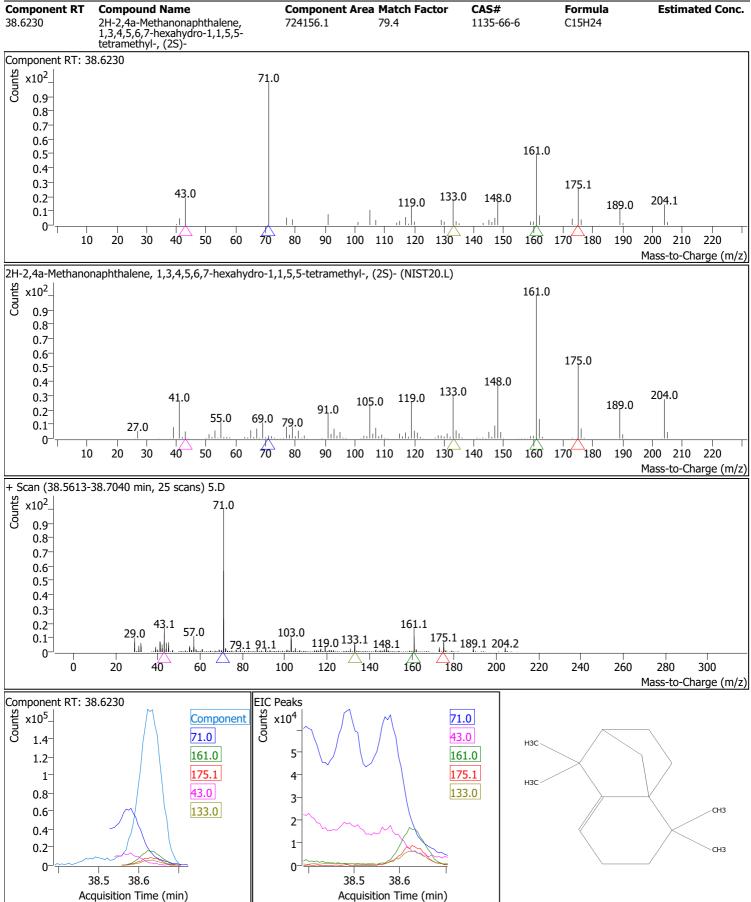


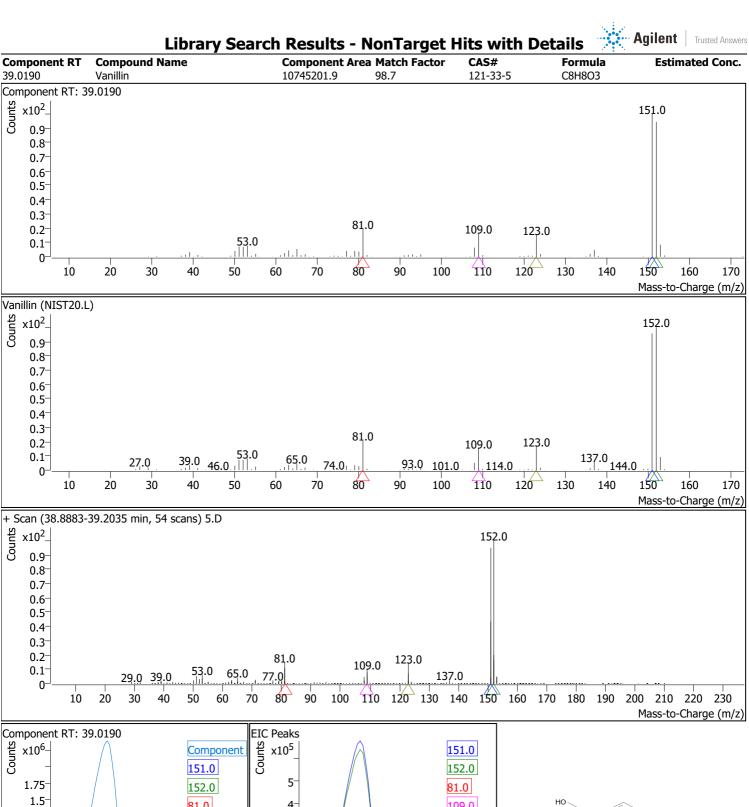


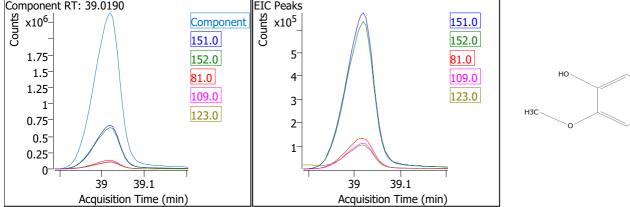


Acquisition Time (min)

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Compound Name Formula** 724156.1 79.4 1135-66-6 C15H24

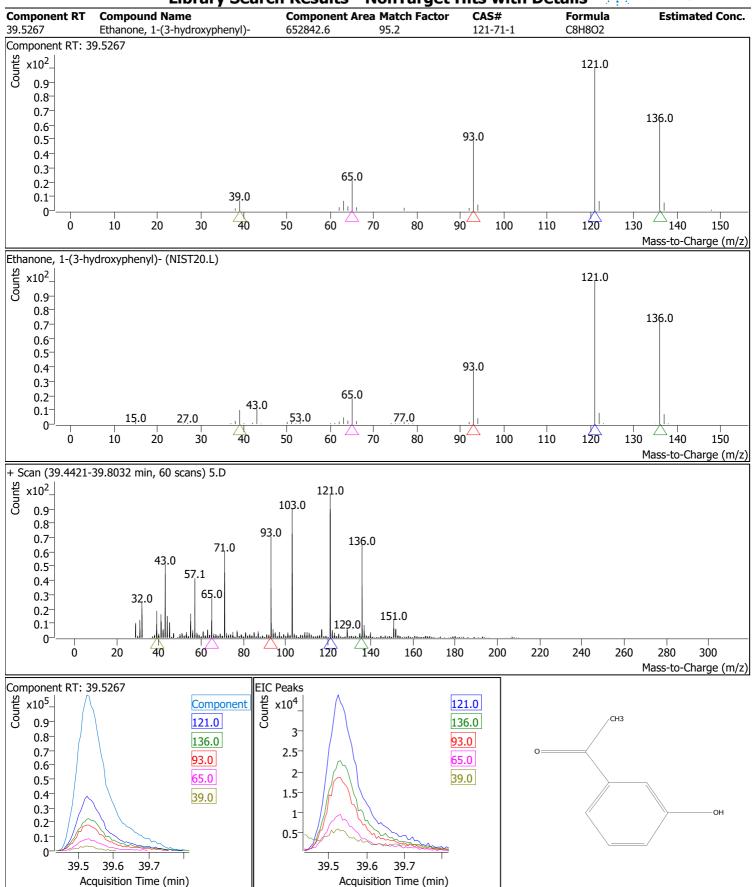




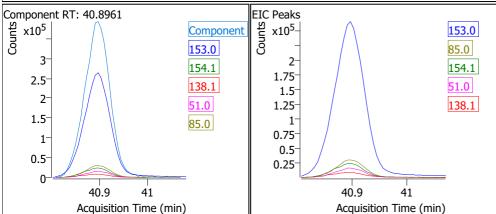


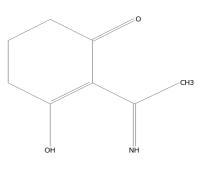






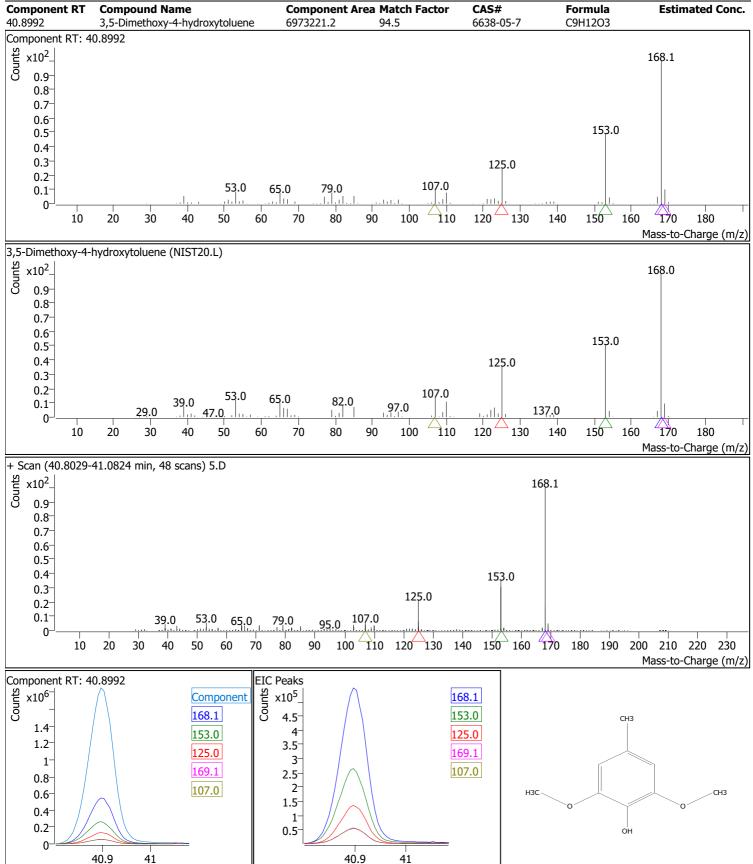
### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1000131-52-4 40.8961 2-Cyclohexen-3-ol-1-one, 2-[1-1465508.6 81.4 C8H11NO2 iminoethyl]-Component RT: 40.8961 x10<sup>2</sup>\_ 153.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 138.1 0.1 51.0 85.0 62.0 96.0 0-140 90 30 40 50 60 70 80 100 110 120 130 150 160 170 Mass-to-Charge (m/z) 2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]- (NIST20.L) $x10^{2}$ 153.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 69.0 83.0 97.0 125.0 49.0 55.0 62.0 112.0 138.0 0 140 30 40 50 60 70 80 90 100 110 120 130 150 160 170 Mass-to-Charge (m/z) + Scan (40.8109-41.0705 min, 44 scans) 5.D x10<sup>2</sup>. 168.1 0.9 0.8 0.7 0.6 0.5 0.4 153.0 0.3 125.0 0.2 0.1 107.0 39.0 79.0 65.0 95.0 100 110 120 130 140 150 160 170 180 190 200 210 220 230 10 20 40 50 60 70 80 90 Mass-to-Charge (m/z) Component RT: 40.8961 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup> 153.0 Component 85.0 153.0 3 2 154.1 154.1 1.75 2.5 138.1 51.0 1.5





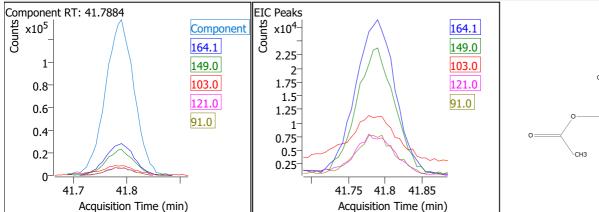




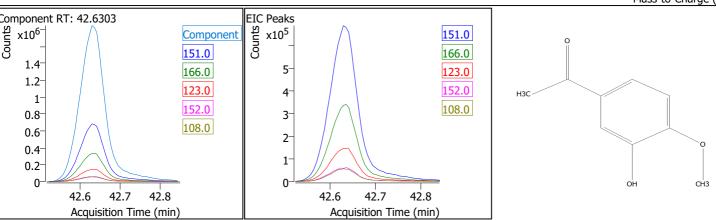


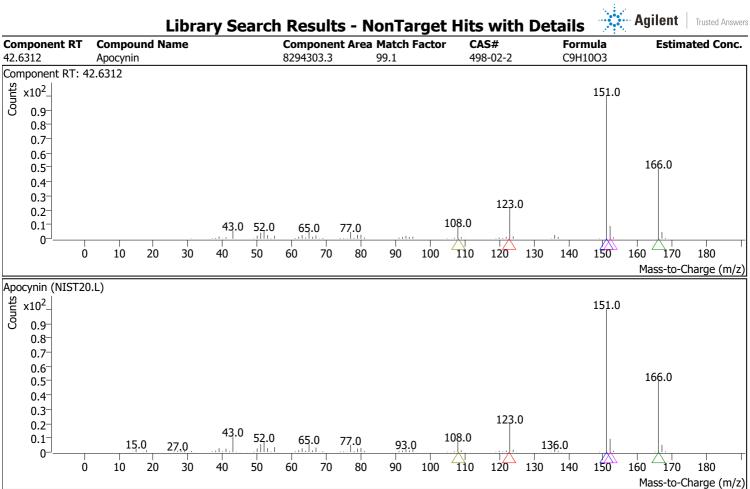
Acquisition Time (min)

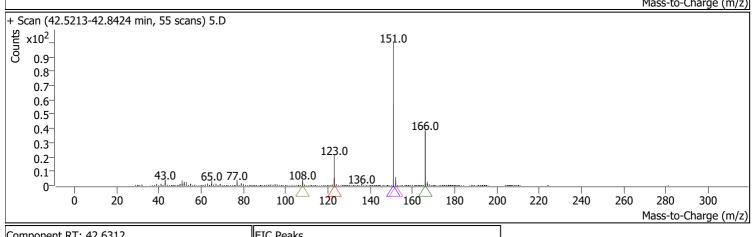
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 93-28-7 41.7884 Phenol, 2-methoxy-4-(2-propenyl)-, 515705.0 85.6 C12H14O3 acetate Component RT: 41.7884 Counts x10<sup>2</sup>. 164.1 0.9 149.0 8.0 0.7 0.6 0.5 0.4 103.0 0.3 91.0 121.0 77.0 137.0  $0.2^{-}$ 0.1 0-**15**0 30 40 50 60 70 80 90 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-(2-propenyl)-, acetate (NIST20.L) Counts  $x10^{2}$ 164.0 0.9 0.8 0.7 0.6 0.5 149.0 0.4 77.0 0.3 55.0 103.0 91.0 131.0 0.2 51.0 121.0 65.0 137.0 0.1 43.0 |82.0 70.0 59.0 0 150 90 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (41.7008-41.8859 min, 32 scans) 5.D x10<sup>2</sup>. 71.1 164.1 0.9 0.8 0.7 149.0 43.0 0.6 0.5 0.4 103.0 0.3 32.0 77.085.0 0.2 121.0 137.0 57.0 0.1 اعتبارين والمانين المتاريخ الماريخ الماريخ المتاريخ المتاريخ المتاريخ الماريخ الماريخ الماريخ الماريخ الماريخ 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 10 20 30 40 50 60 70 80 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 41.7884 x10<sup>4</sup>-164.1 x10<sup>5</sup> Component

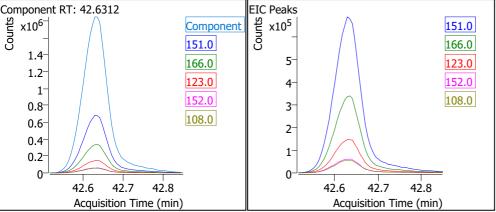


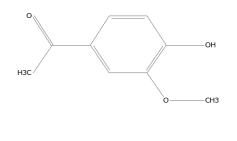
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-8293589.4 6100-74-9 42.6303 98.9 C9H10O3 Component RT: 42.6303 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 166.0 0.5 0.4 0.3 123.0 $0.2^{-}$ 108.0 0.1 43.0 52.0 65.0 77.0 0-110 150 10 20 30 40 50 60 70 80 90 100 120 130 140 160 170 180 Mass-to-Charge (m/z) Ethanone, 1-(3-hydroxy-4-methoxyphenyl)- (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 166.0 0.5 0.4 0.3 123.0 0.2 43.0 108.0 0.1 52.0 65.0 77.0 93.0 136.0 28.0 15.0 0 110 150 170 10 20 30 40 50 60 70 80 90 100 120 130 140 160 180 Mass-to-Charge (m/z) + Scan (42.5213-42.8424 min, 55 scans) 5.D x10<sup>2</sup>\_ 151.0 0.9 0.8 0.7 0.6 0.5 166.0 0.4 0.3 123.0 0.2 0.1 65.0 77.0 43.0 108.0 136.0 0 Ó 100 120 140 160 200 220 260 20 40 60 80 180 240 280 300 Mass-to-Charge (m/z) Component RT: 42.6303 EIC Peaks Counts Counts x10<sup>6</sup> x10<sup>5</sup> 151.0 Component 166.0 151.0 1.4 5 166.0 123.0 1.2 123.0 152.0 4 НЗС 1

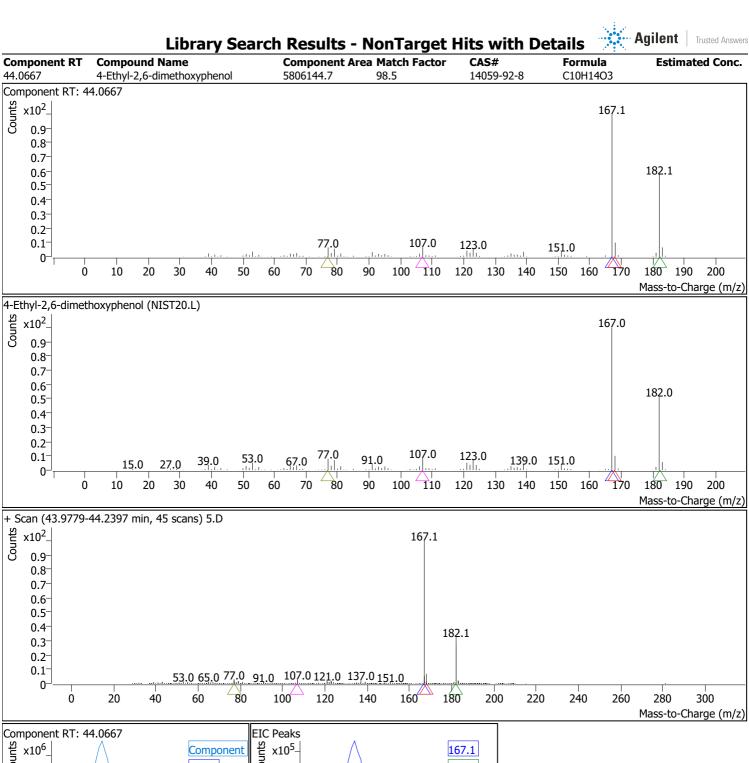


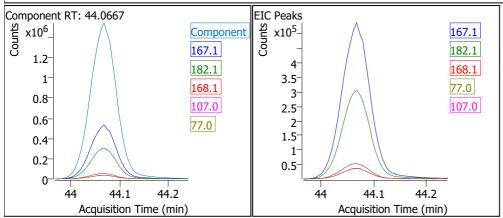


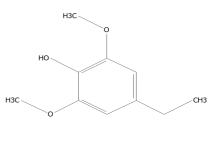












#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-44.3276 16734060.1 91.2 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3276 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 $0.2^{-}$ 122.0 43.0 0.1 77.0 66.0 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 85.0<sup>9</sup>1.0 131.0 147.0 164.0 173.0 0 100 130 180 20 30 50 60 80 110 120 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2041-44.5073 min, 52 scans) 5.D x10<sup>2</sup>. 137.1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 180.1 74.0 0.2 122.0 43.0 55.0 0.1 171.1 0 Ó 100 140 180 20 40 60 80 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3276 **EIC Peaks** Counts Counts x10<sup>6</sup> x10<sup>6</sup> 137.0 Component 180.0 137.0 3 1.4 180.0 122.0 2.5 1.2 138.0 122.0 2-1

44.3

44.4

Acquisition Time (min)

94.0

138.0

94.0

1.5

0.5

1

44.3

44.4

Acquisition Time (min)

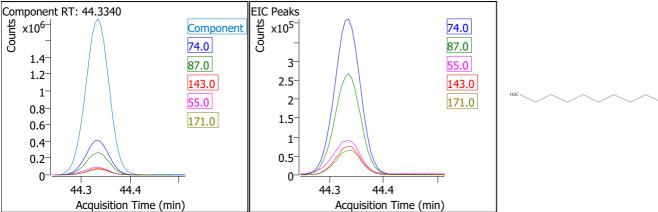
0.8

0.6

 $0.4^{-}$ 

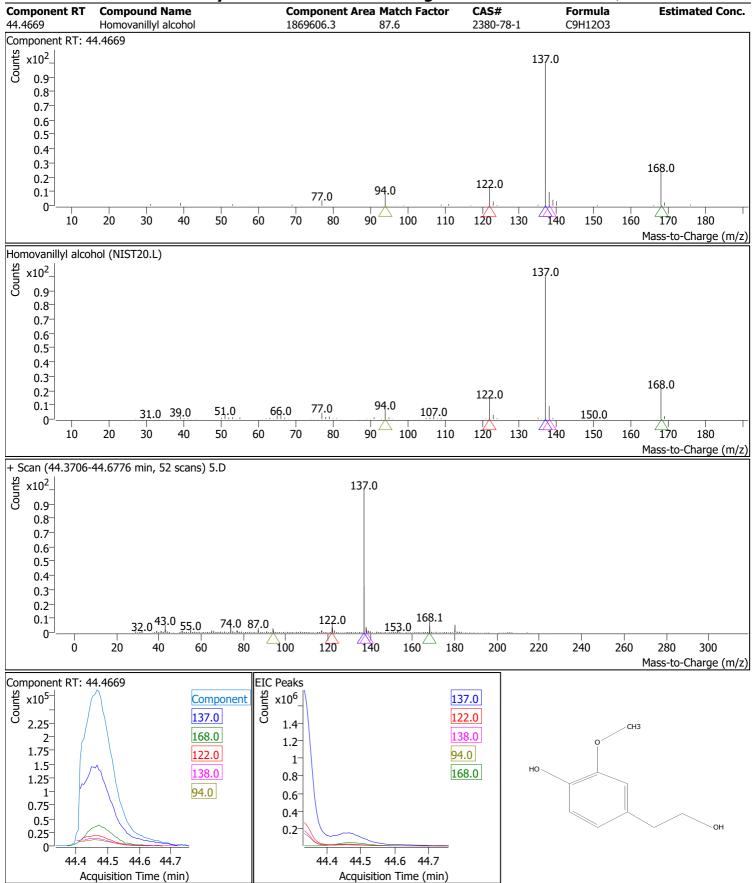
 $0.2^{-1}$ 

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3340 Dodecanoic acid, methyl ester 6278172.1 86.9 111-82-0 C13H26O2 Component RT: 44.3340 Counts $x10^{2}$ 74.0 0.9 0.8 87.0 $0.7^{-}$ 0.6 0.5 0.4 0.3 143.0 171.0 183.0 55.0 41.0 0.2 69.0 0.1 130 140 150 160 170 180 190 200 210 220 230 240 50 70 100 110 120 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10<sup>2</sup>\_ 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 <del>\_\_9</del>0 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 -10 10 20 30 40 50 60 70 80 Mass-to-Charge (m/z) + Scan (44.2457-44.5133 min, 46 scans) 5.D st x10<sup>2</sup> 0.9 137.1 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 180.1 0.2 122.0 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: 44.3340



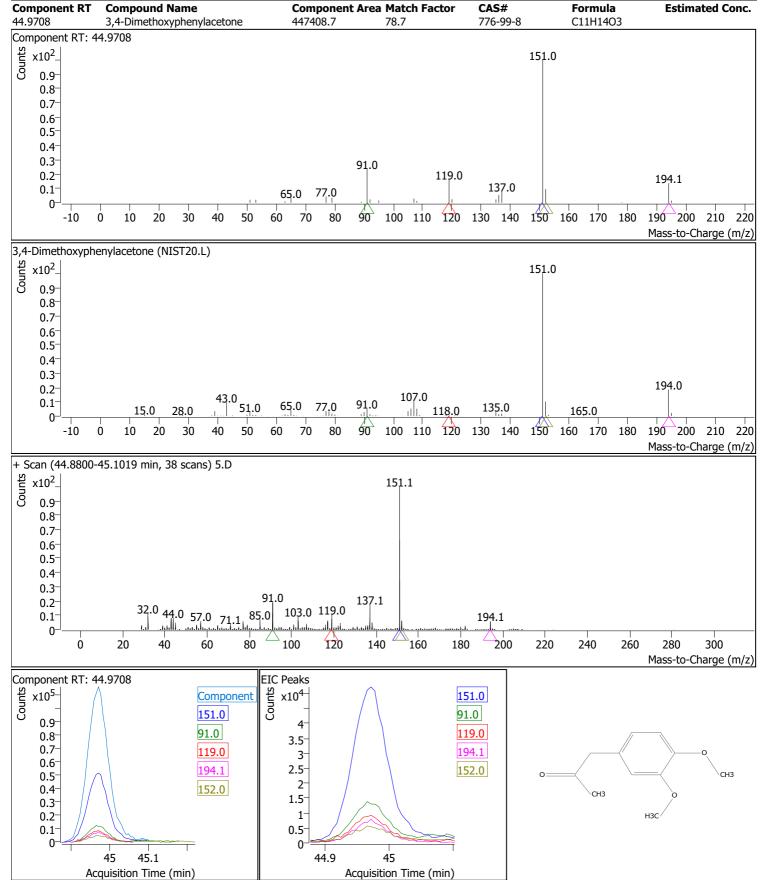












## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 45.5971 109-02-4 Morpholine, 4-methyl-458139.7 75.8 C5H11NO Component RT: 45.5971 v10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 0.4 71.0 0.3 101.0 57.0 0.2 0.1 98.0 75.0 55 100 105 10 15 20 25 30 35 60 85 95 110 Mass-to-Charge (m/z) Morpholine, 4-methyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 43.0 0.8 0.7 0.6 0.5 0.4 101.0 0.3 71.0 0.2 15.0 0.1 28.0 56.0 68.0 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 (45.5063-45.6965 min, 33 scans) 5.D st x10<sup>2</sup> 0.9 99.0 0.8 0.7 0.6 43.0 0.5 $0.4^{-}$ 0.3 117.0 0.2 55.0 0.1 29.0 130.1 164.1 181.1 91.0 20 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 45.5971 Counts Counts x10<sup>4</sup> 43.0 Component 43.0 71.0 3 71.0 57.0 6 2.5 101.0 55.0



101.0

НЗС

2-

1.5

1 0.5

45.5

45.6

45.7

Acquisition Time (min)

57.0

55.0

5

4

3 2

45.6

45.7

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3757-32-2 45.6016 Pentanoic acid, 4-oxo-, 2-methylpropyl 1035409.0 83.1 C9H16O3 Component RT: 45.6016 x10<sup>2</sup>\_ 99.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 0.3 $0.2^{-}$ 71.0 117.0 130.0 0.1 0-120 40 70 100 130 0 10 20 30 50 60 80 90 110 140 150 160 170 Mass-to-Charge (m/z) Pentanoic acid, 4-oxo-, 2-methylpropyl ester (NIST20.L) St x10<sup>2</sup> 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 0 120 40 100 130 10 20 30 50 60 70 80 90 110 140 150 160 170 Mass-to-Charge (m/z) + Scan (45.4825-45.8095 min, 56 scans) 5.D st x10<sup>2</sup> 0.9 99.0 0.8 0.7 0.6 43.0 0.5 0.4 0.3 0.2 117.0 71.0 55.0 32.0 130.1 0.1 181.1 196.1 0 Ó 40 100 120 200 260 280 20 60 80 140 160 180 220 240 300 Mass-to-Charge (m/z) Component RT: 45.6016 **EIC Peaks** Counts Counts x10<sup>4</sup>-99.0 x10<sup>5</sup> Component 99.0 43.0 7 1.6 43.0 117.0 1.4 6 1.2 117.0 71.0 5

45.7

Acquisition Time (min)

45.6

130.0

1-

0.8

0.6

0.4

45.6

45.7

Acquisition Time (min)

71.0

130.0

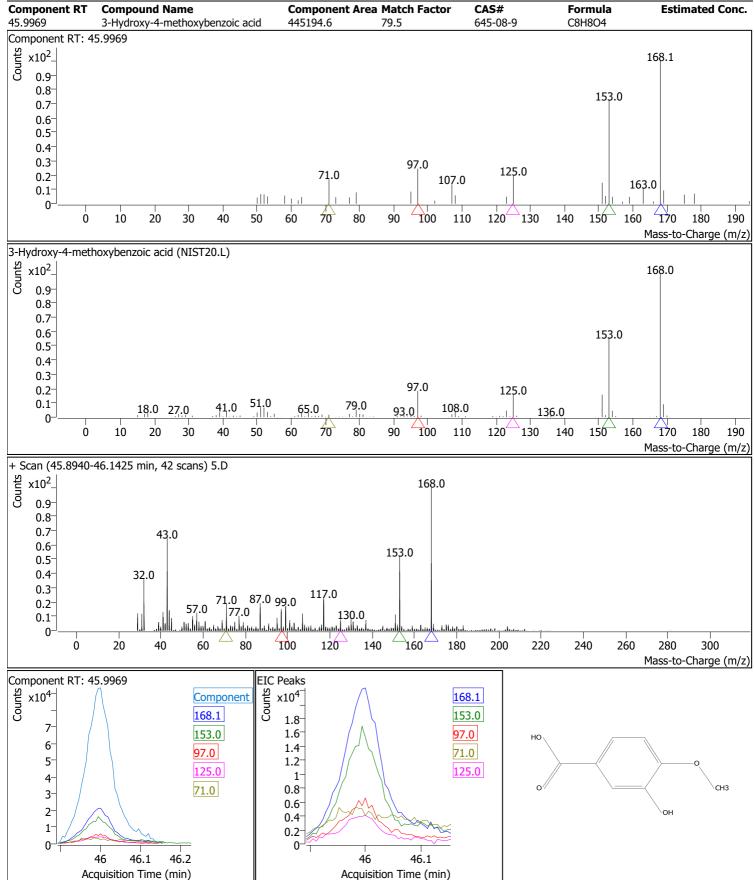
4

3

2







### **Library Search Results - NonTarget Hits with Details** --- Agilent Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 46.4911 1-Propanone, 1-(4-hydroxy-3-920678.4 92.8 1835-14-9 C10H12O3 methoxyphenyl)-Component RT: 46.4911 Counts x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 $0.2^{-}$ 123.0 0.1 108.0 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) Counts $x10^{2}$ 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 0.1 52.0 65.0 93.0 29.0 39.0 136.0 164.0 0 110 10 20 30 50 60 70 80 90 100 120 130 140 150 160 180 190 200 Mass-to-Charge (m/z) + Scan (46.3922-46.5706 min, 31 scans) 5.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 180.1 0.2 0.1 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 50 60 70 80 Mass-to-Charge (m/z) Component RT: 46.4911 **EIC Peaks** st x10<sup>5</sup>-Counts x10<sup>5</sup>-151.0 Component СНЗ 180.0 151.0 0.9 1.6 180.0 123.0 0.8

46.5

46.6

Acquisition Time (min)

152.0

108.0

1.4

1.2

0.8

0.6

0.4

0.2

46.5

46.6

Acquisition Time (min)

1

123.0

152.0

108.0

 $0.7^{-}$ 

0.6

0.5

0.4

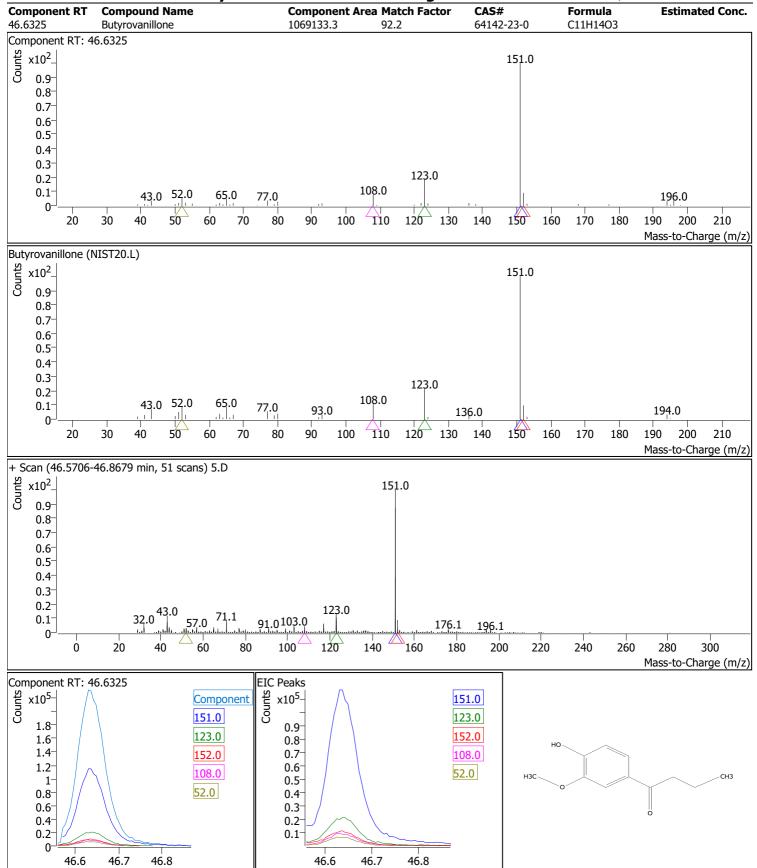
0.3

0.2

0.1







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.** 6766-82-1 47.3550 2,6-Dimethoxy-4-propylphenol 1630239.2 93.0 C11H16O3 Component RT: 47.3550 $x10^{2}$ 167.1 0.9 0.8 0.7 0.6 0.5 0.4 196.1 0.3 0.2 151.0 0.1 123.0 77.0 106.0 190 200 120 130 140 150 160 170 10 20 50 60 70 90 100 110 Mass-to-Charge (m/z) 2,6-Dimethoxy-4-propylphenol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 167.0 0.8 0.7 0.6 0.5 0.4 0.3 196.0 0.2 0.1 77.0 53.0 29.0 39.0 106.0 91.0 151.0 181.0 120 130 140 150 160 170 180 190 200 10 20 50 60 70 80 90 100 110 Mass-to-Charge (m/z) + Scan (47.2731-47.5398 min, 45 scans) 5.D st x10<sup>2</sup> 0.9 167.1 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 196.1 0.2

151.1

160

140

123.0

120

176.1

180

167.1

196.1

168.1

151.0

123.0

200

220

**H3C** 

HO

нзс

240

260

280

300 Mass-to-Charge (m/z)

-CH3

0.1

X10<sup>5</sup>

3.5

2.5

1.5

0.5

3

2

1

47.3

Ó

Component RT: 47.3550

20

47.4

Acquisition Time (min)

32.043.0 57.0

47.5

60

Component 167.1

196.1

168.1

151.0

123.0

40

77.0 91.0103.0

Counts x10<sup>5</sup>

100

EIC Peaks

1.4

1.2

0.8

0.6

0.4

0.2

47.3

1

80

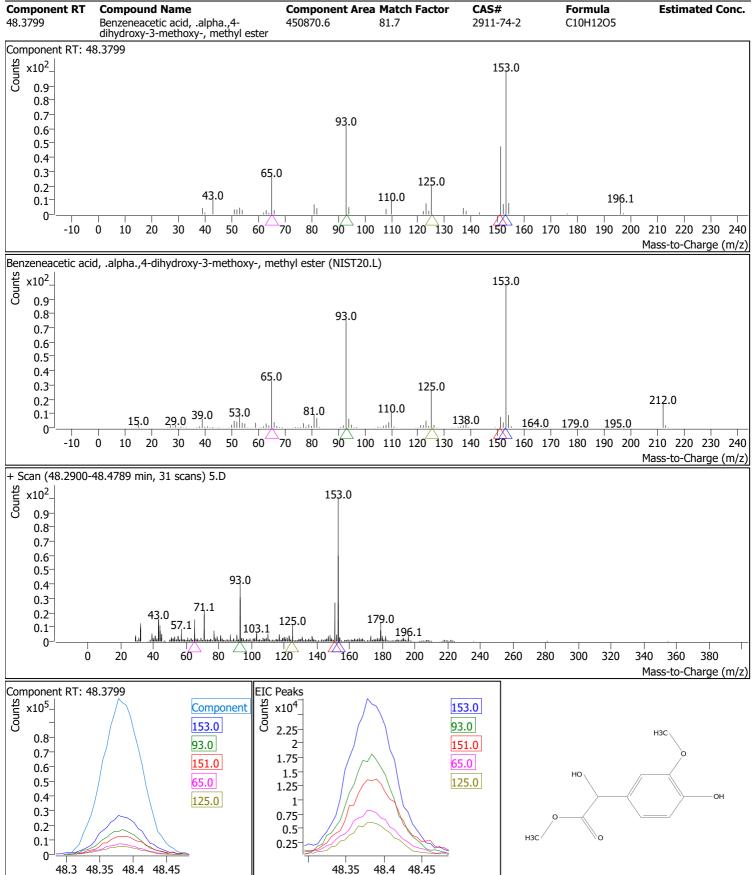
47.4

Acquisition Time (min)

47.5

# **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.** 2305-13-7 48.9878 Benzenepropanol, 4-hydroxy-3-6476909.6 96.6 C10H14O3 methoxy-Component RT: 48.9878 x10<sup>2</sup>\_ 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 60 70 80 90 100 110 120 130 150 160 170 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 0.2 122.0 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 (48.8717-49.2047 min, 57 scans) 5.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 182.1 0.3 0.2 65.0 77.0 91.0 107.0 $^{122.0}$ 0.1 31.0 43.0 149.0 0 Ó 40 100 140 180 260 20 60 80 120 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 48.9878 **EIC Peaks** Counts Counts x10<sup>6</sup> x10<sup>5</sup> 137.0 Component 137.0 182.1 182.1 3-138.1 1 2.5 138.1 122.0 0.8 122.0 2 123.0



0.6

0.4

0.2

48.9

49

49.1

Acquisition Time (min)

123.0

1.5

0.5

1

48.9

49

49.1

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 49.3686 Benzaldehyde, 4-hydroxy-3,5-2353548.5 96.0 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3686 x10<sup>2</sup>\_ 182.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 111.0 167.0 96.0 139.0 65.0 0.1 79.0 0-0 10 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 190 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 0.2 167.0 139.0 65.0 93.0 39.0 51.0 79.0 0.1 15.0 29.0 153.0 123.0 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 (49.2782-49.5927 min, 53 scans) 5.D x10<sup>2</sup>\_ 182.0 0.9 0.8 0.7 0.6 0.5 131.0 194.1 0.4 0.3 0.2 159.0 $96.0_{\,111.0}$ 77.0 0.1 32.0 51.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) Component RT: 49.3686 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup> 182.0 Component 0 181.0 182.0 4 1.2 181.0 111.0 3.5 1 111.0 167.0 3 0.8 2.5 167.0 183.0

49.4

49.5

Acquisition Time (min)

0.6

0.4

0.2

183.0

2

1

49.4

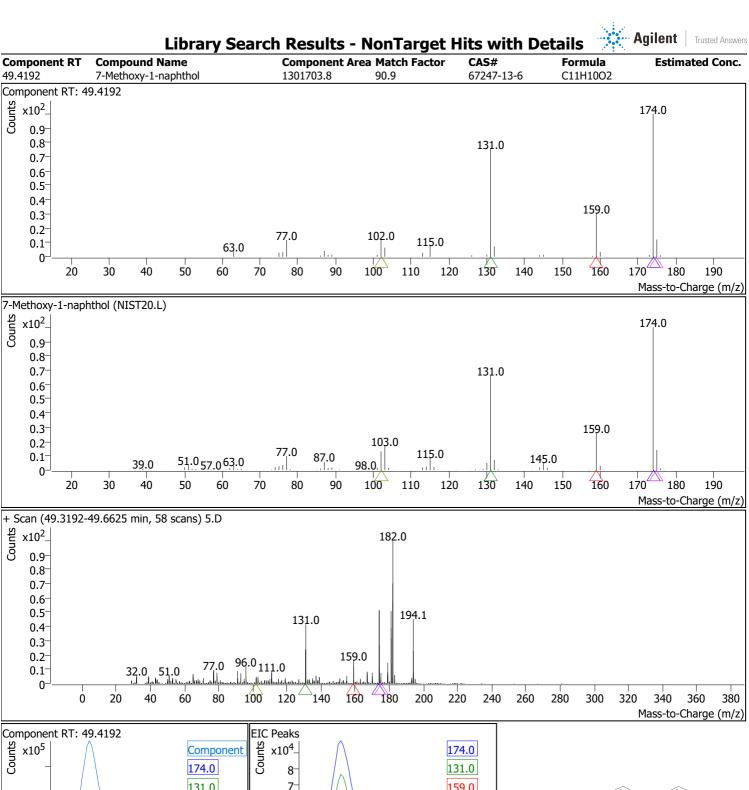
49.5

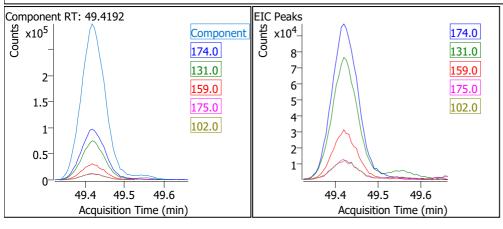
Acquisition Time (min)

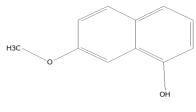
1.5

0.5

ОΉ

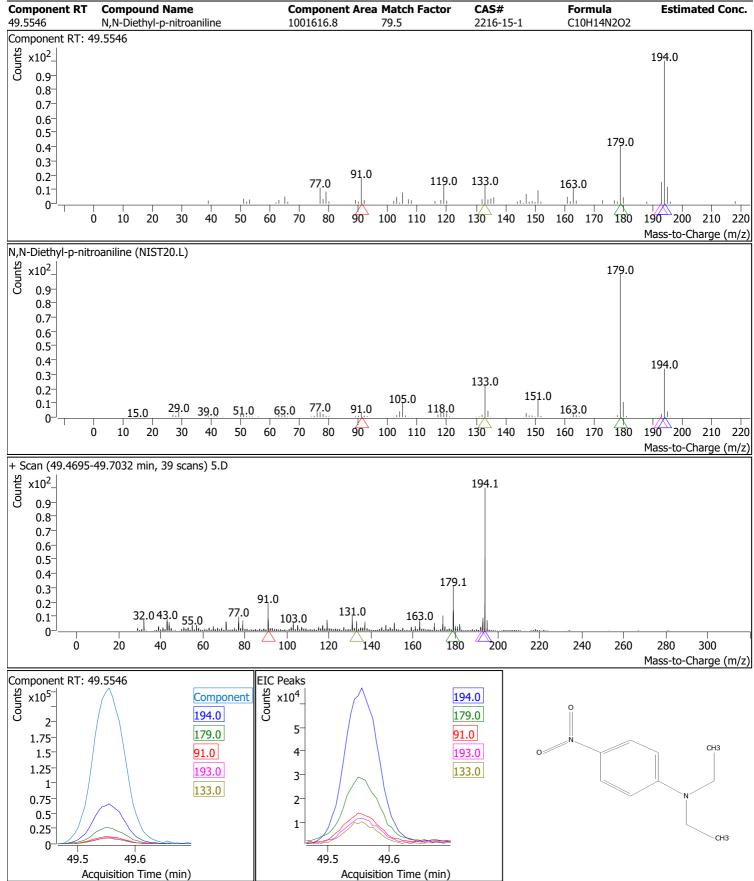






# **Library Search Results - NonTarget Hits with Details**





#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 49.5546 2-Propenoic acid, 3-(4-hydroxy-3-1007538.9 80.3 1135-24-6 C10H10O4 methoxyphenyl) Component RT: 49.5546 x10<sup>2</sup>\_ 194.1 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 $0.2^{-}$ 119.0 133.0 77.0 163.0 0.1 0-180 10 20 30 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 179.0 133.0 0.2 77.0 105.0 0.1 18.0 28.0 63.0 89.0 123.0 149,0 164.0 0 130 140 180 20 30 50 60 70 80 90 100 110 120 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4698-49.7032 min, 39 scans) 5.D x10<sup>2</sup>\_ 194.1 0.9 0.8 0.7 0.6 0.5 0.4 179.1 0.3 91.0 0.2 32.043.0 55.0 131.0 77.0 163.0 0.1 103.0 n 180 Ó 20 40 60 80 100 120 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.5546 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>4</sup> 194.1 Component 179.0 194.1 CH3 2 5 179.0 91.0 1.75 91.0 4 193.0 1.5 НО

49.6

Acquisition Time (min)

133.0

1.25

0.75

0.5

49.5

49.6

Acquisition Time (min)

1

193.0

133.0

3-

2-

49.5

ОН

# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 50.6433 Phenylacetylformic acid, 4-hydroxy-3- 483869.0 76.0 1081-71-6 C10H10O5 methoxy-Component RT: 50.6433 Counts x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 210.1 0.3 164.1 $0.2^{-}$ 193.0 71.0 149.0 91.0 122.0 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 -10 10 20 50 60 90 Mass-to-Charge (m/z) Phenylacetylformic acid, 4-hydroxy-3-methoxy- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 0.4 210.0 0.3 0.2 164.0 0.1 65.0 77.0 51.0 107.0 28.0 149.0 0 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 10 20 70 80 Mass-to-Charge (m/z) + Scan (50.5069-50.7060 min, 34 scans) 5.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 71.0 0.6 0.5 0.4 32.0 0.3 210.1 43.0 164.1 117.0 193.0 0.2 77.0 91.0 57.0 149.0 179.0 0.1 0 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 50.6433 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>5</sup> 137.0 Component 71.0 137.0 2.25 0.8 2 210.1 210.1 $0.7^{-1}$ 1.75

50.6

Acquisition Time (min)

193.0

164.1

50.7

НЗС

0.6

0.5

0.4

0.3

0.2

0.1

50.6

Acquisition Time (min)

164.1

193.0

71.0

50.7

1.5

1.25

0.75

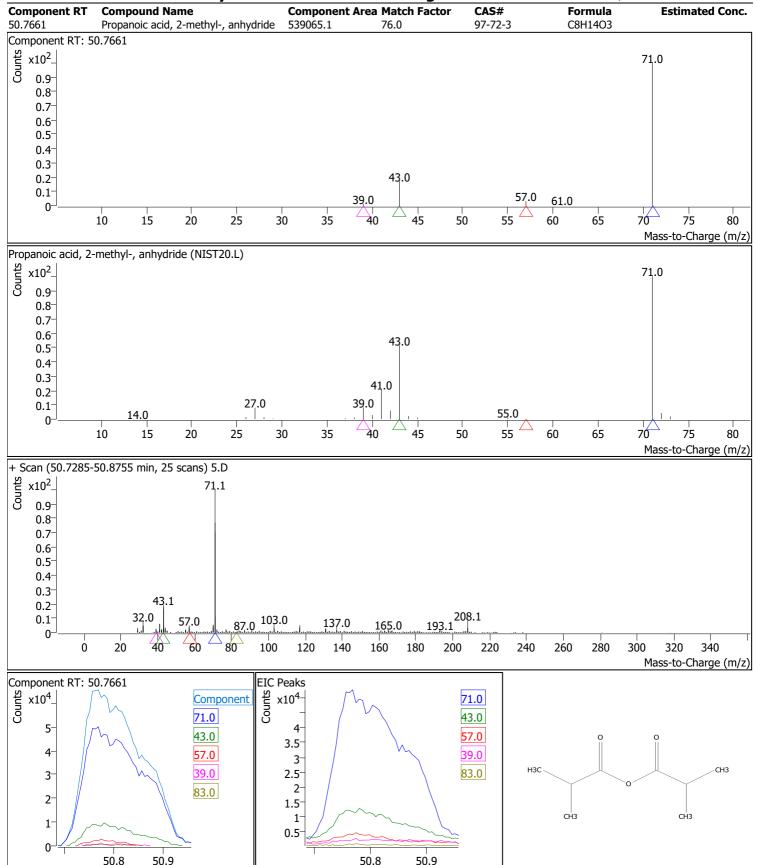
0.5

0.25

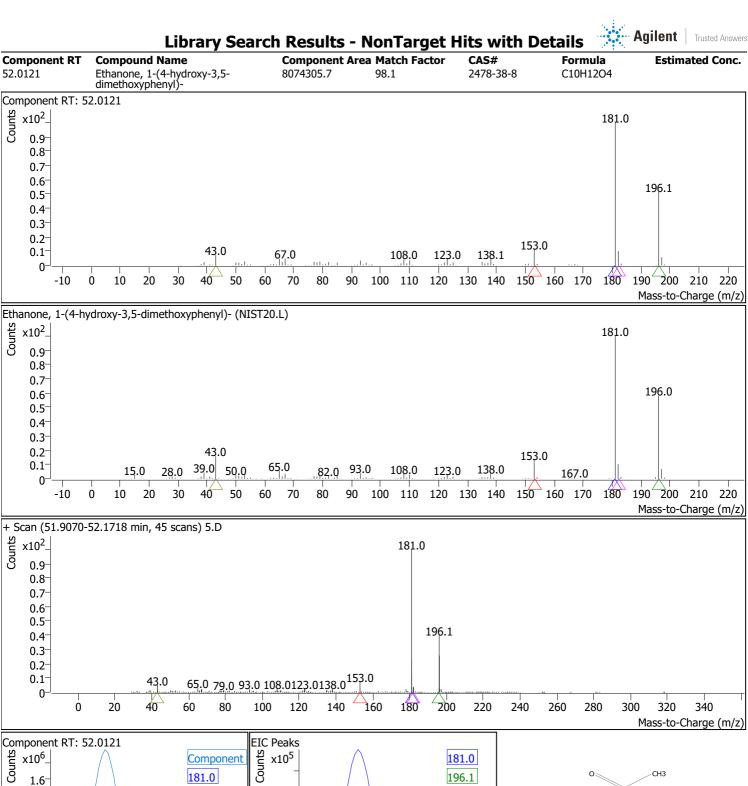
1

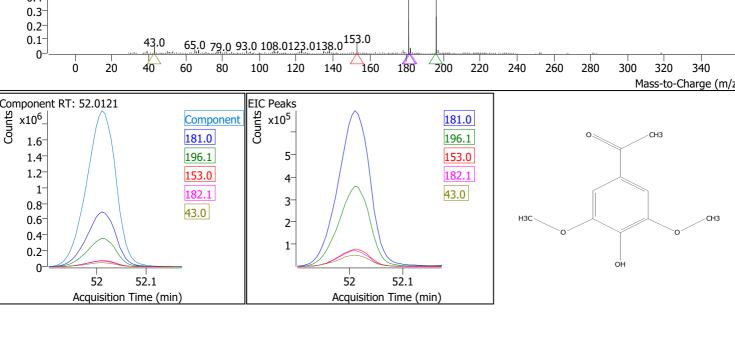


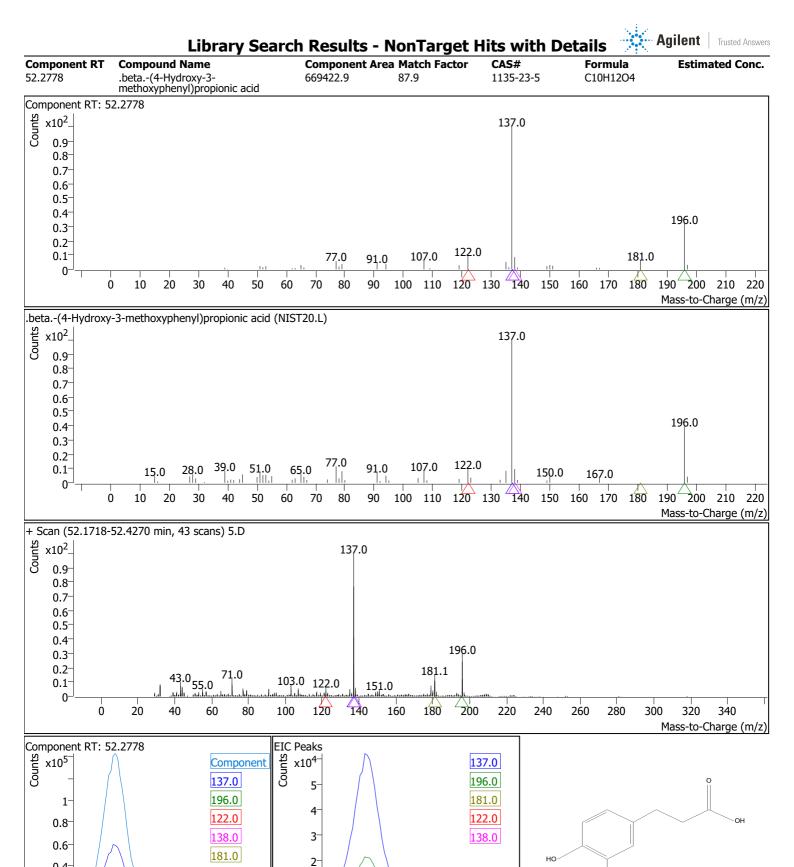




Acquisition Time (min)







52.3

52.4

Acquisition Time (min)

0.4

52.2

52.3

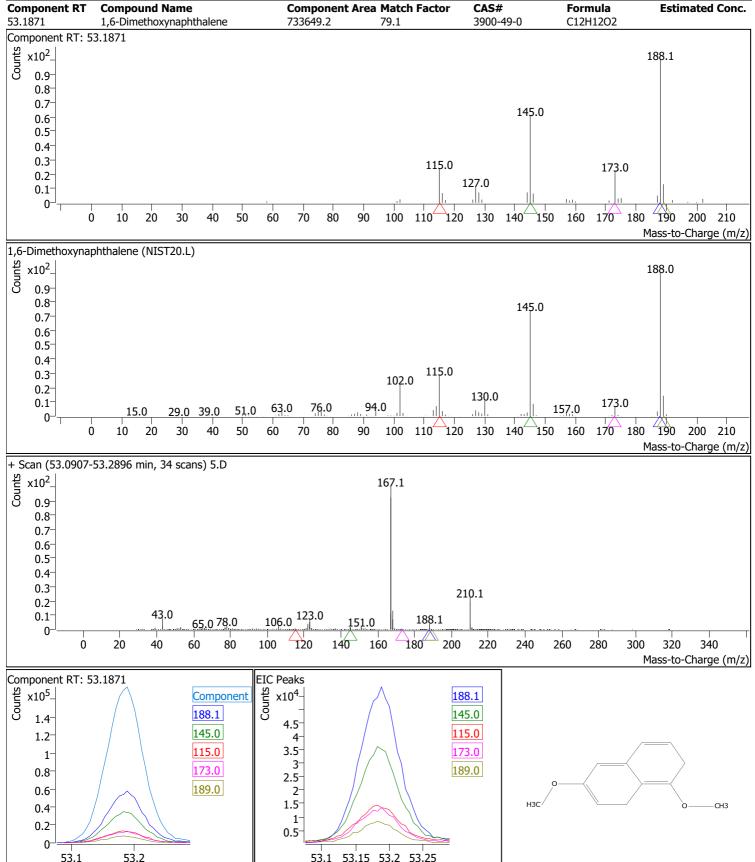
52.4

Acquisition Time (min)

СНЗ



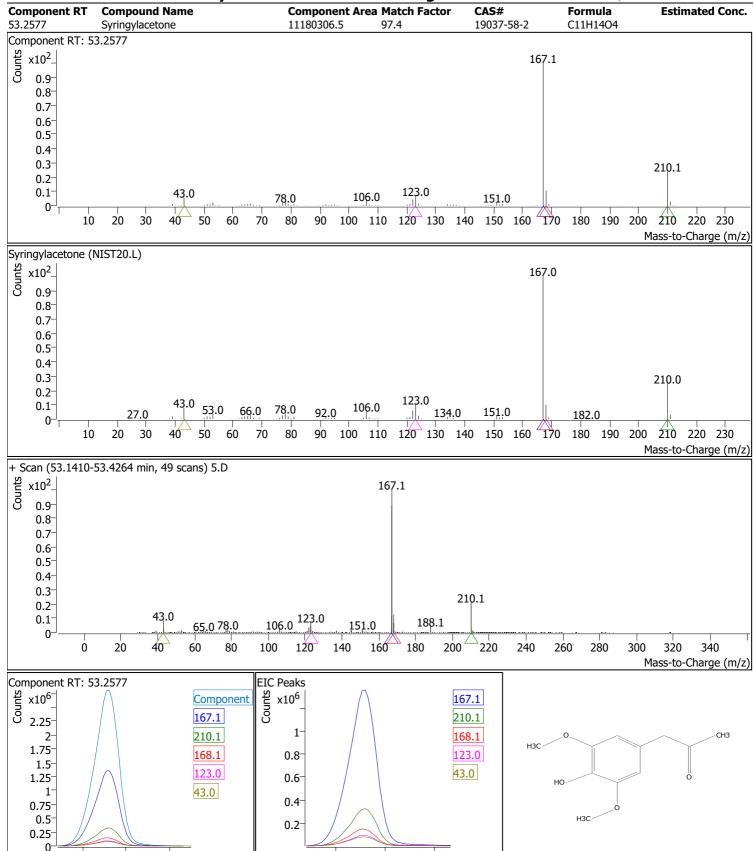




Acquisition Time (min)







Acquisition Time (min)

53.4

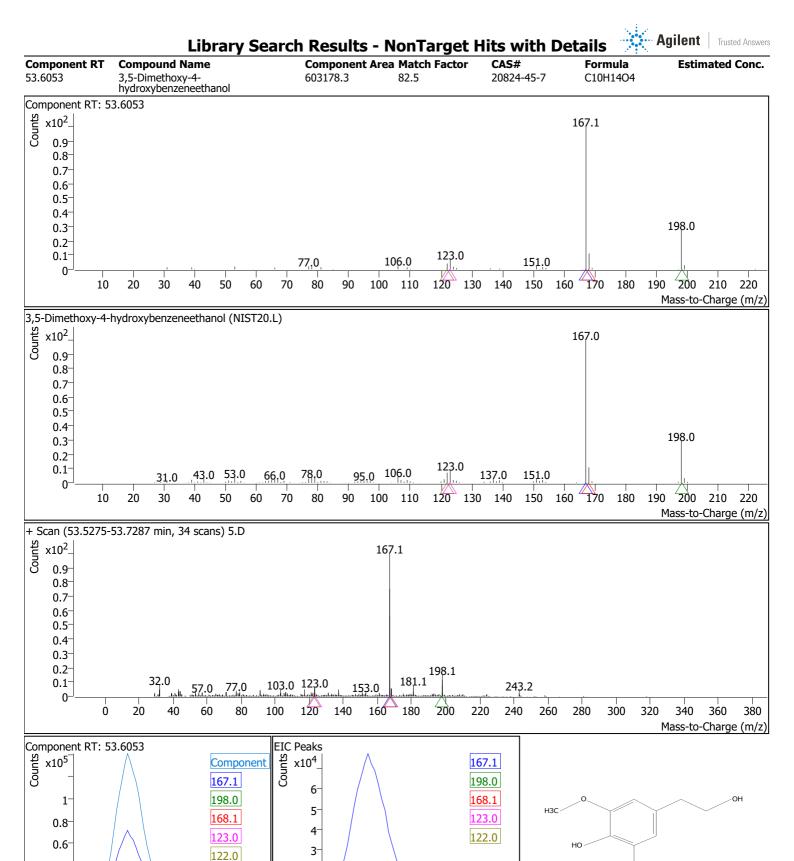
53.2

53.2

53.3

Acquisition Time (min)

53.4



53.7

Acquisition Time (min)

2-

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)-55.2315 1486376.3 92.3 5650-43-1 C11H14O4 Component RT: 55.2315 x10<sup>2</sup>\_ 181.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 210.0 $0.2^{-}$ 153.0 0.1 108.0 67.0 123.0 138.0 224.0 0 150 160 170 180 190 200 210 220 230 10 20 30 50 60 70 80 90 100 110 120 130 140 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 67.0 93.0 138.0 53.0 82.0 29.0 39.0 166.0 0 120 130 140 150 160 170 180 190 200 210 220 230 10 20 30 50 60 70 80 90 100 110 Mass-to-Charge (m/z) + Scan (55.0972-55.4421 min, 59 scans) 5.D x10<sup>2</sup>\_ 181.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 210.1 103.0 137.0153.0 0.1 43.0 67.0 n 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) Component RT: 55.2315 **EIC Peaks** Counts Counts x10<sup>5</sup>\_ x10<sup>5</sup>-181.0 Component 181.0 210.0 1 2 -CH3 210.0 182.0 1.75 0.8 182.0 153.0 H3C 1.5

55.2

55.3

Acquisition Time (min)

55.4

153.0

123.0

0.6

 $0.4^{\circ}$ 

0.2

1.25

0.75 0.5

0.25

55.2

55.3

Acquisition Time (min)

55.4

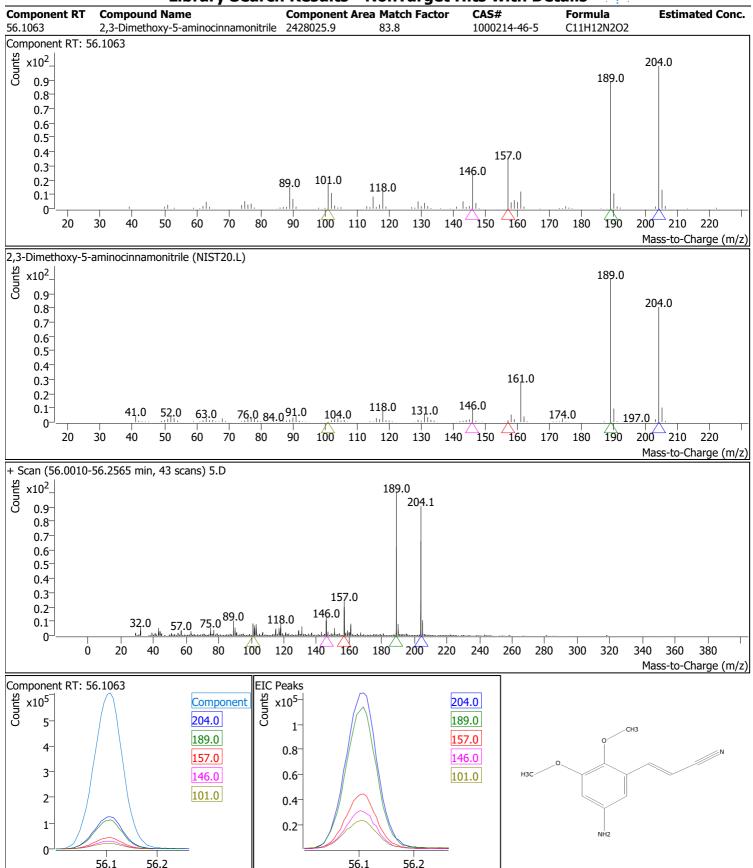
123.0

-OH

-CH3

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

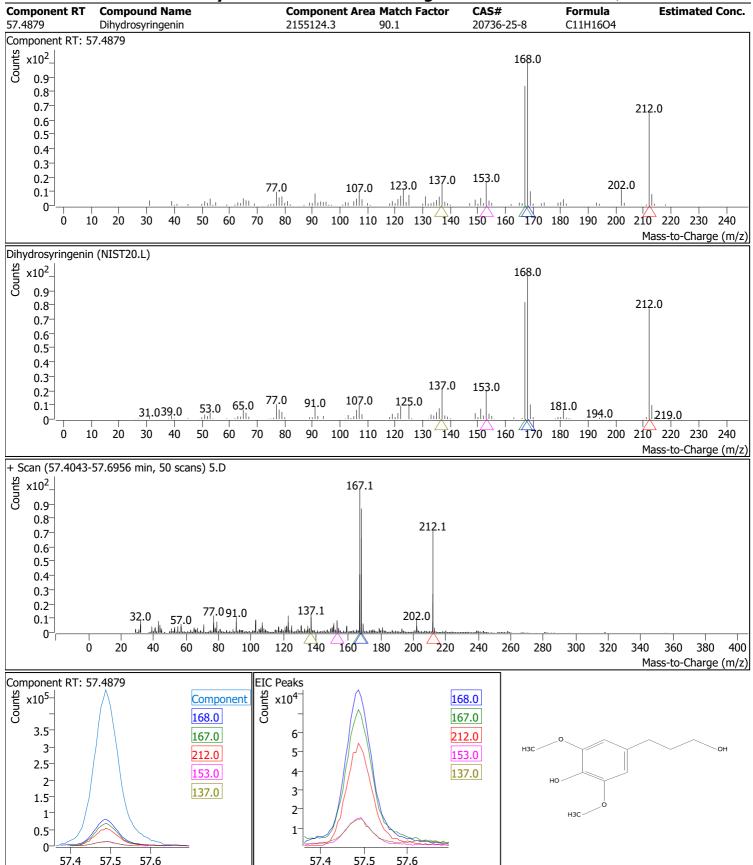




Acquisition Time (min)







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.** 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol 57.4879 2150845.1 89.6 63543-12-4 C11H16O4 Component RT: 57.4879 x10<sup>2</sup>\_ 168.1 0.9 8.0 0.7 212.1 0.6 0.5 0.4 0.3 153.0 $0.2^{-}$ 137.0 123.0 202.1 77.0 107.0 0.1 . طالت ب 0-100 110 120 130 140 150 160 170 180 190 10 20 30 50 60 80 90 200 210 220 230 240 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 (57.4043-57.6956 min, 50 scans) 5.D x10<sup>2</sup>. 167.1 0.9 0.8 212.1 0.7 0.6 0.5 0.4 0.3 0.2 77.091.0 137.1 202.0 32.0 57.0 0.1 0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 340 360 380 400 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 57.4879 Counts Counts x10<sup>5</sup>x10<sup>4</sup> 168.1 Component 168.1 167.1 3.5 6 167.1 212.1 3 5 212.1 153.0 2.5

57.5

57.6

Acquisition Time (min)

137.0

4

3

2

57.4

153.0

137.0

2

0.5

57.5

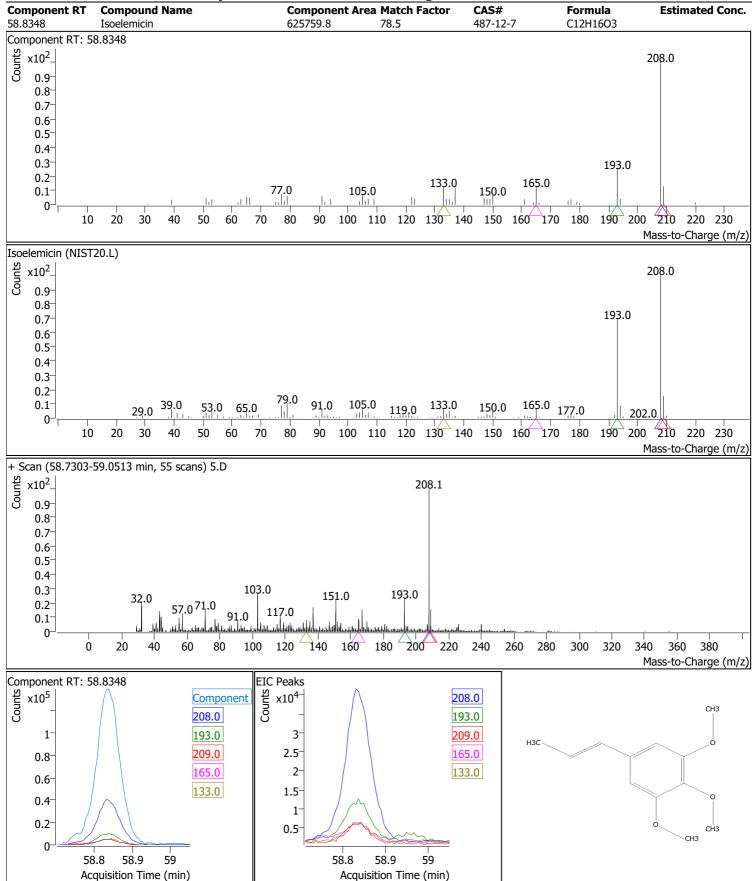
57.6

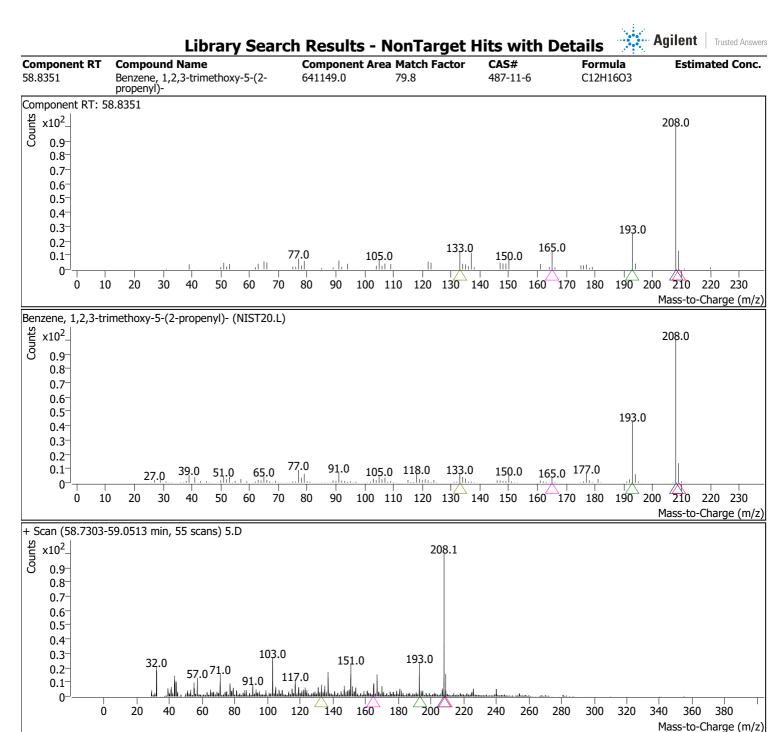
Acquisition Time (min)

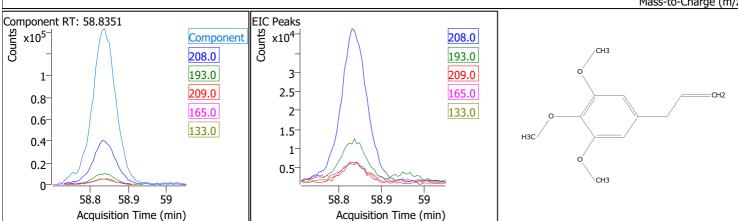
1.5











### **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 66.3352 (E)-9-Octadecenoic acid ethyl ester 1251163.7 89.2 6114-18-7 C20H38O2 Component RT: 66.3352 v10<sup>2</sup> 0.9 55.0 0.8 69.0 88.0 $0.7^{-}$ 41.0 0.6 0.5 0.4 0.3 0.2 0.1 0 20 40 80 100 120 140 180 200 220 260 280 300 320 340 Mass-to-Charge (m/z) (E)-9-Octadecenoic acid ethyl ester (NIST20.L) st x10<sup>2</sup>\_ 0.9-55.0 69.0 0.8 0.7 83.0 97.0 0.6 41.0 0.5 0.4 111.0 264.0 0.3 222.0 0.2 123.0 29.0 180.0 155.0 310.0 0.1 201.0 235.0 281.0 20 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) + Scan (66.2577-66.4300 min, 29 scans) 5.D St x10<sup>2</sup> 0.9 55.0 43.0 0.8 117.0 $0.7^{-}$ 101.0 0.6 167.1 83.1 0.5 181.0 $0.4^{-}$ 137.0 264.2 0.3 29.0 0.2 0.1 20 40 TDO 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 -20 Mass-to-Charge (m/z) Component RT: 66.3352 **EIC Peaks** Counts x10<sup>5</sup> Counts x10<sup>4</sup> 55.0 Component 55.0 69.0 1.8 2.5 69.0 88.0 1.6 2 88.0 1.4 83.0

66.3

Acquisition Time (min)

97.0

66.4

1.2

0.8

0.6

0.2

66.2

1

83.0

97.0

66.4

1.5

1

0.5

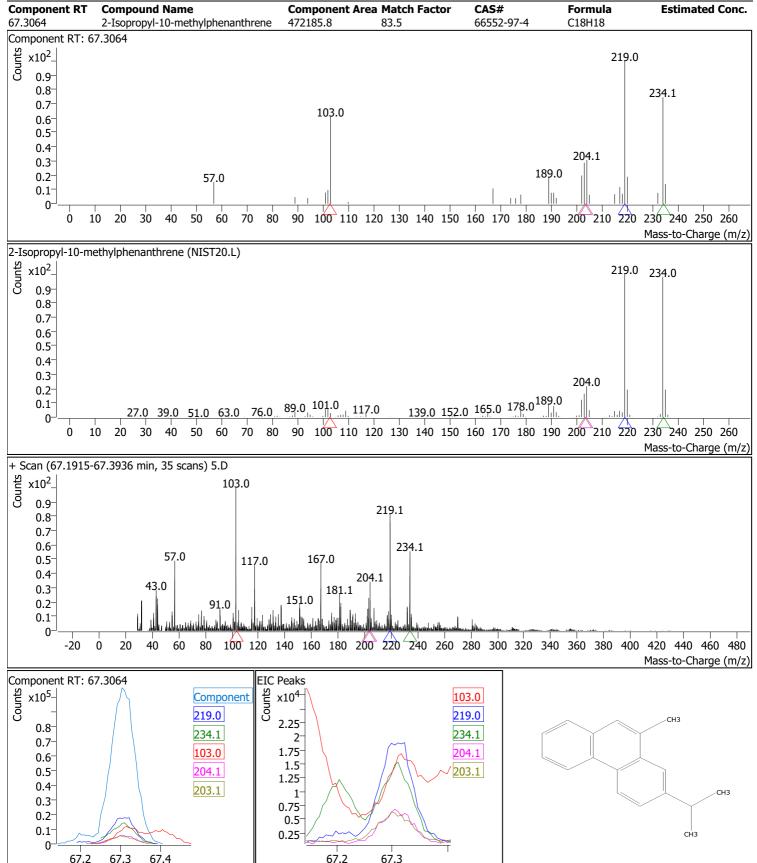
0

66.2

66.3

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

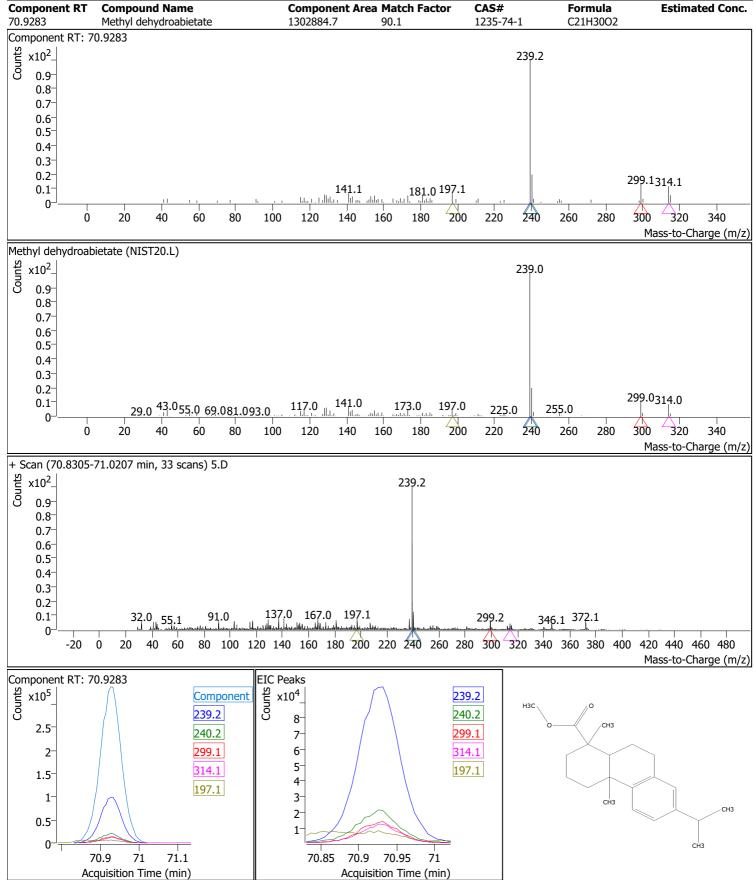




Acquisition Time (min)

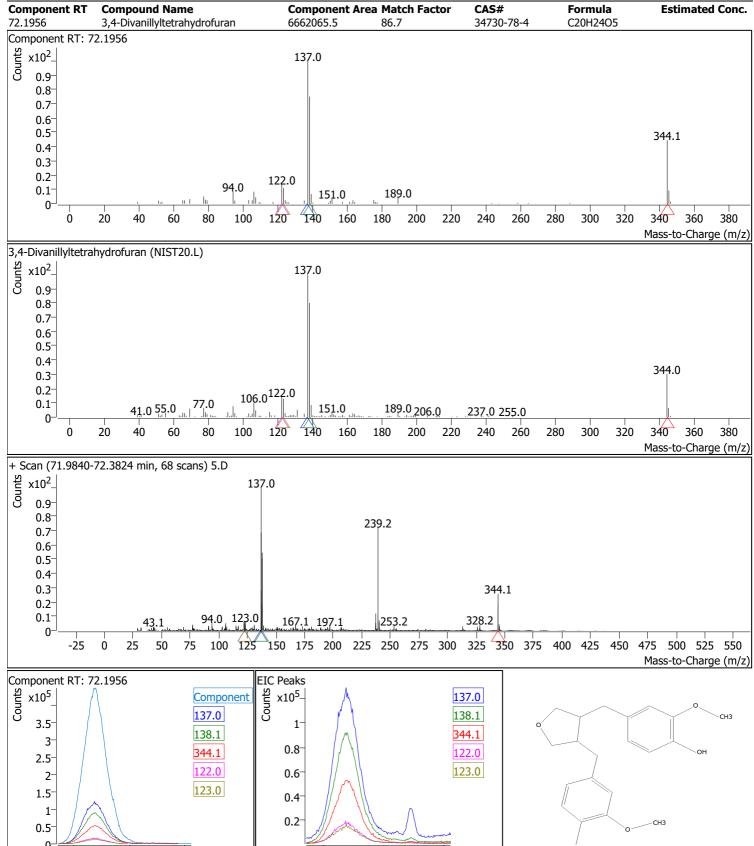












Acquisition Time (min)

73

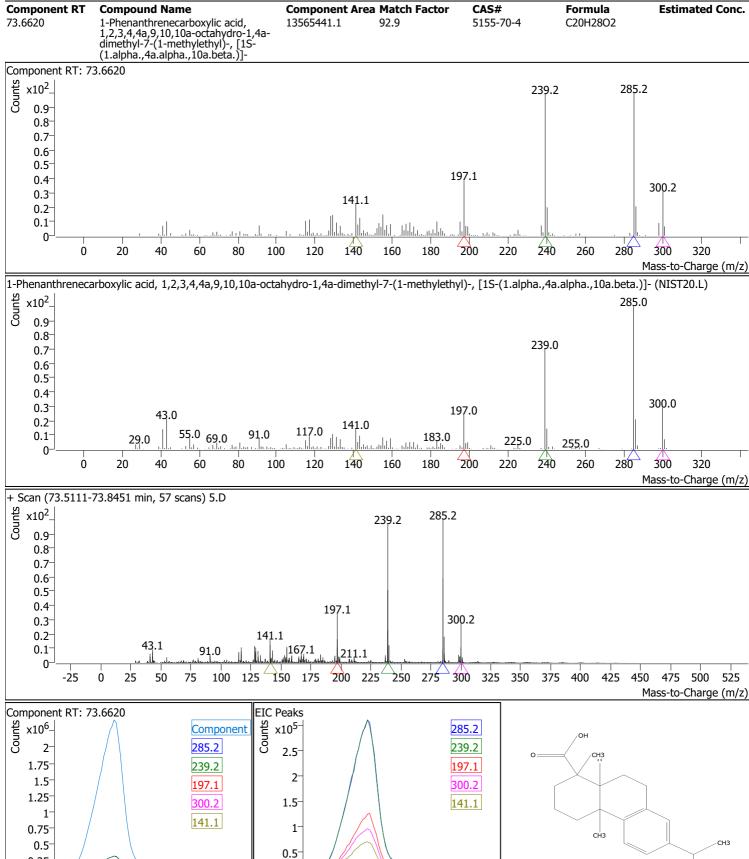
72

72

72.5

Acquisition Time (min)

73



Acquisition Time (min)

73.6

73.8

0.25

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 75.9073 873882.8 81.0 22318-87-2 C18H22O4 Component RT: 75.9073 $x10^{2}$ 151.0 0.9 0.8 $0.7^{\circ}$ 0.6 0.5 0.4 0.3 0.2 302.0 65.077.0 91.0 108.0123.0 0.1 60 100 120 300 -20 20 40 140 160 180 200 220 240 260 280 320 340 Mass-to-Charge (m/z) 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether (NIST20.L) x10<sup>2</sup>\_ 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 0.1 165.0 181.0196.0211.0226.0241.0256.0 300 20 120 180 200 220 240 260 320 340 -20 40 60 80 100 140 160 280 Mass-to-Charge (m/z) + Scan (75.8132-76.0291 min, 37 scans) 5.D Counts x10<sup>2</sup>\_ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 181.0 207.0 0.2 137.0 43.0 0.1 69.1 91.0 302.1 150 300 325 350 375 125 175 200 225 250 275 400 425 475 500 525 550 -25 0 25 50 100 450 Mass-to-Charge (m/z) Component RT: 75.9073 EIC Peaks Counts v10<sup>5</sup> x10<sup>5</sup>-151.0 Component 151.0 152.0 1 302.0 91.0 1.4 0.8 1.2 302.0 152.0 1 123.0 91.0 0.6 0.8

75.9

76

Acquisition Time (min)

123.0

 $0.4^{-}$ 

0.2

75.8

0.6

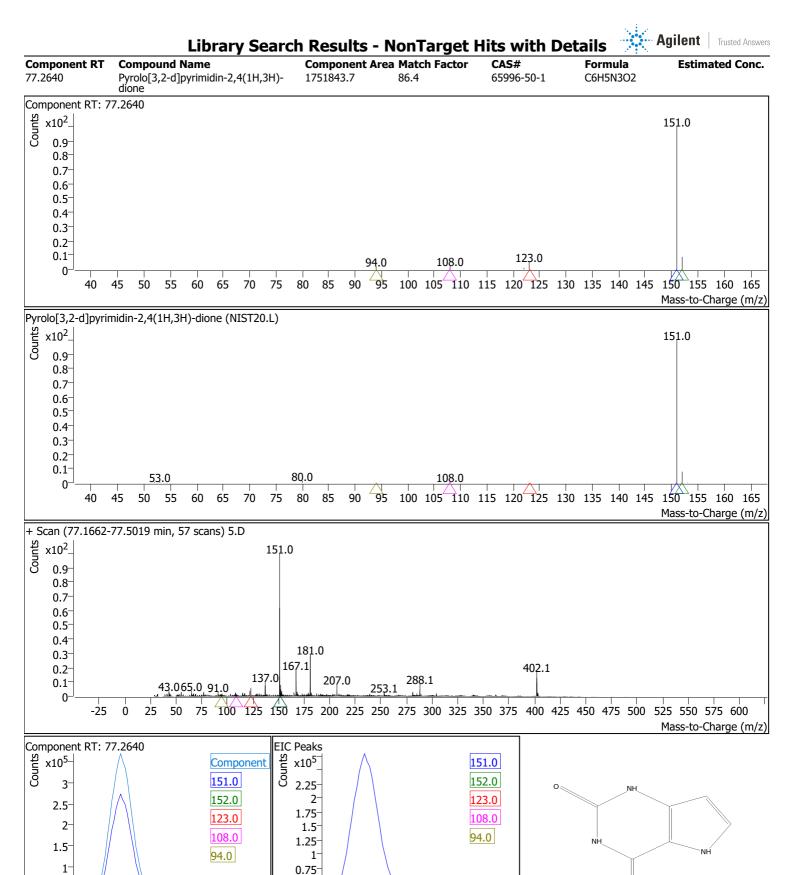
0.4

0.2

75.8

75.9

76



0.25

77.2

77.3

77.4

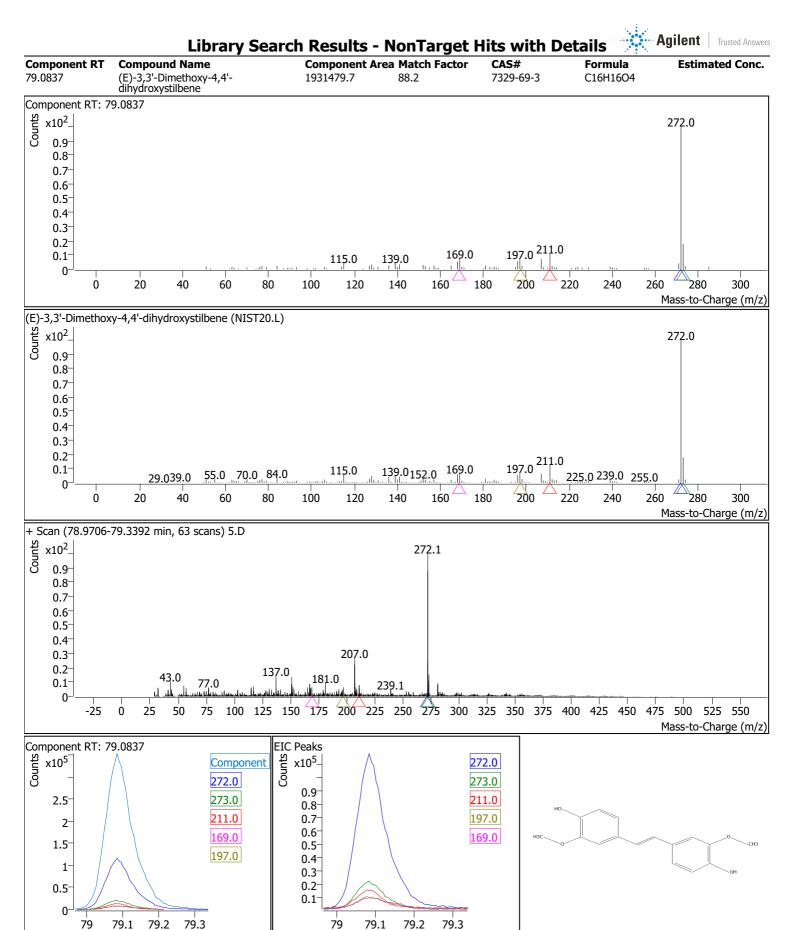
Acquisition Time (min)

0.5

77.2

77.3

77.4



Acquisition Time (min)