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

Dil.



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

**File Name** 4.D **Sample Name** Acq. Method File

240501 scan Acq. Date-Time 5/1/2024 6:09:15 PM

**Instrument Name GCMSD**  **Path Name** D:\MassHunter\GCMS\1\data\RBEL\240501 scan **Sample Type** Sample Acq. Method Path

1

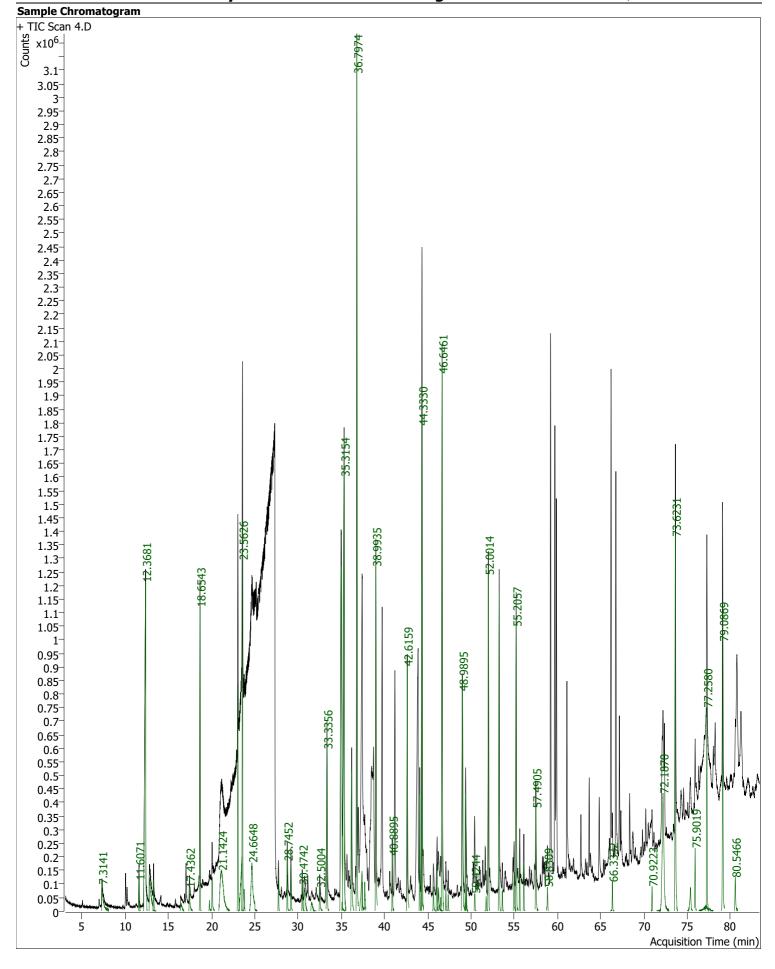
D:\MassHunter\GCMS\1\methods\RBEL\ Acq. Operator

Component R	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
7.3141	1,3-Propanediol	504-63-2	C3H8O2	1202732.8	94.8	
11.6071	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	528254.6	82.0	
12.3681	Butyrolactone	96-48-0	C4H6O2	10540151.4	96.8	
12.8058	Methyltartronic acid	595-98-2	C4H6O5	1691916.6	94.9	
13.2899					78.3	
	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	532351.4		
16.4719	2,2-Dimethyl-2-sila-1,3-dioxacyclohexane	14879-83-5	C5H12O2Si	309458.3	77.2	
17.4362	Silane, diethoxydimethyl-	78-62-6	C6H16O2Si	544676.0	75.3	
18.6543	Diisoamyl ether	544-01-4	C10H22O	4244738.5	98.2	
19.7524	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	167867.0	85.4	
20.0568	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	658804.5	95.3	
21.1424	1,3,5-Trioxane	110-88-3	C3H6O3	4088997.3	81.6	
23.0353	1-Octanol	111-87-5	C8H18O	3434766.0	98.7	
23.5037	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	2002503.1	92.6	
23.5626	Phenol, 2-methoxy-	90-05-1	C7H8O2	5846632.4	97.9	
23.7721	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-	21835-00-7	C7H10O2	319272.0	78.5	
24.6648	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	2725027.1	91.7	
27.7300	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	521798.4	82.1	
28.7452	Naphthalene	91-20-3	C10H8	774394.9	97.5	
29.1709	Creosol	93-51-6	C8H10O2	734304.1	96.7	
30.4742			C4H8O2		79.1	
	1,3-Dioxane	505-22-6		454800.7		
30.7369	Catechol	120-80-9	C6H6O2	876657.4	93.0	
31.5746	5-Hydroxymethylfurfural	67-47-0	C6H6O3	360007.4	82.3	
32.5004	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	520439.7	95.2	
33.3356	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	2515777.9	97.4	
34.9749	2,3-dihydroxypropyl isobutyrate	1010458-45-6	C7H14O4	12232779.8	78.5	
35.0843	Phenol, 5-ethenyl-2-methoxy-	621-58-9	C9H10O2	202572.3	82.6	
35.3154	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	11843195.3	78.6	
35.3163	Butanoic acid, anhydride	106-31-0	C8H14O3	11248701.5	79.7	
36.1877	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	2781061.4	82.1	
36.7974	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	12715578.1	99.1	
37.3896	Ethylamine, 2-((p-bromoalphamethylalpha	3565-72-8	C18H22BrNO	1629293.7	75.7	
	phenylbenzyl)oxy)-N,N-dimethyl-					
37.4168	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	394237.8	78.1	
37.7057	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	475586.9	78.5	
38.9935	Vanillin	121-33-5	C8H8O3	5678104.3	98.5	
40.8895	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	847530.0	93.6	
42.6159	Apocynin	498-02-2	C9H10O3	4014973.2	99.2	
44.0555	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	1629043.1	97.5	
44.2950	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	5445870.8	94.2	
44.3330	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6342821.8	95.2	
45.6451	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	435378.6	81.3	
46.0653	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	936058.2	92.6	
46.2195	Oxazolidin-2-one	497-25-6	C3H5NO2	634933.3	80.5	
46.2202	3-Pentanol, 2,2,4,4-tetramethyl-	14609-79-1	C9H20O	744700.7	78.0	
46.4841	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	210231.0	81.4	
46.6461	, = , = , , , ,	64142-23-0				
	Butyrovanillone		C11H14O3	8738295.8	89.8	
47.0820	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	306538.1	76.4	
47.3540	Homosyringaldehyde	87345-52-6	C10H12O4	224103.1	82.6	
48.9895	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	5515590.4	96.4	
49.3613	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2047327.7	96.5	
49.4171	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	307367.8	84.8	
49.4533	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	449347.7	82.9	
50.4244	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	321466.5	91.8	
51.7398	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	4899-74-5	C10H12O4	212350.2	89.7	
52.0014	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	5359990.6	98.5	
53.2410	Syringylacetone	19037-58-2	C11H14O4	4823009.2	97.3	
53.6141	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	276859.3	75.6	
54.9715	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	733657.1	88.0	
55.2057 FF 6331	Butylsyringone	69271-91-6	C12H16O4	4574151.5	93.0	
55.6221	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	700159.4	89.0	
56.0995	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	712035.6	79.3	
57.4905	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	1812481.3	92.3	
58.8309	Isoelemicin	487-12-7	C12H16O3	404594.3	77.8	
66.3332	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C20H38O2	421940.8	78.5	

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

Agilent	Trusted Answers
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Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
70.9223	Methyl dehydroabietate	1235-74-1	C21H30O2	359827.9	75.8	
72.1870	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6222168.8	88.7	
73.6231	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	6817161.6	93.1	
75.3519	Undecane, 4-cyclohexyl-	13151-79-6	C17H34	739647.2	77.0	
75.9019	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	1003347.8	80.1	
77.0919	8-Benzylquinoline	28748-19-8	C16H13N	604940.0	84.3	
77.2580	.alphaAmino-3'-hydroxy-4'-methoxyacetophenone	90765-44-9	C9H11NO3	3636759.4	76.5	
79.0869	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	5180261.7	89.1	
80.5466	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	757240.5	83.0	



#### -- 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 7.3141 1,3-Propanediol 1202732.8 94.8 C3H8O2 Component RT: 7.3141 y x10<sup>2</sup> 0.9 57.0 0.8 0.7 31.0 0.6 0.5 0.4 0.3 45.0 0.2 0.1 39.0 15 25 55 65 70 75 5 10 20 30 35 40 45 50 80 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 28.0 31.0 0.8 0.7 57.0 0.6 0.5 0.4 0.3 43.0 0.2 15.0 0.1 39.0 55.0 18.0 75.0 55 70 5 10 15 20 25 30 35 40 45 50 65 75 80 Mass-to-Charge (m/z) + Scan (7.2738-8.1054 min, 140 scans) 4.D st x10<sup>2</sup> 0.9 58.0 31.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 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: 7.3141 **EIC Peaks** Counts Counts x10<sup>4</sup> $x10^{4}$ 57.0 Component 57.0 58.0 8 2 7-58.0 1.75 31.0 6 1.5 31.0 43.0 5 1.25 45.0 45.0

1-

0.75

0.5

0.25

7.4

7.6

7.8

Acquisition Time (min)

43.0

4

3

2

1

7.6

7.8

#### ... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-(2-methoxyethoxy)propanoic acid, O-acetyl-11.6071 528254.6 82.0 1000506-61-7 C8H14O5 Component RT: 11.6071 x10<sup>2</sup>\_ 29.0 59.0 43.0 0.9 8.0 0.7 0.6 103.0 0.5 0.4 0.3 $0.2^{-}$ 0.1 0-30 60 0 10 20 40 50 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) 2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L) $x10^{2}$ 0.9 0.8 59.0 0.7 0.6 0.5 0.4 103.0 0.3 0.2 29.0 0.1 15.0 87.0 73.0 117.0 130.0 147.0 0 30 40 130 0 10 20 50 70 80 90 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (11.5140-11.7503 min, 40 scans) 4.D x10<sup>2</sup>. 0.9 103.0 0.8 87.0 0.7 0.6 57.0 0.5 31.0 0.4 0.3 0.2 0.1 117.0 0 30 200 210 220 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) Component RT: 11.6071 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>5</sup> 103.0 Component 29.0 43.0 0.9 1.75 59.0 57.0 0.8 1.5 $0.7^{-}$ 59.0 43.0

11.6

11.7

Acquisition Time (min)

29.0

нзс

1.25

0.75

0.5

0.25

0

1

103.0

57.0

0.6

0.5

 $0.4^{-}$ 

0.3

0.2

11.6

11.7

#### --- 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 12.3681 Butyrolactone 10540151.4 96.8 C4H6O2 Component RT: 12.3681 v10<sup>2</sup> 0.9 42.0 0.8 0.7 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 0.1 15 40 10 20 25 30 35 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) st x10<sup>2</sup>\_ 0.9-42.0 0.8 28.0 0.7 0.6 0.5 0.4 0.3 86.0 56.0 39.0 0.2 0.1 53.0 | 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.1274-12.4877 min, 61 scans) 4.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 86.0 29.0 0.3 0.2 56.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 12.3681 Counts Counts x10<sup>6</sup> x10<sup>5</sup> 42.0 Component 42.0 41.0 3 1 41.0 86.0 2.5 0.8 29.0 86.0

56.0

2-

1-

12.2

12.3

12.4

Acquisition Time (min)

12.5

1.5

0.5

29.0

56.0

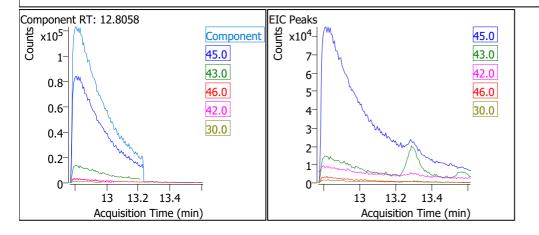
0.6

0.4

0.2

12.2 12.3 12.4 12.5

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 595-98-2 12.8058 Methyltartronic acid 1691916.6 C4H6O5 Component RT: 12.8058 v10<sup>2</sup> 0.9 45.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 0.2 0.1 30.0 0 30 70 110 120 130 10 20 50 60 80 90 100 140 Mass-to-Charge (m/z) Methyltartronic acid (NIST20.L) st x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 29.0 0.2 19.0 0.1 90.0 30 0 10 20 **4**0 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (12.7694-13.2309 min, 78 scans) 4.D St x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 29.0 0.1 87.0 102.0 56.0



80

100

120

140

160

180

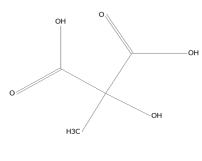
200

220

240

60

20



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.** 2-(2-methoxyethoxy)propanoic acid, O-acetyl-13.2899 532351.4 78.3 1000506-61-7 C8H14O5 Component RT: 13.2899 x10<sup>2</sup>. 103.0 0.9 43.0 8.0 0.7 87.0 0.6 57.0 0.5 31.0 0.4 0.3 $0.2^{-}$ 0.1 0-30 0 10 20 40 50 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) 2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L) $x10^{2}$ 43.0 0.9 0.8 59.0 0.7 0.6 0.5 0.4 103.0 0.3 0.2 29.0 0.1 15.0 87.0 73.0 117.0 130.0 147.0 0 30 40 90 130 0 10 20 50 60 70 80 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (13.2202-13.4509 min, 39 scans) 4.D x10<sup>2</sup>. 0.9 0.8 0.7 0.6 0.5 103.0 0.4 0.3 87.0 29.0 57.0 0.2 0.1 30 40 200 210 220 230 10 20 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) EIC Peaks Component RT: 13.2899 Counts Counts x10<sup>4</sup> x10<sup>5</sup> 103.0 Component 43.0 103.0 0.9 1.8 43.0 87.0 0.8 1.6

13.3

13.4

Acquisition Time (min)

57.0

31.0

нзс

1.4

1.2

0.8

0.6

 $0.4^{\circ}$ 

0.2

1

87.0

57.0

31.0

0.7

0.6

 $0.5^{-}$ 

0.4

0.3

0.2

0.1

13.3

13.4

#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 309458.3 14879-83-5 16.4719 2,2-Dimethyl-2-sila-1,3-C5H12O2Si dioxacyclohexane Component RT: 16.4719 x10<sup>2</sup> 117.0 0.9 8.0 0.7 0.6 0.5 59.0 0.4 75.0 0.3 43.0 $0.2^{-}$ 31.0 89.0 0.1 133.0 0-60 30 35 50 55 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 Mass-to-Charge (m/z) 2,2-Dimethyl-2-sila-1,3-dioxacyclohexane (NIST20.L) $x10^{2}$ 117.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 31.0 45.0 87.0 0.2 75.0 59.0 0.1 101.0 132.0 0 30 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 35 Mass-to-Charge (m/z) + Scan (16.3883-16.8164 min, 73 scans) 4.D x10<sup>2</sup>. 117.0 32.0 0.9 0.8 0.7 0.6 0.5 0.4 89.0 61.0 0.3 103.0 75.0 0.2 0.1 190 200 210 220 230 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 16.4719 **EIC Peaks** Counts Counts x10<sup>4</sup> $x10^{3}$ 117.0 Component 117.0 43.0 2 6 59.0 61.0 1.75 5 61.0 1.5 4

16.5 16.6 16.7

Acquisition Time (min)

1.25

0.75

0.5

16.4 16.5 16.6 16.7

Acquisition Time (min)

1

75.0

43.0

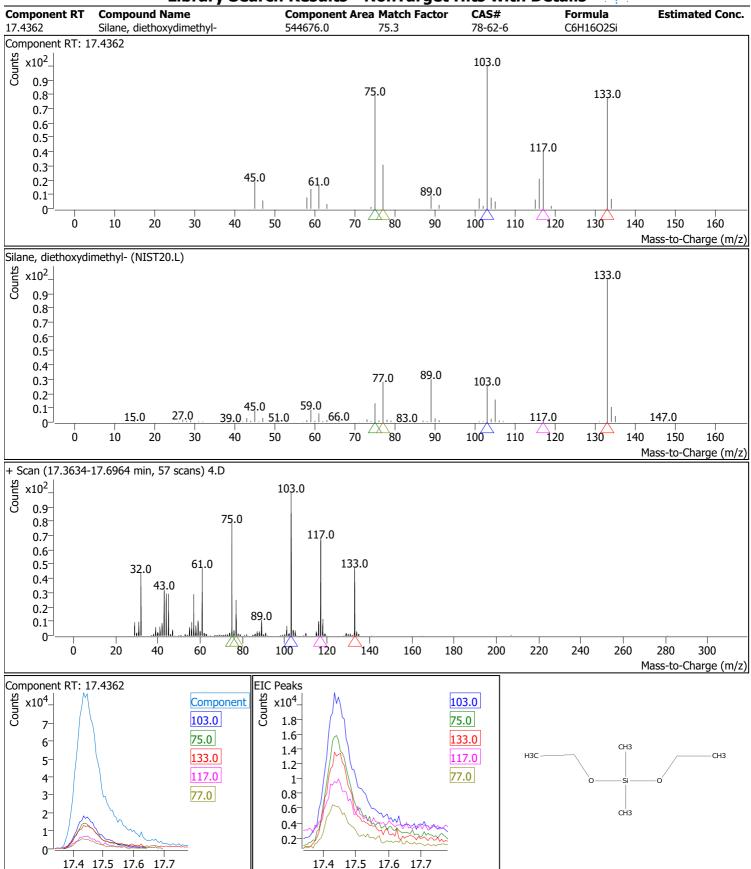
3

2-

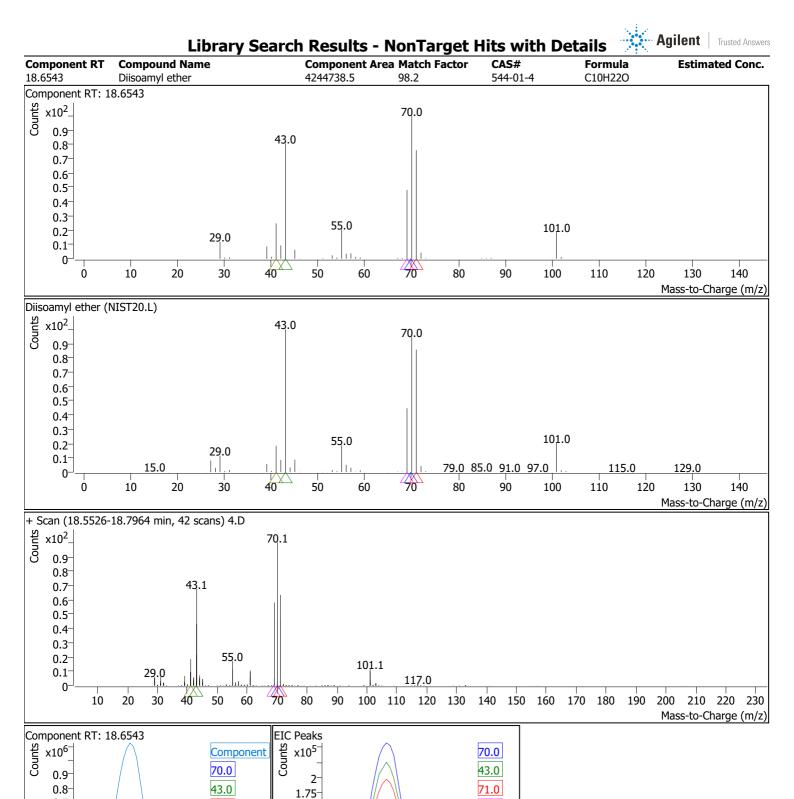
CH3







Acquisition Time (min)



18.7

Acquisition Time (min)

69.0

41.0

0.7

0.6

0.5

0.4

0.3

0.2

18.6

18.7

Acquisition Time (min)

71.0

69.0

41.0

1.5

1.25

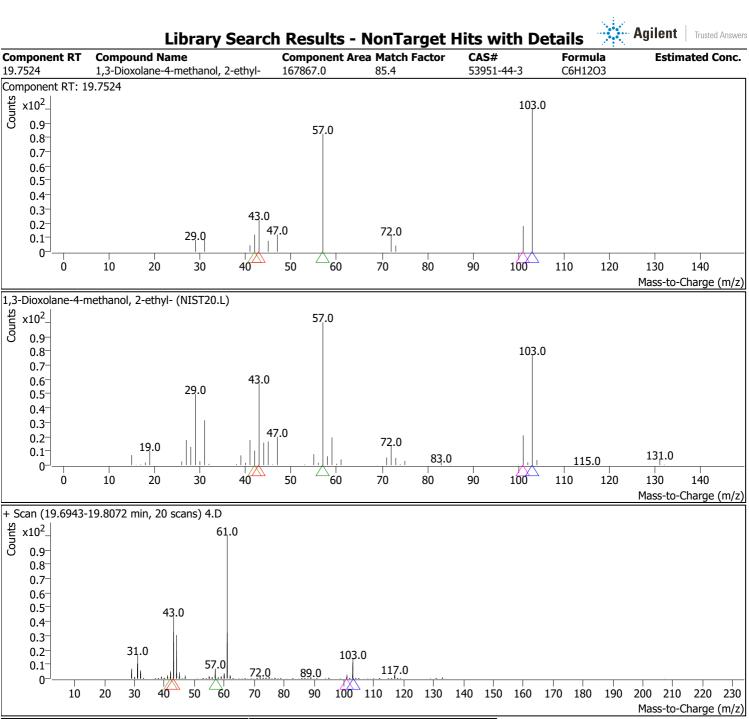
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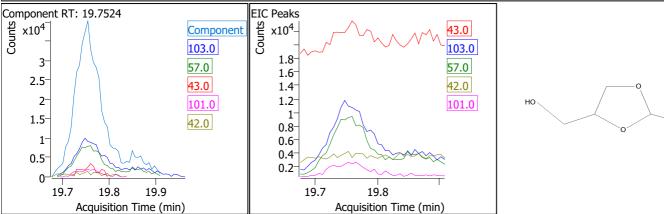
0.5

0.25

18.6

1





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20.1

20.2

Acquisition Time (min)

20.3

41.0

1-

0.5

0

0.4

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.** 4088997.3 110-88-3 21.1424 1,3,5-Trioxane 81.6 C3H6O3 Component RT: 21.1424 v10<sup>2</sup> 0.9 61.0 89.0 0.8 43.0 0.7 0.6 0.5 0.4 31.0 0.3 0.2 0.1 47.0 <del>\_\_9</del>0 75 10 15 20 25 30 35 40 45 50 55 65 70 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 0.4 29.0 0.3 0.2 0.1 44.0 14.0 56.0 <del>\_\_9</del>0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.8120-22.0846 min, 215 scans) 4.D st x10<sup>2</sup> 0.9 0.8 43.0 0.7 0.6 0.5 0.4 0.3 31.0 0.2 89.0 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: 21.1424 **EIC Peaks** Counts stuno 1.2x10<sup>5</sup> 61.0 Component 61.0 43.0 1.2 89.0 31.0 1 43.0 89.0 0.8 0.8 31.0 60.0 0.6 0.6

21.5

Acquisition Time (min)

22

60.0

0.4

0.2

21

0.4

0.2

21

21.5

#### --- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0353 1-Octanol 3434766.0 98.7 111-87-5 C8H18O Component RT: 23.0353 v10<sup>2</sup> 0.9 56.0 41.0 0.8 70.0 $0.7^{-}$ 84.0 0.6 0.5 0.4 0.3 0.2 0.1 70 55 100 105 110 115 120 125 130 135 140 45 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 55 20 25 35 40 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9530-23.2262 min, 46 scans) 4.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 56.1 70.1 84.1 0.1 103.0 117.0 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) EIC Peaks Component RT: 23.0353 Counts x10<sup>5-</sup> Counts x10<sup>5</sup>\_ 56.0 Component 56.0 55.0 0.8 6 55.0 41.0 0.7 5 70.0 41.0 0.6

23.1

Acquisition Time (min)

23.2

69.0

4

3

2

1

23

23.1

Acquisition Time (min)

23.2

70.0

69.0

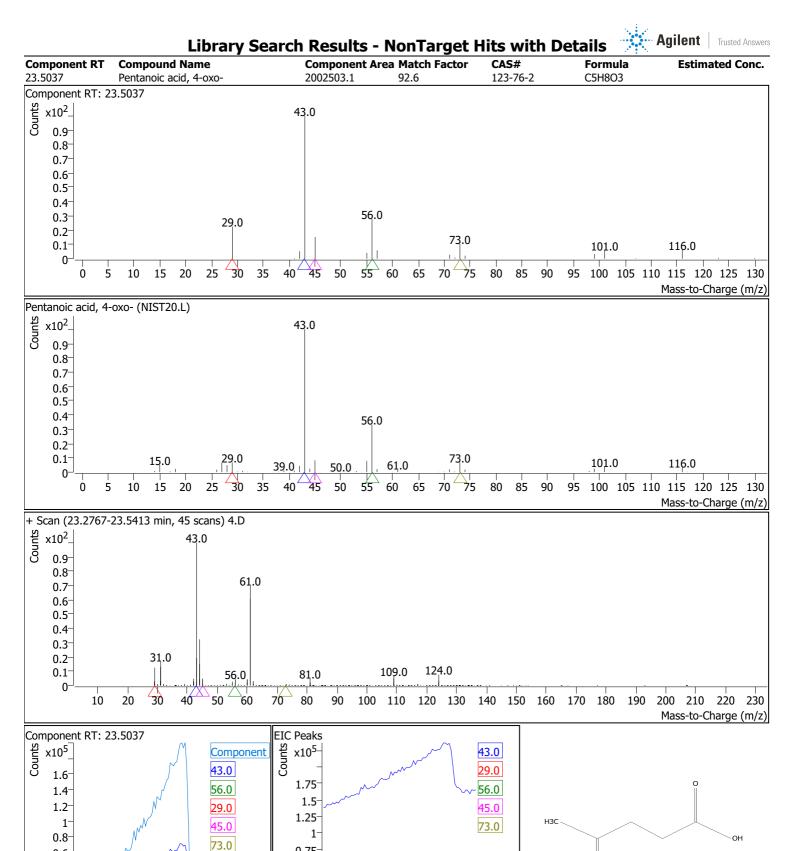
0.5<sup>-</sup> 0.4<sup>-</sup>

0.3

0.2

 $0.1^{\circ}$ 

23



23.2 23.3 23.4 23.5

Acquisition Time (min)

0.75

0.5

0.25

0.6

0.4

0.2

23.2 23.3 23.4 23.5

#### --- 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 23.5626 Phenol, 2-methoxy-5846632.4 97.9 C7H8O2 Component RT: 23.5626 v10<sup>2</sup> 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 53.0 29.0 0.1 39.0 30 80 110 10 20 40 50 60 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 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 10 20 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4640-23.7792 min, 54 scans) 4.D st x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 109.0 124.0 0.3 81.0 31.0 0.2 0.1 53.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.5626 Counts Counts x10<sup>5</sup> 109.0 Component 109.0 124.0 1 124.0 81.0 2.5 0.8 81.0 2-



53.0

29.0

1.5

0.5

1

23.5

23.6

23.7 Acquisition Time (min)

0.6

0.4

0.2

23.5

23.6

23.7

Acquisition Time (min)

29.0

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.7721 2-Cyclopenten-1-one, 2-hydroxy-3,4-319272.0 78.5 21835-00-7 C7H10O2 dimethyl-Component RT: 23.7721 x10<sup>2</sup>. 126.0 0.9 0.8 0.7 111.0 0.6 0.5 83.1 0.4 0.3 97.0 70.1 41.1 55.0 $0.2^{-}$ 0.1 0 <del>\_\_\_\_</del>85 35 40 45 50 55 60 65 70 75 80 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl- (NIST20.L) $x10^{2}$ 126.0 0.9 0.8 0.7 0.6 0.5 111.0 69.0 0.4 83.0 0.3 41.0 55.0 0.2 98.0 0.1 110 115 125 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 120 130 Mass-to-Charge (m/z) + Scan (23.7050-23.8743 min, 29 scans) 4.D x10<sup>2</sup>. 43.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 55.0 117.0 0 30 110 120 130 140 150 190 200 210 220 230 10 20 40 50 60 70 80 100 160 170 180 Mass-to-Charge (m/z) Component RT: 23.7721 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 29.0 Component CH3 126.0 126.0 6 3 29.0 111.0 5 2.5 111.0 83.1

23.75 23.8

Acquisition Time (min)

84.1

23.85

4

3

2

1

83.1

84.1

23.75 23.8 23.85

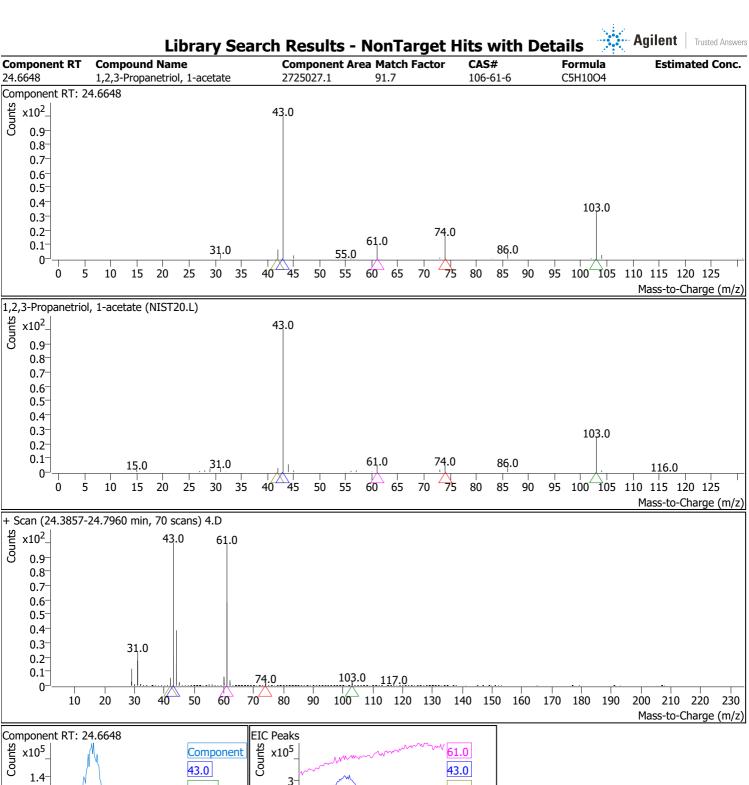
Acquisition Time (min)

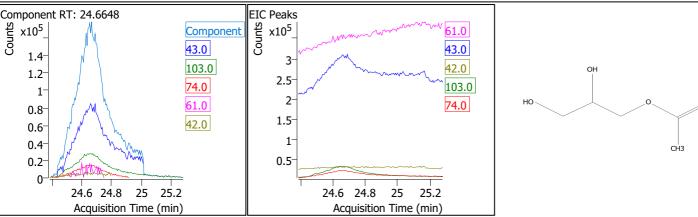
2

1.5

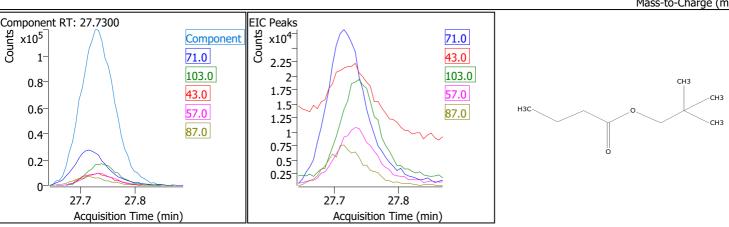
1<sup>-</sup> 0.5

0-





#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7300 Butanoic acid, 2,2-dimethylpropyl 521798.4 82.1 23361-69-5 C9H18O2 Component RT: 27.7300 x10<sup>2</sup>\_ 71.0 0.9 8.0 0.7 103.0 0.6 0.5 0.4 43.0 57.0 0.3 87.0 $0.2^{-}$ 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 <sub>93.0</sub> 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 (27.6512-27.7809 min, 22 scans) 4.D x10<sup>2</sup>. 71.1 43.0 0.9 0.8 0.7 0.6 61.0 0.5 103.0 0.4 57.0 0.3 31.0 0.2 87.0 0.1 117.0 70 90 100 110 120 130 140 150 190 200 210 220 230 10 20 30 40 50 60 80 160 170 180 Mass-to-Charge (m/z) Component RT: 27.7300 **EIC Peaks**



### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 91-20-3 28.7452 Naphthalene 97.5 C10H8 Component RT: 28.7452 y x10<sup>2</sup> 0.9 128.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 0.2 102.0 0.1 100 105 110 115 120 125 130 135 140 55 85 95 Mass-to-Charge (m/z) Naphthalene (NIST20.L) St x10<sup>2</sup> 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 20 25 30 35 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (28.6549-28.9998 min, 59 scans) 4.D St x10<sup>2</sup>\_ 0.9 128.1 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 0.2 103.0 57.0 0.1 117.0 77.0 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: 28.7452 EIC Peaks Counts Counts x10<sup>5</sup> 128.0 Component 128.0 127.0 0.8 1.4 127.0 129.0 0.7 1.2 129.0 102.0 0.6 1 0.5

126.0

102.0

126.0

0.4

0.3

0.2

0.1

28.7

28.8

28.9

Acquisition Time (min)

0.8

0.6

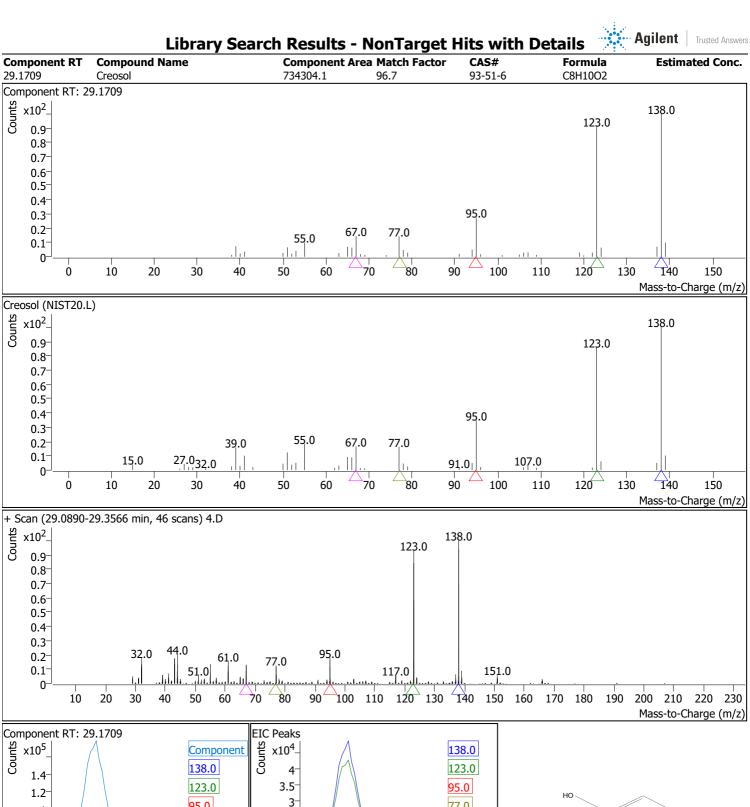
0.4

0.2

28.7

28.8

28.9



#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 505-22-6 30.4742 1,3-Dioxane 454800.7 C4H8O2 Component RT: 30.4742 v10<sup>2</sup> 0.9 87.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 59.0 0.1 30 25 75 10 15 20 50 55 65 70 80 90 95 Mass-to-Charge (m/z) 1,3-Dioxane (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 87.0 0.8 0.7 0.6 28.0 0.5 0.4 0.3 0.2 58.0 41.0 0.1 15.0 55.0 70.0 5 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (30.3795-30.7301 min, 59 scans) 4.D st x10<sup>2</sup> 0.9 87.0 0.8 0.7 110.0 0.6 0.5 $0.4^{-}$ 0.3 0.2 59.0 81.0 145.0 0.1 92.0 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) EIC Peaks Component RT: 30.4742 Counts Counts x10<sup>4</sup> 87.0 Component 87.0 31.0 8 3.5 7 31.0 59.0 3 6 59.0 42.0 2.5 5 41.1 41.1 2

30.5

30.6

Acquisition Time (min)

30.7

4

3 2

1

30.5

30.6

Acquisition Time (min)

30.7

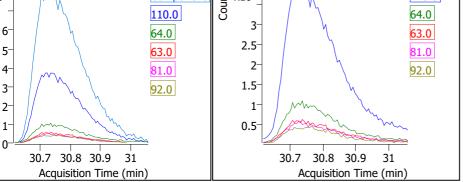
42.0

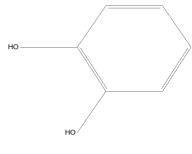
1.5

0.5

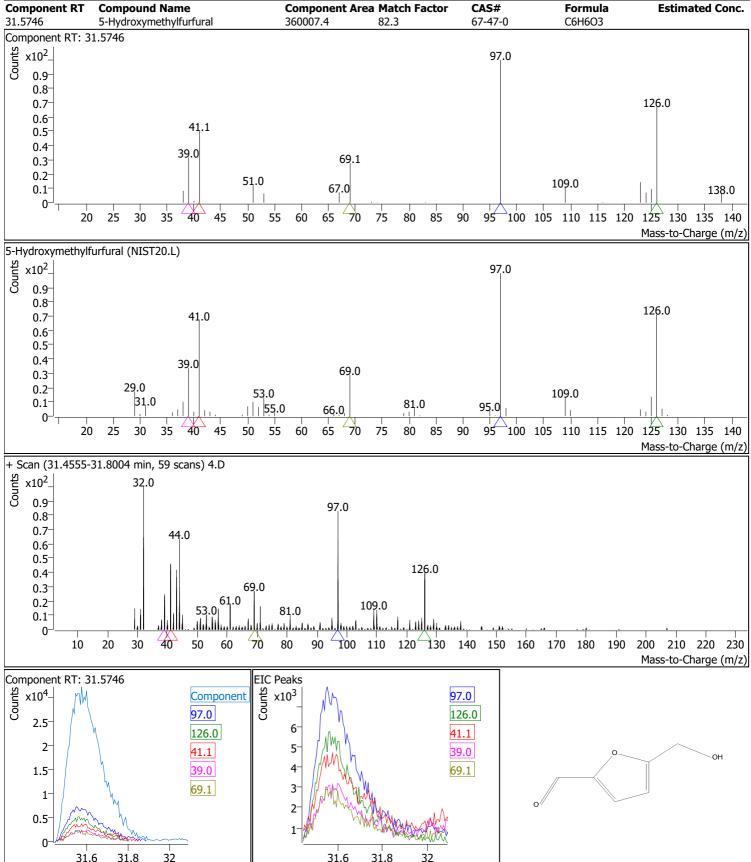
1

#### --- 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 30.7369 Catechol 876657.4 93.0 C6H6O2 Component RT: 30.7369 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 95 100 105 110 115 120 125 10 35 50 55 75 80 85 90 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 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 (30.6237-31.0571 min, 73 scans) 4.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 32.0 44.0 81.0 92.0 103.0 0.1 57.0 ا...اناسب 69.0 129.0 90 10 20 30 40 50 60 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 30.7369 Counts Counts x10<sup>4</sup> 110.0 Component 110.0 64.0 3 6 64.0 63.0 2.5 5

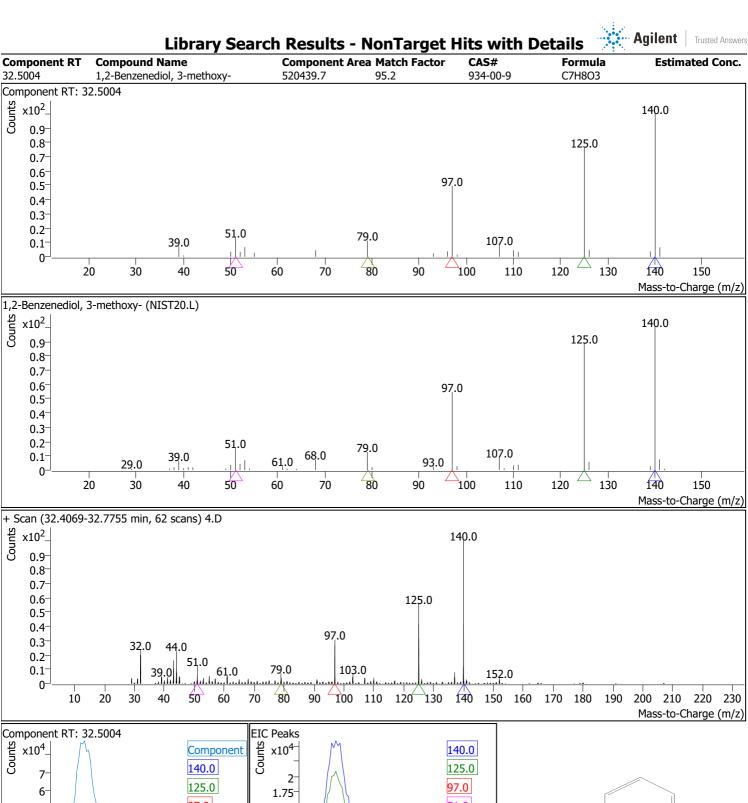


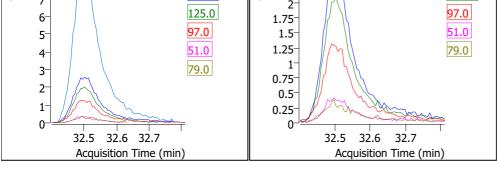






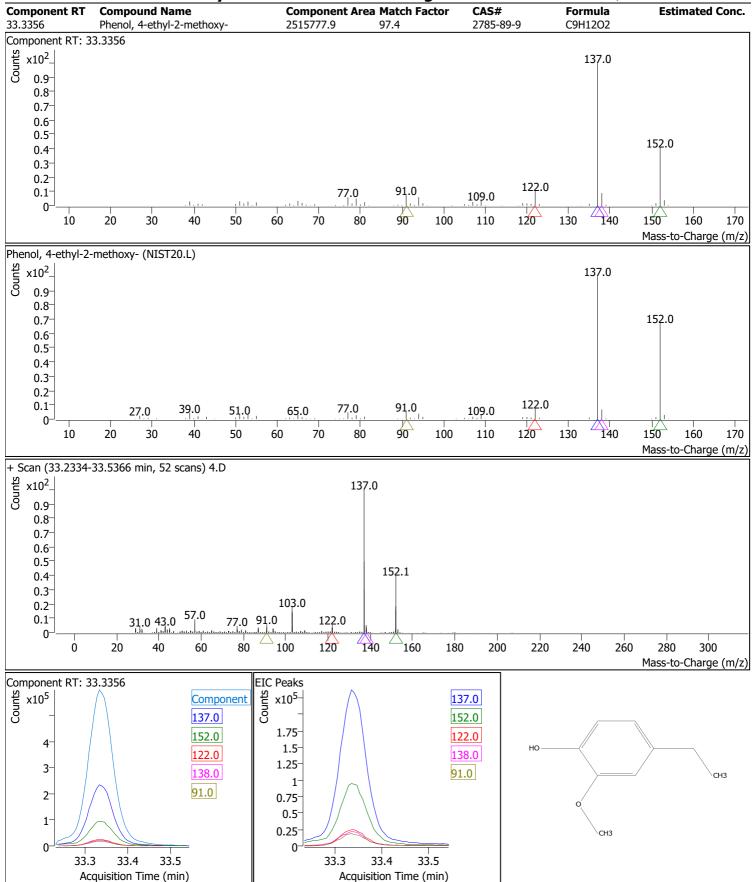
Acquisition Time (min)





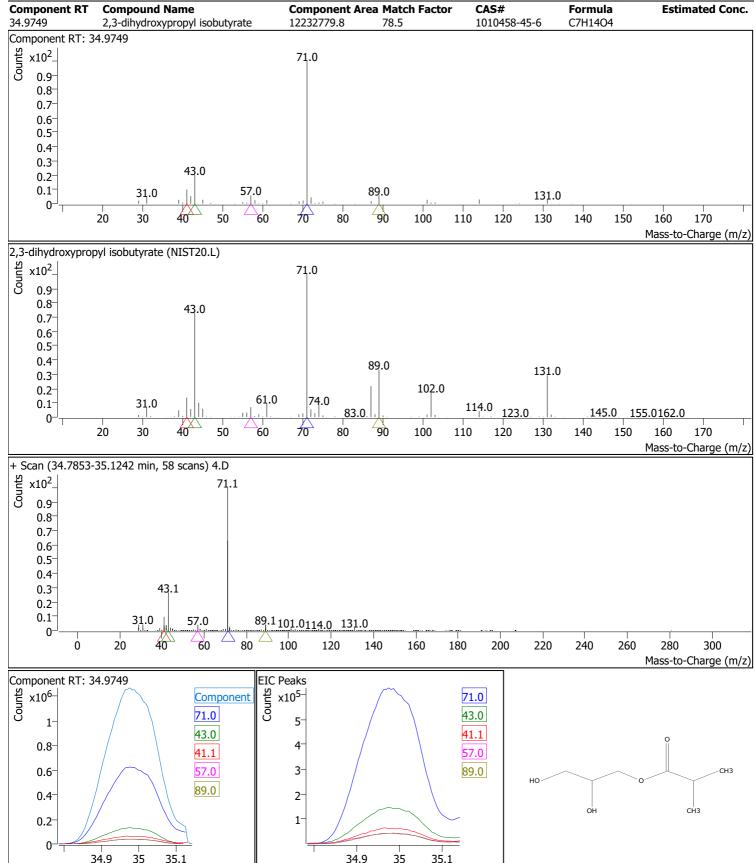




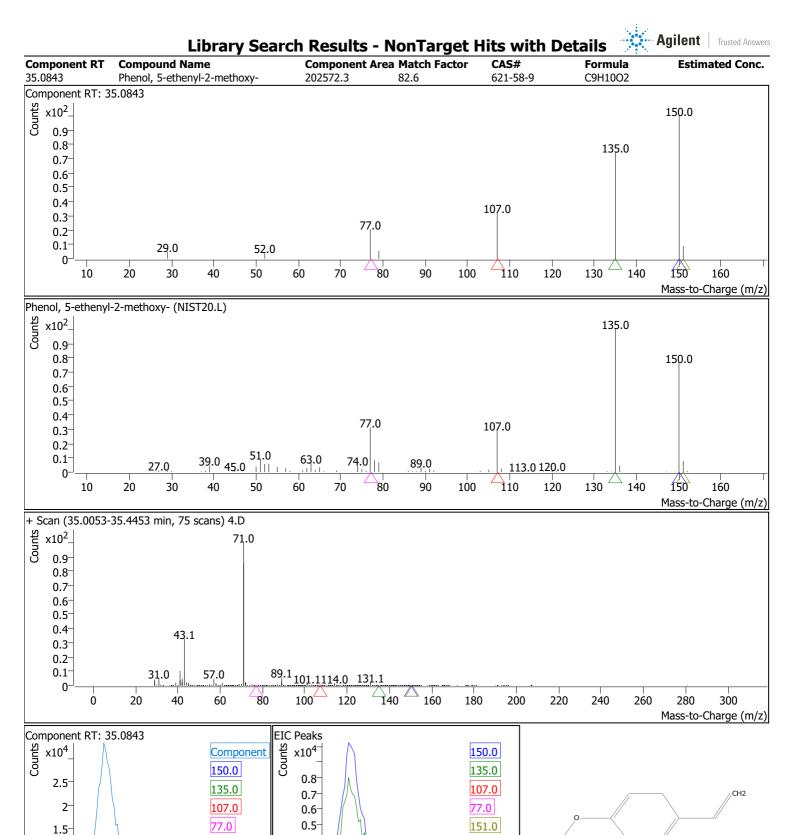


## **Library Search Results - NonTarget Hits with Details**





Acquisition Time (min)



35.1 35.2 35.3

Acquisition Time (min)

35.4

 $0.4^{-}$ 

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

151.0

35.1 35.2 35.3 35.4

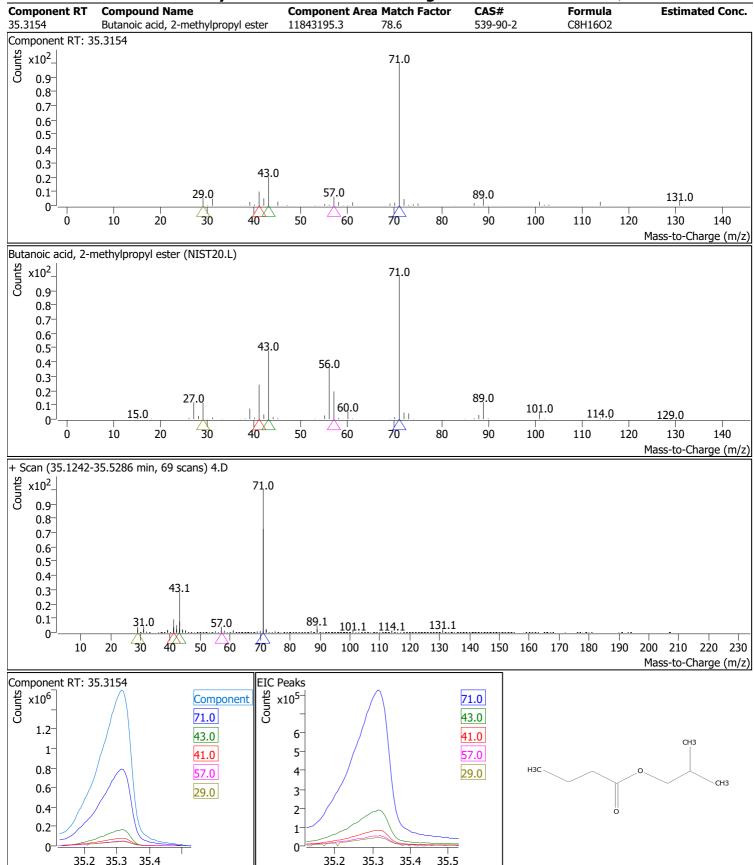
Acquisition Time (min)

1

0.5

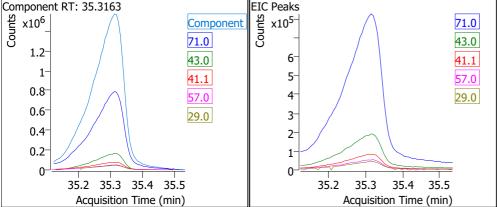
# **Library Search Results - NonTarget Hits with Details**

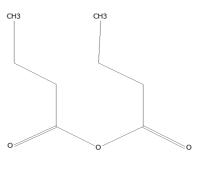




Acquisition Time (min)

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.3163 Butanoic acid, anhydride 11248701.5 C8H14O3 Component RT: 35.3163 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.1 57.0 0.1 29.0 89.0 <del>3</del>0 10 20 25 40 55 60 65 75 85 90 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 95 Mass-to-Charge (m/z) + Scan (35.1242-35.5286 min, 69 scans) 4.D st x10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 43.1 0.3 0.2 0.1 57.0 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 35.3163 **EIC Peaks** Counts Counts x10<sup>5</sup> 71.0 Component CH3 CH3 71.0 43.0 1.2 6 43.0 41.1 1





#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.1877 2-Furanmethanol, tetrahydro-2781061.4 82.1 97-99-4 C5H10O2 Component RT: 36.1877 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 10 25 55 60 65 90 100 105 110 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 53.0,57.0 61.0 15.0 67.0 102.0 10 15 20 25 35 40 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.0721-36.4383 min, 62 scans) 4.D st x10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 0.1 57.0 131.0 10 20 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: 36.1877 **EIC Peaks** Counts Counts x10<sup>5-</sup> 71.0 Component 71.0 43.0 2.25 43.0 41.1 3.5 2 1.75 131.0 41.1 3

31.0

1.5

1.25

0.75

0.5

36.1

36.2

36.3

Acquisition Time (min)

36.4

0.25

131.0

31.0

2.5

1.5

0.5

2

1

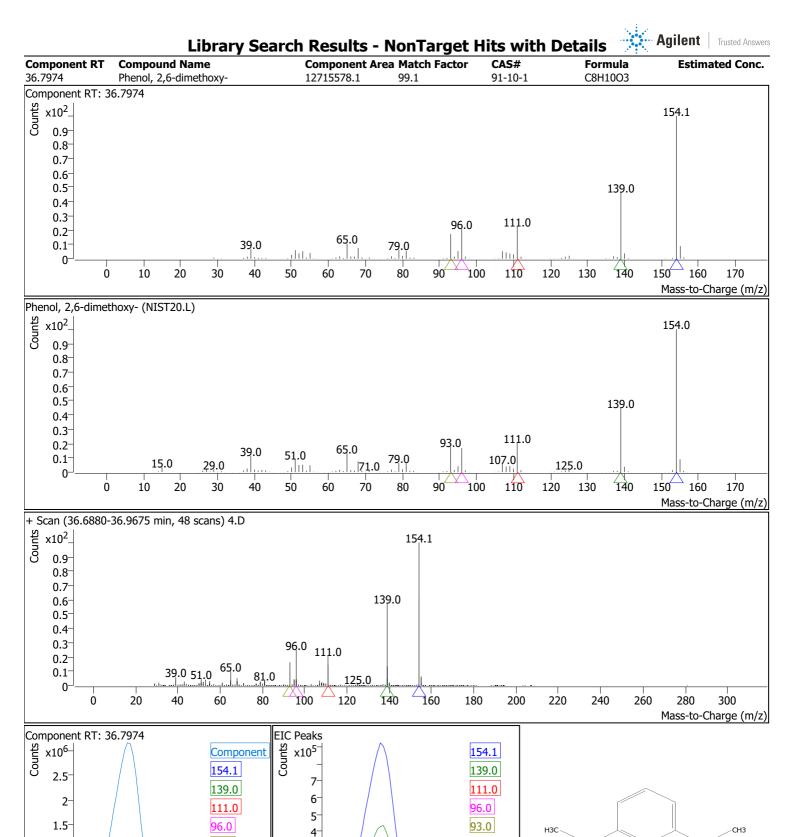
36.1

36.2

36.3

Acquisition Time (min)

36.4





36.8

36.9

Acquisition Time (min)

93.0

1

0.5

36.8

36.9

Acquisition Time (min)

3

2-

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Ethylamine, 2-((p-bromo-alpha.-methyl-alpha.-phenylbenzyl)oxy)-N,N-dimethyl-37.3896 1629293.7 75.7 3565-72-8 C18H22BrNO Component RT: 37.3896 $x10^{2}$ 58.0 0.9 0.8 0.7 0.6 0.5 0.4 42.0 0.3 0.2 0.1 0 20 30 40 70 100 110 120 130 140 150 160 170 50 80 90 180 Mass-to-Charge (m/z) Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl- (NIST20.L) $x10^{2}$ 58.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 30.0 42.0 72.0 103.0 165.0 0 40 30 70 20 50 90 100 120 130 140 150 160 80 110 170 180 Mass-to-Charge (m/z) + Scan (37.0511-37.6751 min, 105 scans) 4.D Counts x10<sup>2</sup>\_ 45.0 0.9 0.8 0.7 0.6 0.5 0.4 103.0 71.0 0.3 0.2 29.0 87.0 117.0 0.1 137.0 40 60 20 180 200 220 240 260 280 300 80 100 120 140 160 Mass-to-Charge (m/z) Component RT: 37.3896 EIC Peaks Counts st x10<sup>5</sup>x10<sup>4</sup> 58.0 Component 42.0 58.0 1.2 42.0 59.0 5 1

37.4

Acquisition Time (min)

37.6

59.0

37.4 37.6

Acquisition Time (min)

3

2

37.2

0.8

0.6

0.4

0.2

CH3

СНЗ

СНЗ

#### --- 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 37.4168 Phenol, 2-methoxy-4-propyl-394237.8 78.1 C10H14O2 Component RT: 37.4168 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 94.0 66.0 107.0 160 - 170 120 10 20 30 40 50 60 70 100 110 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 150 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 180 Mass-to-Charge (m/z) + Scan (37.3481-37.4967 min, 26 scans) 4.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 103.0 58.0 0.3 29.0 71.0 0.2 137.0 87.0 117.0 0.1 166.1 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 37.4168 EIC Peaks Counts Counts x10<sup>4</sup> 137.0 Component 137.0 166.0 4.5 0.8 166.0 122.0 0.7

37.4

37.45

Acquisition Time (min)

37.5

122.0

138.0

94.0

37.4 37.45 37.5

Acquisition Time (min)

0.6

0.5

 $0.4^{-}$ 

0.3

0.2-

0.1

3.5

3

2

1

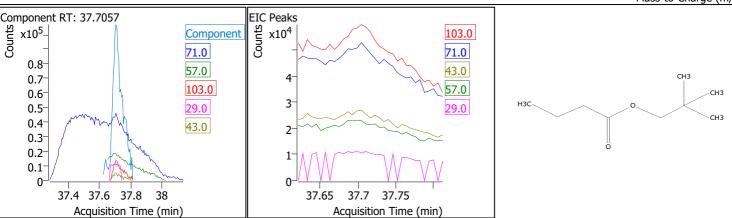
2.5

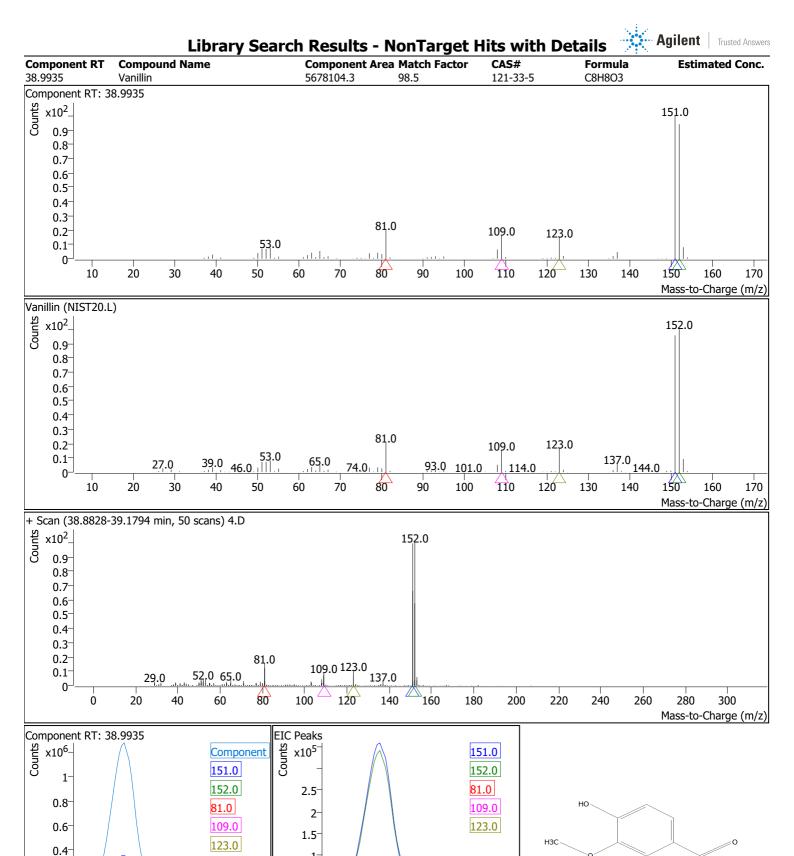
1.5

138.0

94.0

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 37.7057 Butanoic acid, 2,2-dimethylpropyl 475586.9 78.5 23361-69-5 C9H18O2 Component RT: 37.7057 x10<sup>2</sup>\_ 71.0 0.9 8.0 0.7 0.6 0.5 57.0 0.4 0.3 103.0 29.0 $0.2^{-}$ 43.0 0.1 89.0 74.0 30 60 70 150 10 20 50 80 90 100 110 120 130 140 160 170 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> 0.1 36.0 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 (37.6275-37.8000 min, 30 scans) 4.D x10<sup>2</sup>. 103.0 71.0 0.9 0.8 0.7 0.6 0.5 43.0 0.4 0.3 57.0 0.2 29.1 89.0 0.1 131.0 161.0 0 <del>6</del>0 Ó 20 40 80 200 220 240 260 280 100 120 140 160 180 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 37.7057







39

39.1

Acquisition Time (min)

1-

38.9

0.5

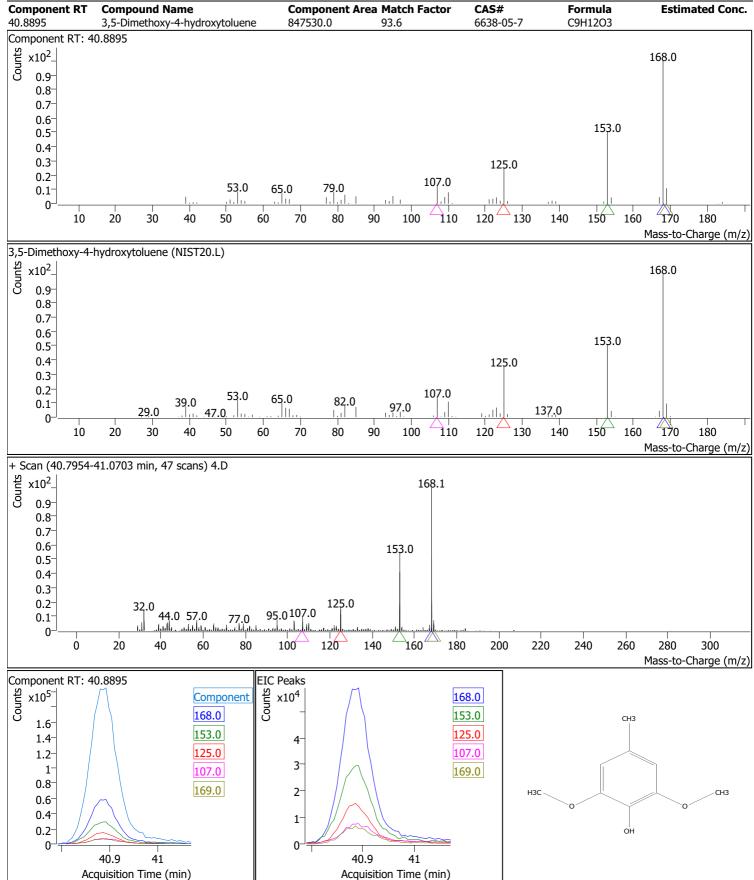
0.2

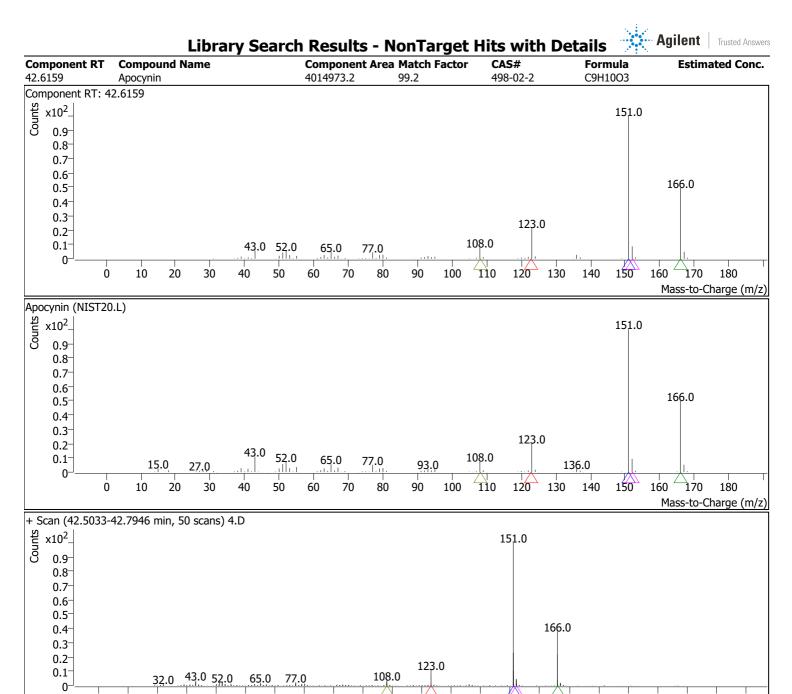
39

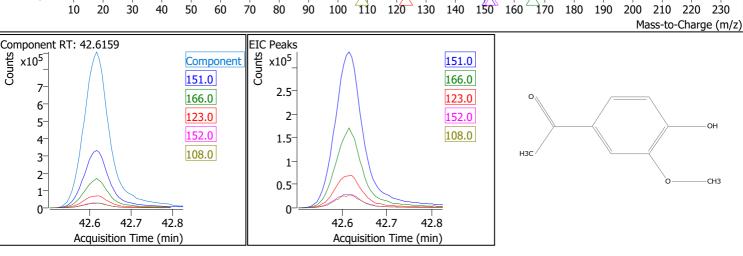
39.1





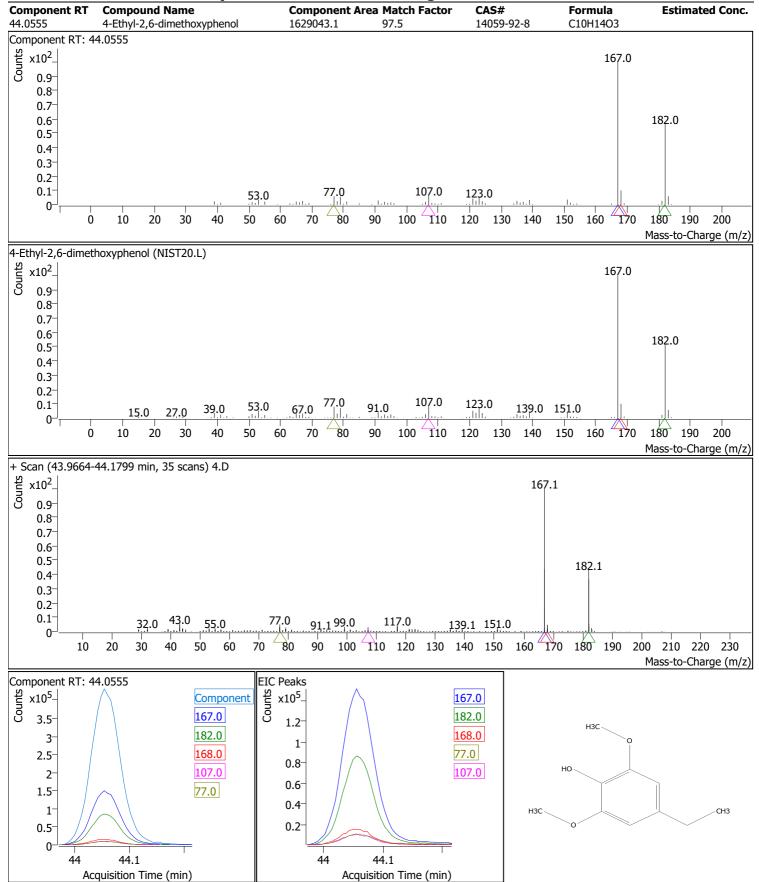




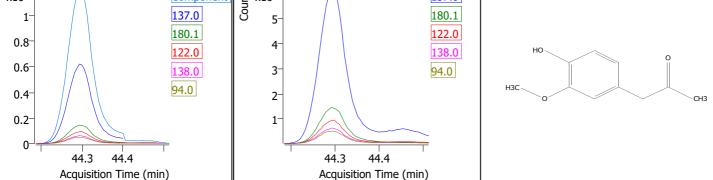


# **Library Search Results - NonTarget Hits with Details**

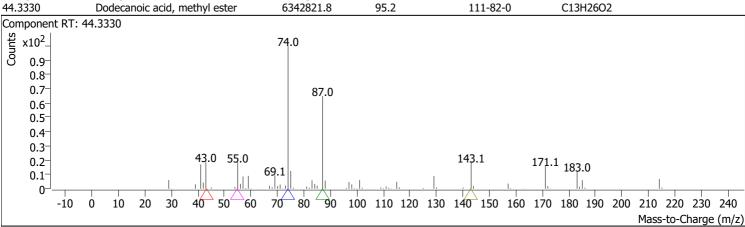




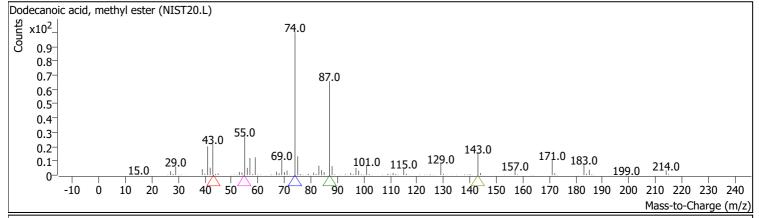
### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-44.2950 5445870.8 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.2950 Counts x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 $0.2^{-}$ 122.0 0.1 77.0 51.0 66.0 120 180 20 30 40 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 0 100 180 20 30 50 60 80 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.1919-44.5130 min, 55 scans) 4.D x10<sup>2</sup>. 137.0 0.9 0.8 $0.7^{-}$ 0.6 74.0 0.5 0.4 0.3 87.0 0.2 180.1 43.0 <sub>55.1</sub> 122.0 0.1 94.0 171.1 0 **1**40 100 120 180 200 Ó 20 40 60 80 160 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 44.2950 Counts Counts x10<sup>6</sup> x10<sup>5</sup>-137.0 Component 180.1 137.0 1 5 180.1 122.0 0.8

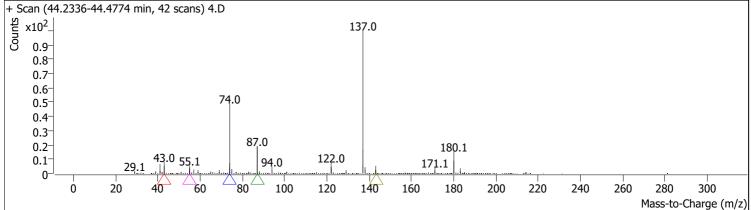


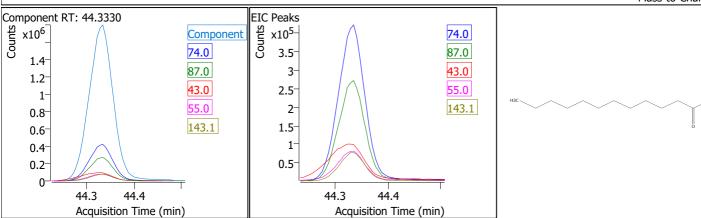
# Library Search Results - NonTarget Hits with Details Compound Name Dodecanoic acid, methyl ester Compound Name Dodecanoic acid, methyl ester Compound Name Compound Area Match Factor 6342821.8 95.2 C13H2602 C13H2602



**Component RT** 







### --- 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 45.6451 Pentanoic acid, 4-oxo-, 2-methylpropyl 435378.6 81.3 C9H16O3 Component RT: 45.6451 x10<sup>2</sup>\_ 99.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 0.3 $0.2^{-}$ 117.0 130.0 57.0 0.1 31.0 40 70 100 130 10 20 30 50 80 90 110 120 140 150 160 170 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 40 100 130 10 20 30 50 60 70 80 90 110 120 140 150 160 170 Mass-to-Charge (m/z) + Scan (45.5417-45.8628 min, 55 scans) 4.D st x10<sup>2</sup> 0.9 99.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 117.0 32.0 0.2 180.0 130.0 165.0 0.1 91.0 0 Ó 20 40 60 80 100 200 260 280 120 140 160 180 220 240 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 45.6451 Counts Counts 99.0 x10<sup>4</sup> x10<sup>4</sup> Component 99.0 43.0 7 3-43.0 117.0 6 2.5 71.0 71.0 5



45.7

Acquisition Time (min)

45.8

130.0

2-

1

45.6

1.5

0.5

117.0

130.0

4

3

2

1

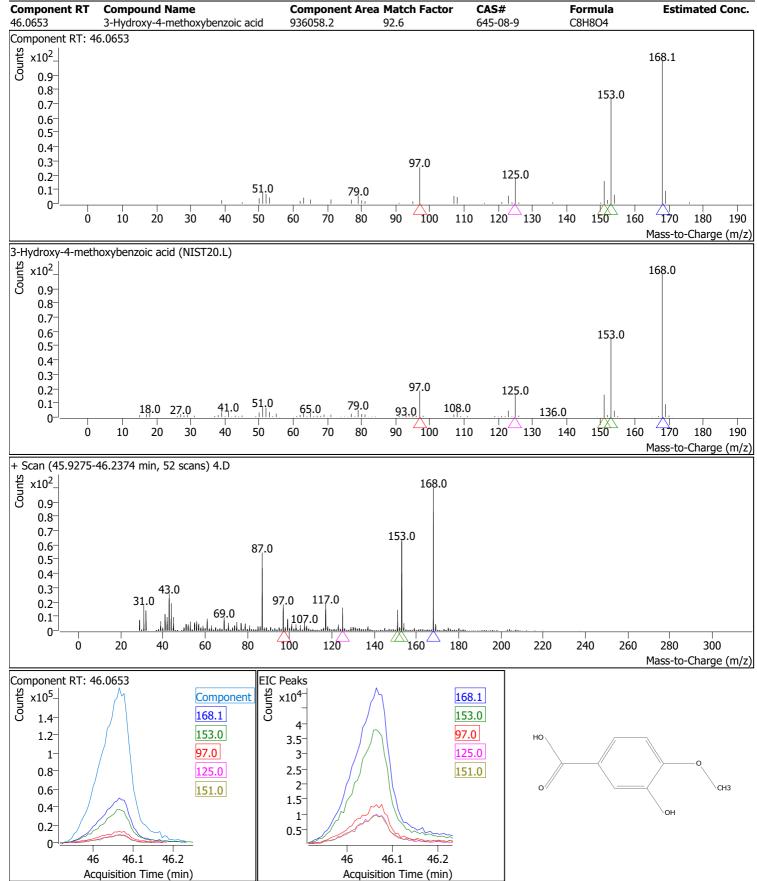
45.6

45.7

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.** 497-25-6 46.2195 Oxazolidin-2-one 634933.3 80.5 C3H5NO2 Component RT: 46.2195 v10<sup>2</sup> 0.9 87.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 42.0 0.1 57.0 40 30 55 85 90 10 15 20 25 35 50 60 65 80 95 Mass-to-Charge (m/z) Oxazolidin-2-one (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 87.0 0.8 0.7 0.6 59.0 0.5 0.4 28.0 0.3 42.0 0.2 0.1 56.0 <del>-7</del>5 5 10 15 20 25 30 35 40 45 50 55 60 65 70 80 90 95 Mass-to-Charge (m/z) + Scan (46.0590-46.5466 min, 83 scans) 4.D st x10<sup>2</sup> 0.9 87.0 151.0 0.8 168.0 117.0 0.7 0.6 0.5 43.0 0.4 32.0 0.3 97.0 0.2 61.0 75.0 180.1 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: 46.2195 Counts x10<sup>4</sup> x10<sup>4</sup> 87.0 Component 87.0 31.0 2.5 31.0 42.0 5 2 42.0 74.0 4 1.5 86.0 86.0

3

2

1

46.2

46.4

Acquisition Time (min)

46.6

74.0

1-

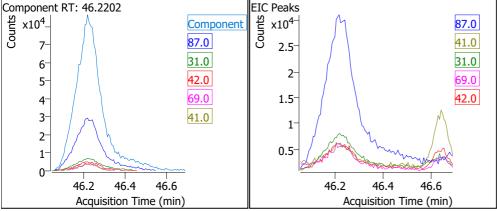
0.5

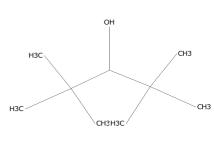
46.2

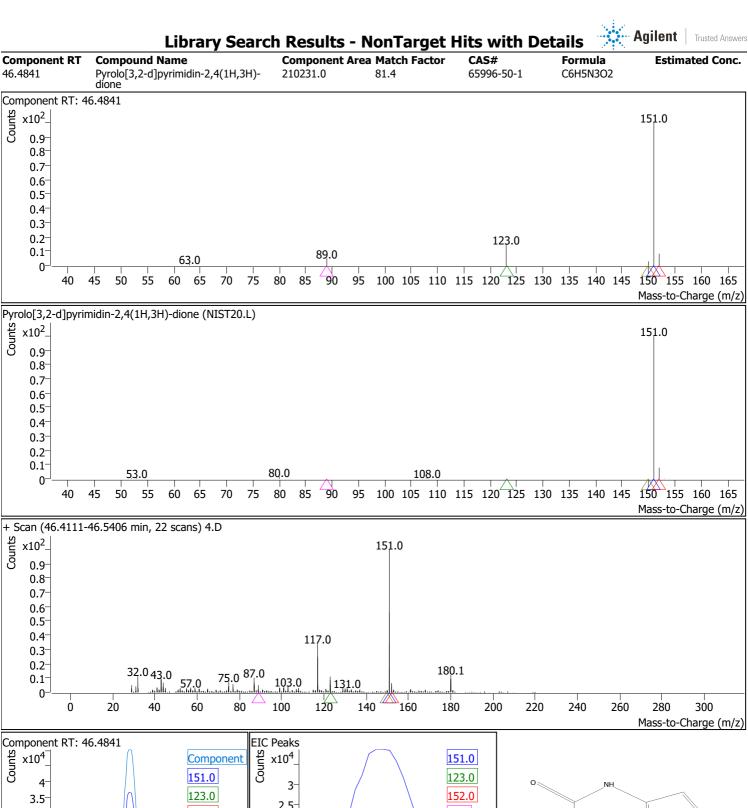
46.4

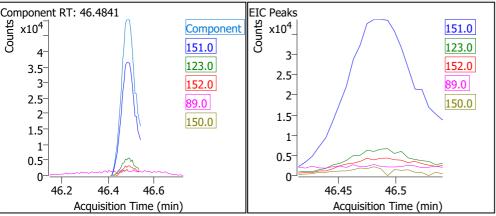
Acquisition Time (min)

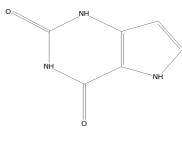
### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 14609-79-1 46.2202 3-Pentanol, 2,2,4,4-tetramethyl-744700.7 78.0 C9H20O Component RT: 46.2202 Counts $x10^{2}$ 87.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 31.0 42.0 0.2 56.0 45.0 0.1 30 70 120 130 10 20 50 60 80 100 110 140 150 160 Mass-to-Charge (m/z) 3-Pentanol, 2,2,4,4-tetramethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 87.0 0.8 0.7 0.6 0.5 57.0 69.0 0.4 0.3 0.2 45.0 0.1 29.0 77.0 83.0 144.0 30 10 20 40 50 60 70 80 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (46.1185-46.6893 min, 97 scans) 4.D St x10<sup>2</sup> 0.9 151.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 108.0 123.0 0.1 43.0 65.0 87.0 196.1 0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 46.2202 EIC Peaks st x10<sup>4</sup> Counts x10<sup>4</sup> 87.0 Component 87.0 41.0 7 2.5 ОН 31.0 31.0 6 2





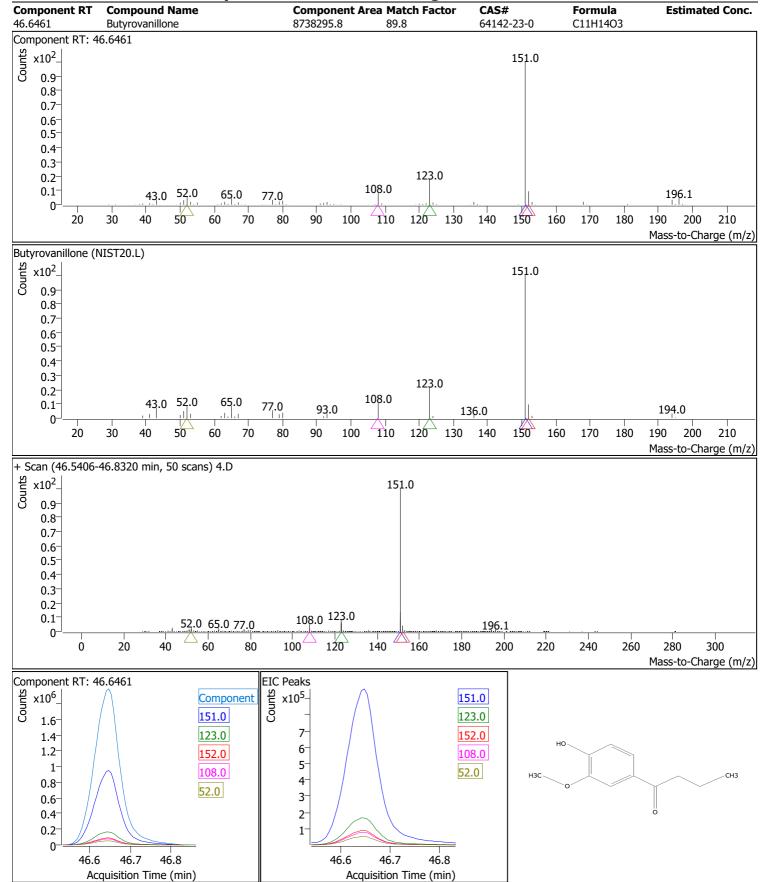












### ... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 47.0820 (E)-2,6-Dimethoxy-4-(prop-1-en-1-306538.1 76.4 C11H14O3 yl)phenol Component RT: 47.0820 x10<sup>2</sup>\_ 194.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 91.0 119.0 131.0 151.0 $0.2^{-}$ 77.0 179.0 0.1 0-**9**0 10 20 30 50 70 80 100 110 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 97.0 85.0 0 90 · 20 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) + Scan (47.0189-47.2148 min, 33 scans) 4.D st x10<sup>2</sup> 194.1 0.8 0.7 43.0 0.6 117.0 99.0 0.5 32.0 87.1 151.0 0.4 0.3 77.0 131.0 0.2 179.0 0.1 0 80 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 47.0820 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 194.0 Component 194.0 91.0 1.4 6 **Н3С** 91.0 151.0 1.2 5 87.0 151.0 1 4 119.0 119.0 НО 0.8

47.05 47.1

47.15

Acquisition Time (min)

3

2

1

47.1

87.0

47.2

Acquisition Time (min)

0.6

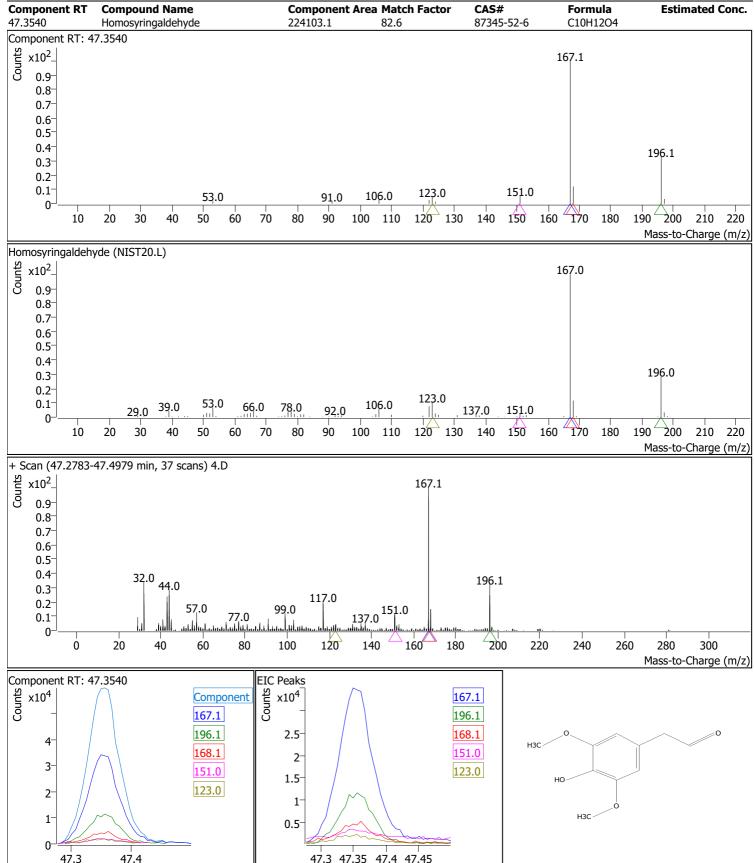
0.4

0.2

НЗС







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 48.9895 Benzenepropanol, 4-hydroxy-3-5515590.4 96.4 C10H14O3 methoxy-Component RT: 48.9895 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 182.0 0.4 0.3 $0.2^{-}$ 122.0 77.0 91.0 0.1 107.0 0-140 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 180 190 200 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 53.0 0.1 31.0 39.0 149.0 164.0 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 (48.8550-49.2340 min, 63 scans) 4.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 <sub>107.0</sub> <sup>122.0</sup> 0.1 149.0 39.0 0 Ó 40 60 100 140 180 260 20 80 120 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 48.9895 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup>\_ 137.0 Component 182.0 137.0 2-6 182.0 1.75 138.0 5 1.5 138.0 122.0 1.25 4 123.0 122.0

49

49.1 49.2

Acquisition Time (min)

1

0.75

0.5

0.25

123.0

3

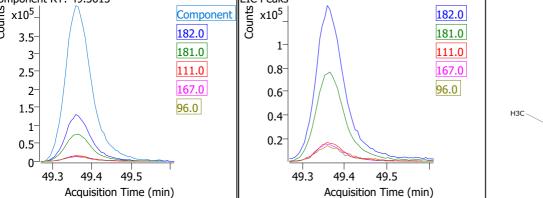
2

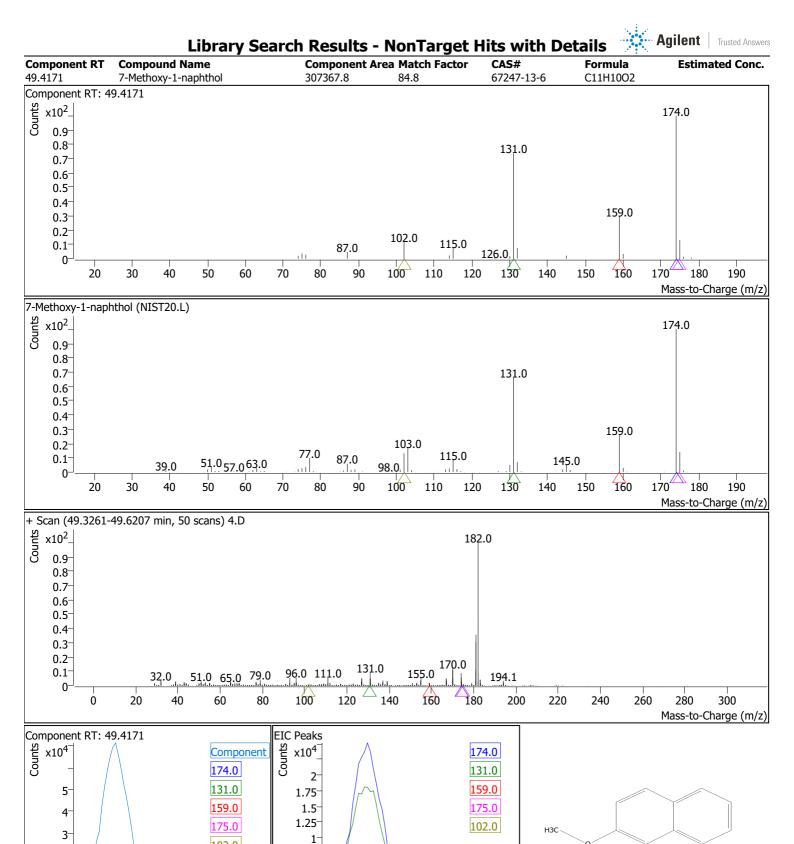
1

49

49.2

### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 49.3613 Benzaldehyde, 4-hydroxy-3,5-2047327.7 96.5 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3613 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 7<u>9</u>.0 0.1 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) 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 0.2 39.0 65.0 93.0 111.0 139.0 167.0 51.0 79.0 15.0 29.0 153.0 0.1 123.0 43.0 0 170 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 180 190 Mass-to-Charge (m/z) + Scan (49.2786-49.6141 min, 56 scans) 4.D x10<sup>2</sup>\_ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 170.0 131.0 96.0 111.0 0.1 155.0 79.0 39.0 51.0 65.0 194.1 0 100 180 Ó 20 40 60 80 120 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3613 **EIC Peaks** Counts Counts x10<sup>5</sup>\_ x10<sup>5</sup> 182.0 Component 0 181.0 182.0 3.5 1 181.0 111.0 3 0.8 2.5 111.0 167.0







49.5

Acquisition Time (min)

49.6

102.0

2-

1

49.4

49.5

Acquisition Time (min)

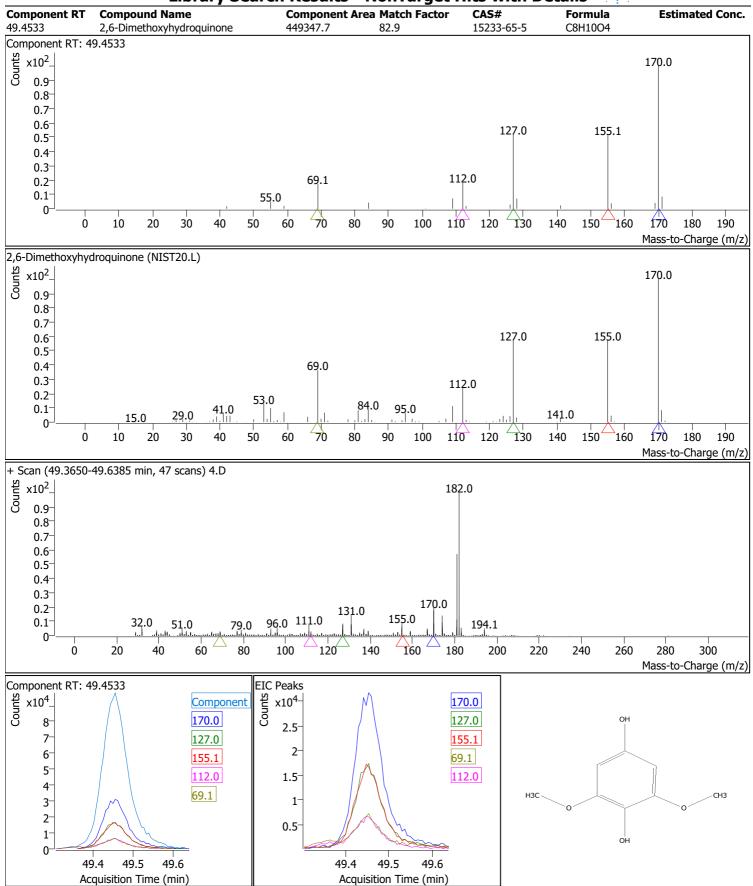
0.75

0.5

0.25







··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 50.4244 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-321466.5 91.8 65996-50-1 C6H5N3O2 Component RT: 50.4244 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3  $0.2^{-}$ 0.1 77.0 148.1 91.0 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 40 55 65 80 85 90 Mass-to-Charge (m/z) Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L)  $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 80.0 108.0 0 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 55 60 65 70 80 85 90 Mass-to-Charge (m/z) + Scan (50.3227-50.5721 min, 42 scans) 4.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 169.0 0.3 81.0 109.0 0.2 53.0 65.0 32.0 95.0 123.0 0.1 183.0 228.1 139.0 0 40 80 120 300 Ó 20 60 100 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) Component RT: 50.4244 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup>-151.0 Component 152.0 151.0 5 4 152.0 77.0 3.5 77.0 148.1 3

50.4

50.5

Acquisition Time (min)

120.0

3

2

1

50.4

50.5

Acquisition Time (min)

148.1

120.0

2.5<sup>-</sup>

1.5<sup>-</sup>

### --- 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-hydroxy-3-(4-hydroxy- 212350.2 3-methoxyphenyl)-51.7398 89.7 4899-74-5 C10H12O4 Component RT: 51.7398 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 196.1 $0.2^{-}$ 122.0 94.0 0.1 77.0 66.0 151.0 208.0 0-140 190 200 120 10 20 30 40 50 60 70 80 90 100 110 130 150 160 170 180 210 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 196.0 0.3 94.0 0.2 122.0 31.0 39.0 0.1 55.0 65.0 107.0 0 190 200 10 20 30 60 70 80 90 100 110 120 130 140 150 160 170 180 210 Mass-to-Charge (m/z) + Scan (51.6671-51.8304 min, 27 scans) 4.D x10<sup>2</sup>. 137.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 0.2 196.0 44.0 151.0 <sup>169.0</sup> 57.071.0 0.1 122.0 0 200 20 40 60 80 100 120 140 160 180 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) Component RT: 51.7398 **EIC Peaks** Counts Counts x10<sup>4</sup> 137.0 x10<sup>4</sup> Component 196.1 137.0 H<sub>3</sub>C 2.5 196.1 122.0 3.5 138.0 122.0 2 3



51.7

Acquisition Time (min)

51.8

94.0

2.5

1.5

0.5

2

1

51.7

Acquisition Time (min)

51.8

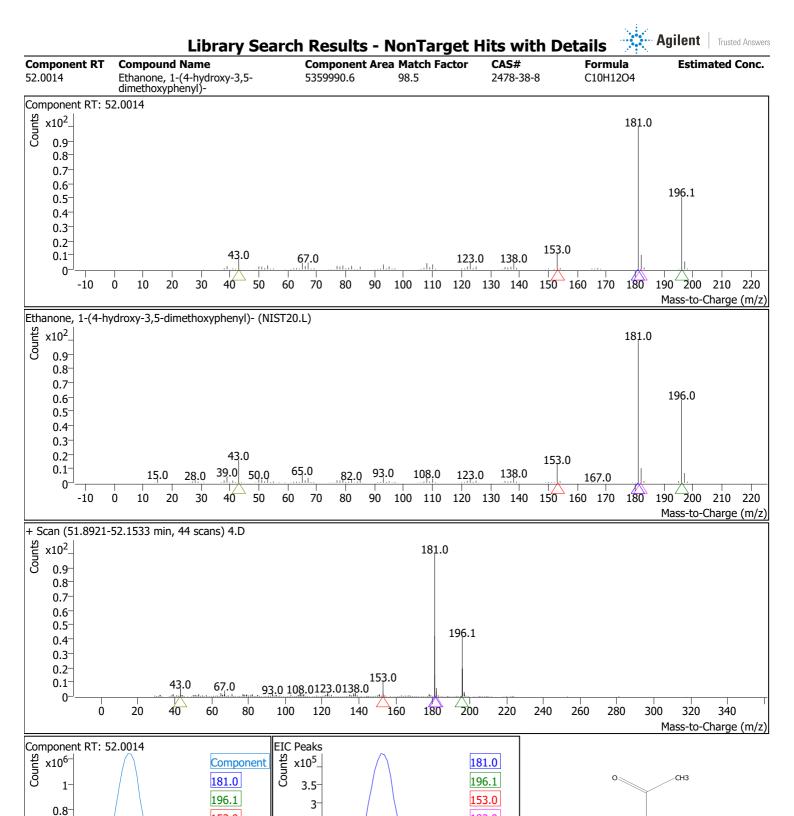
138.0

94.0

1.5

1

51.6



52

52.1

Acquisition Time (min)

182.0

43.0

153.0

182.0

43.0

0.6

0.4

0.2

0

52

52.1

Acquisition Time (min)

2.5

2

1

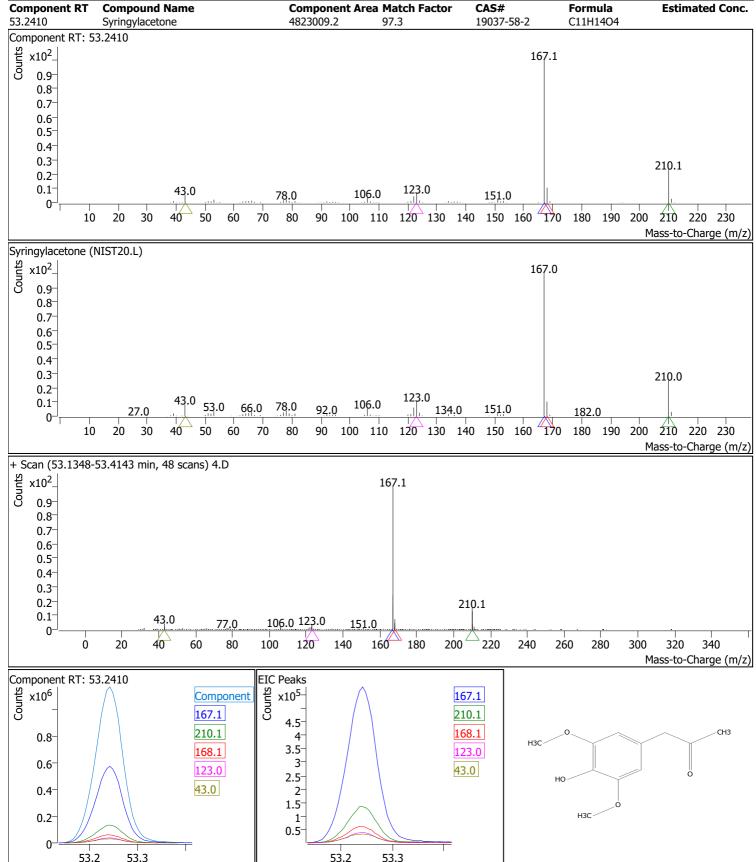
1.5

0.5

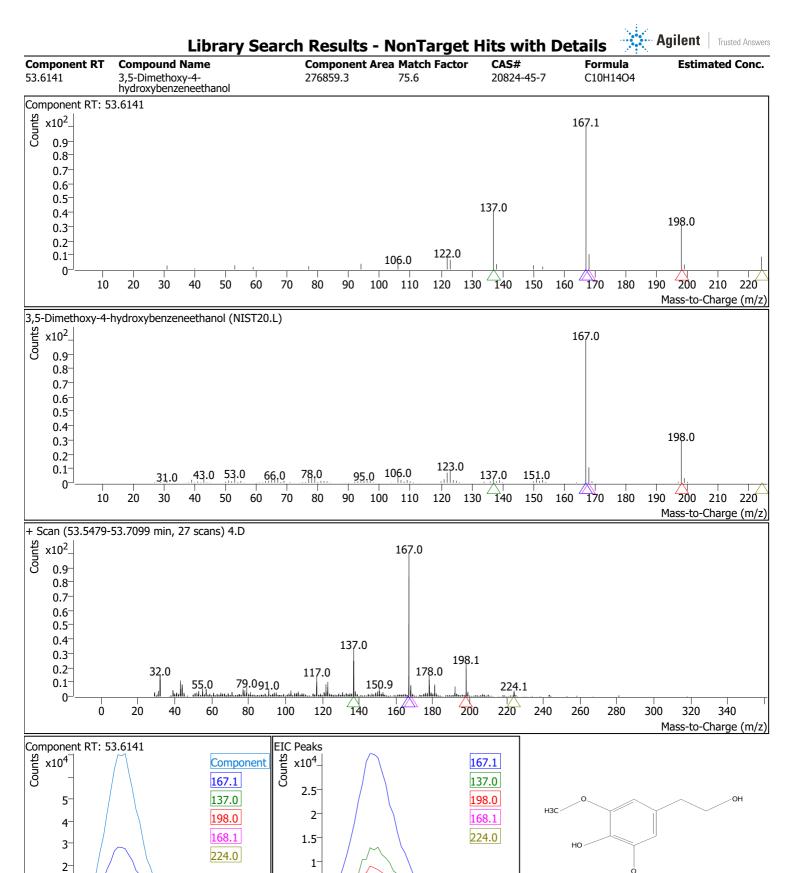
ОН







Acquisition Time (min)



53.6 53.65 53.7

Acquisition Time (min)

0.5

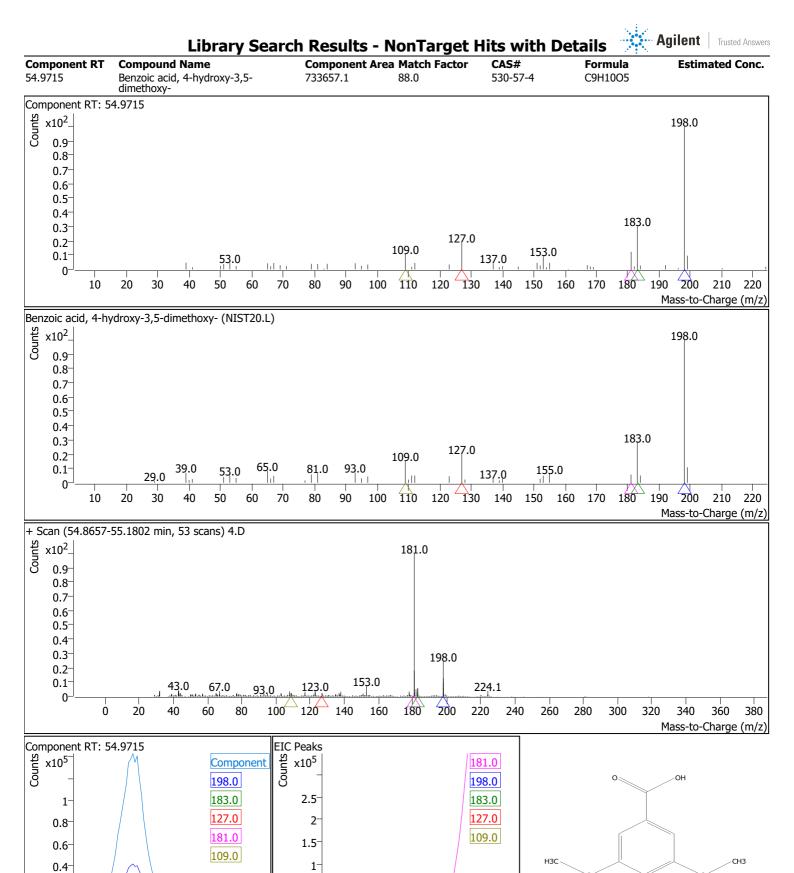
1

53.6

53.7

Acquisition Time (min)

H3C



55

55.1

Acquisition Time (min)

0.5

54.9

0.2

54.9

55

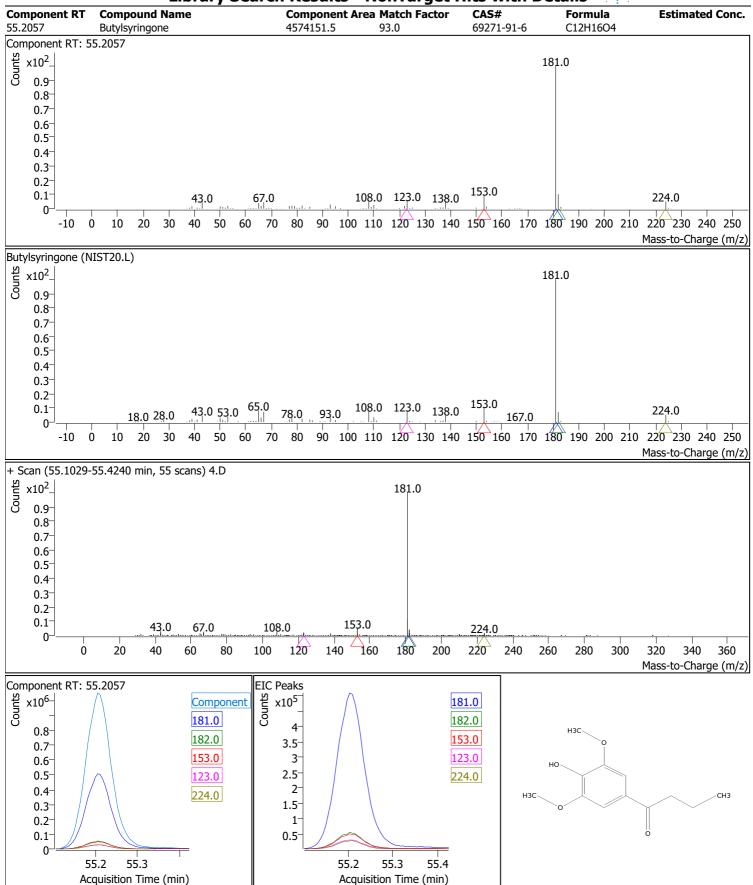
Acquisition Time (min)

55.1

ОН

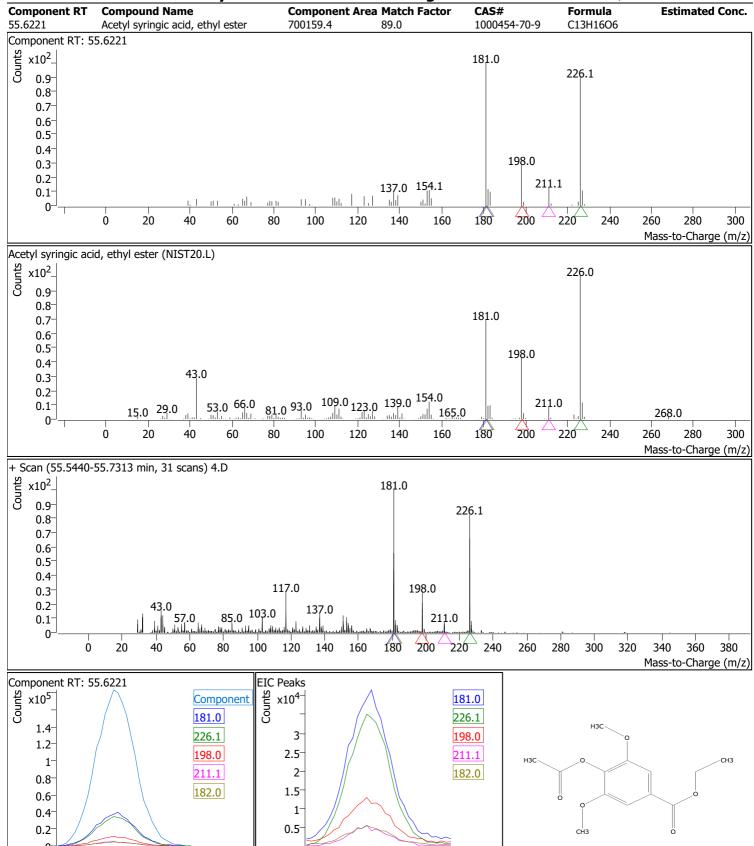












55.6

55.65

Acquisition Time (min)

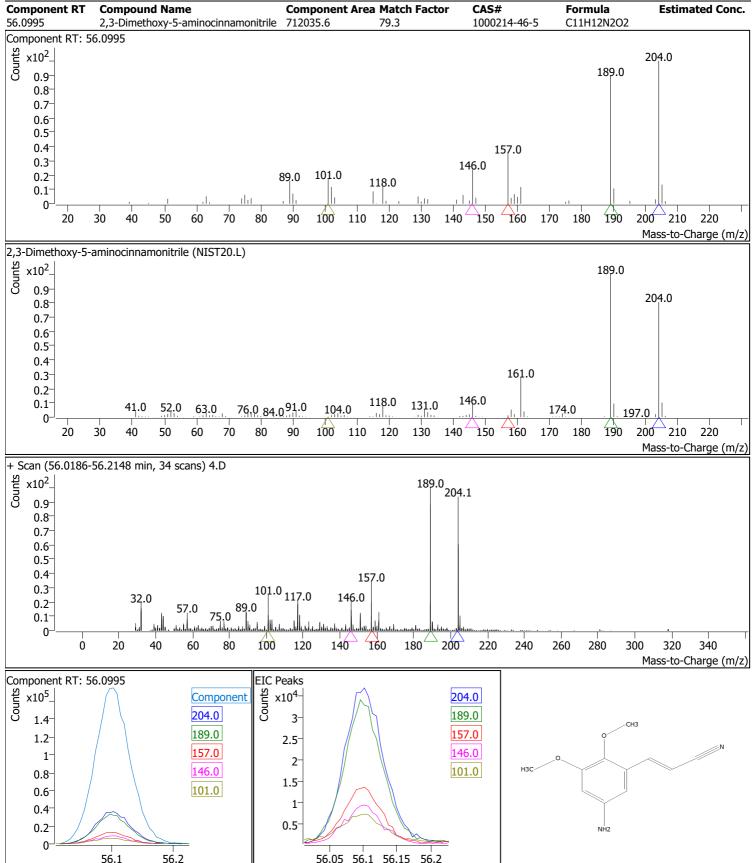
55.7

55.6 55.65

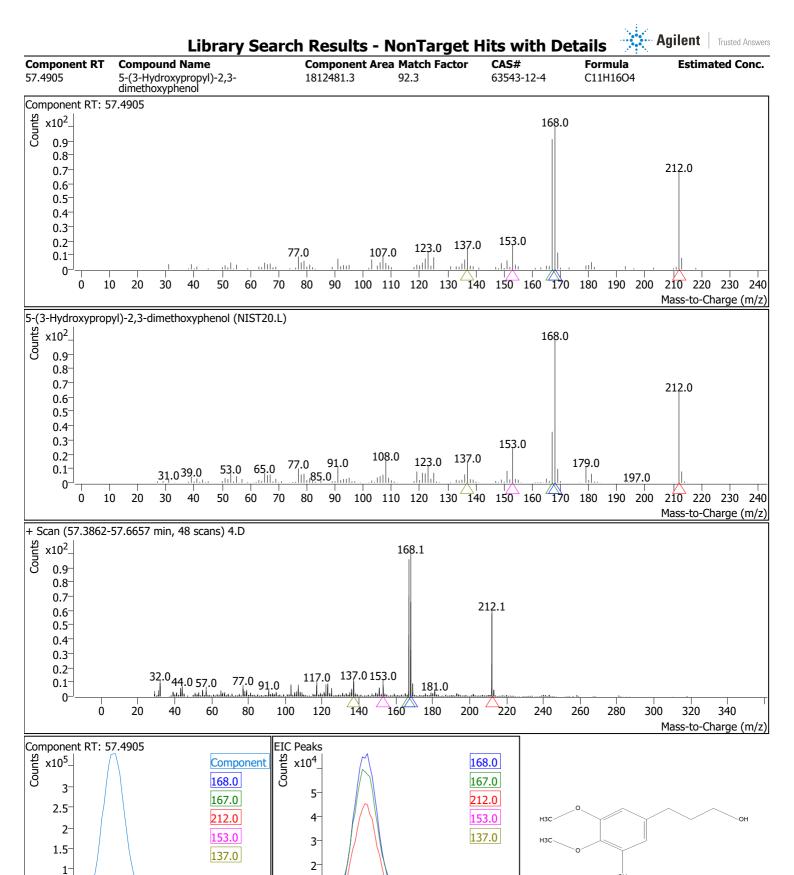
Acquisition Time (min)







Acquisition Time (min)



57.5

57.6

Acquisition Time (min)

57.7

0.5

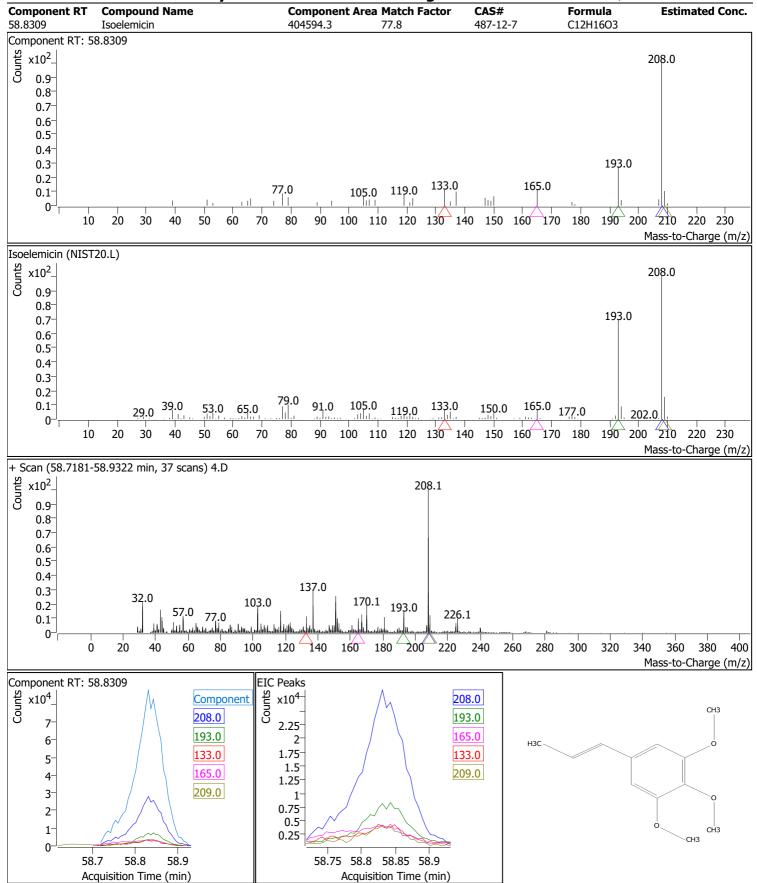
57.5

57.6

Acquisition Time (min)







### Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 6114-18-7 66.3332 (E)-9-Octadecenoic acid ethyl ester 421940.8 78.5 C20H38O2 Component RT: 66.3332 $x10^{2}$ 55.0 0.9 0.8 69.1 88.0 $0.7^{-}$ 97.0 0.6 41.1 264.0 0.5 0.4 0.3 0.2 0.1 310.1 0 20 80 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) (E)-9-Octadecenoic acid ethyl ester (NIST20.L) Counts 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 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) + Scan (66.3252-66.3695 min, 7 scans) 4.D St x10<sup>2</sup> 0.9 117.0 0.8 $0.7^{-}$ 55.1 43.0 0.6 0.5 $0.4^{-}$ 96.1 137.1 167.0 81.0 0.3 0.2 32.0 264.2 207.0 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 Mass-to-Charge (m/z) EIC Peaks Component RT: 66.3332 Counts Sounds x10<sup>5</sup> 0.9 x10<sup>3</sup> 55.0 Component 55.0 69.1 0.8 69.1 83.1 6 0.7 88.0 97.0

88.0

5

4

66.2

66.3

66.4

Acquisition Time (min)

66.5

83.1

97.0

66.2 66.3 66.4 66.5

Acquisition Time (min)

0.6

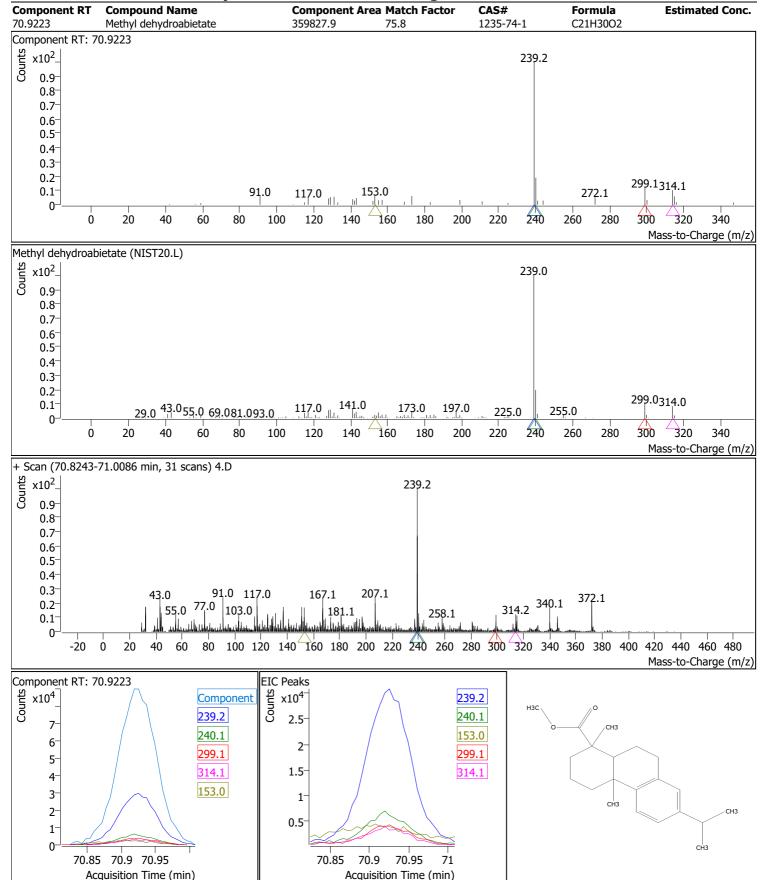
0.5

0.4

0.3 0.2-0.1

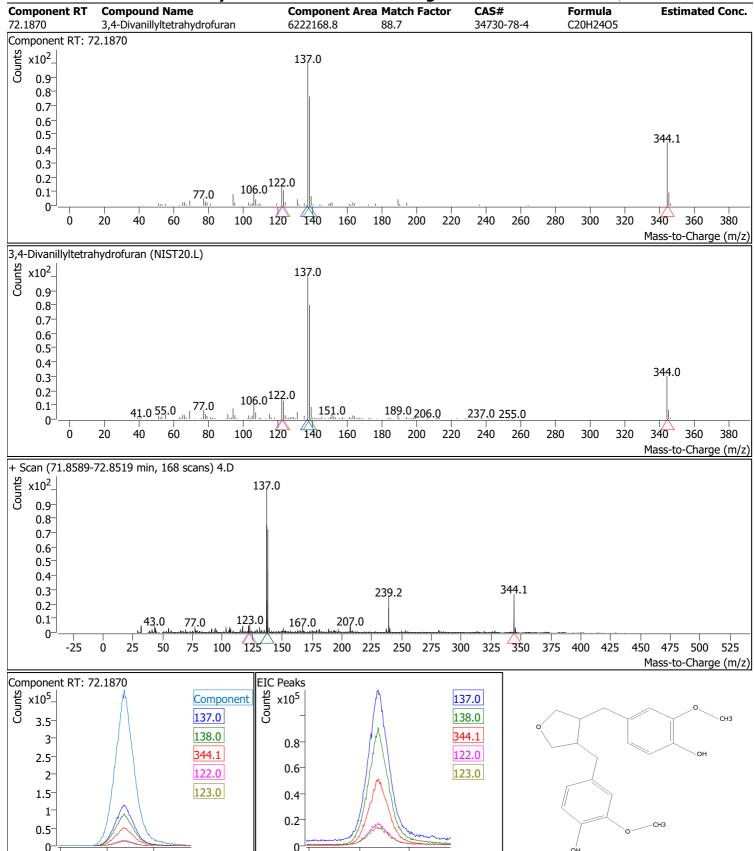








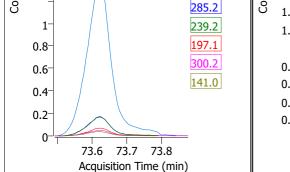


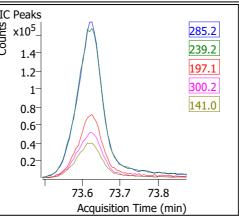


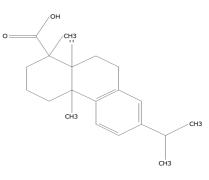
72

72.5 Acquisition Time (min)

72.5







## --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 75.3519 Undecane, 4-cyclohexyl-739647.2 77.0 13151-79-6 C17H34 Component RT: 75.3519 v10<sup>2</sup> 0.9 155.0 55.0 83.0 0.8 69.0 97.0 $0.7^{-}$ 43.0 0.6 0.5 0.4 0.3 0.2 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 80 Mass-to-Charge (m/z) Undecane, 4-cyclohexyl- (NIST20.L) st x10<sup>2</sup> 0.9 83.0 57.0 0.8 0.7 43.0 0.6 0.5 71.0 97.0 0.4 0.3 29.0 0.2 0.1 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 10 20 30 50 Mass-to-Charge (m/z) + Scan (75.2879-75.4443 min, 27 scans) 4.D st x10<sup>2</sup> 0.9 181.0 0.8 $0.7^{-}$ 0.6 0.5 151.0 $0.4^{-}$ 0.3 167.0 207.0 0.2 41.0 137.0 69.1 97.0 280.1 0.1 340.1 25 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 -25 Mass-to-Charge (m/z) EIC Peaks Component RT: 75.3519 v10<sup>4</sup>-Counts x10<sup>3</sup> Component 55.0 155.0 57.0 6 155.0 55.0 6

75.2

75.4 Acquisition Time (min)

69.0

5

57.0

83.0

69.0

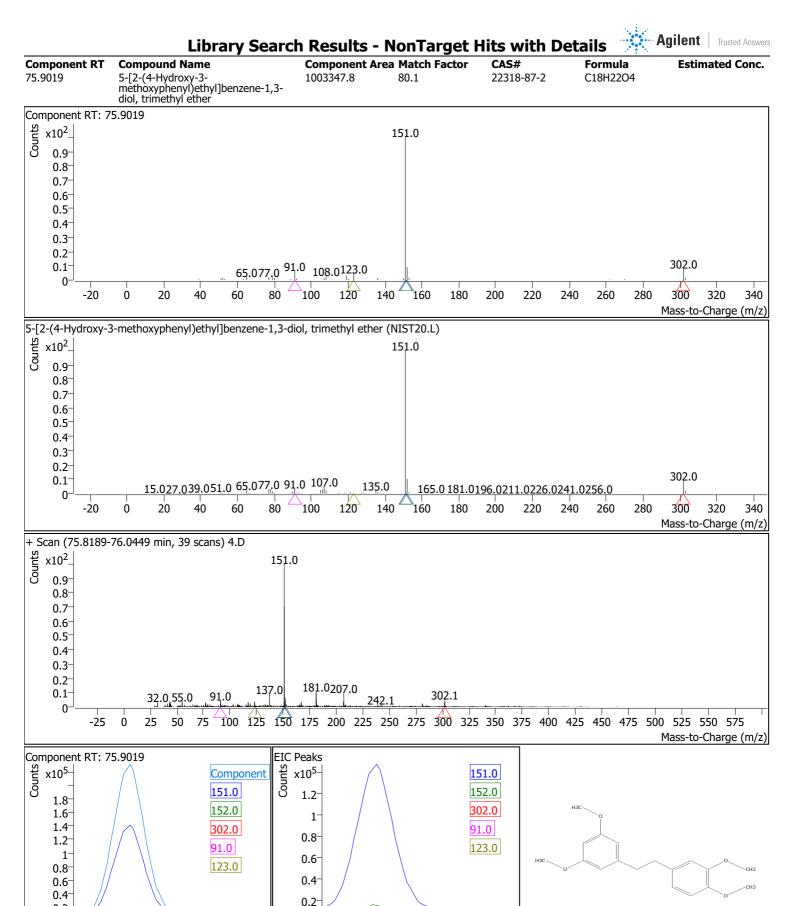
5

4 3

2 1 0-

75.2

75.4



75.9

76

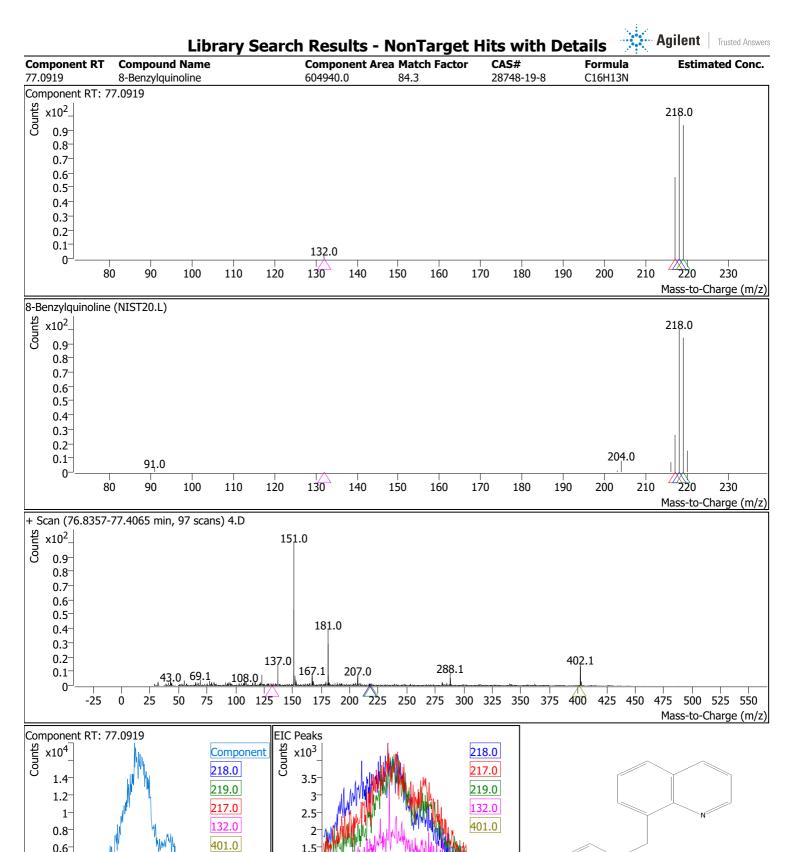
Acquisition Time (min)

0.2

75.9

Acquisition Time (min)

76



77 77.5 Acquisition Time (min)

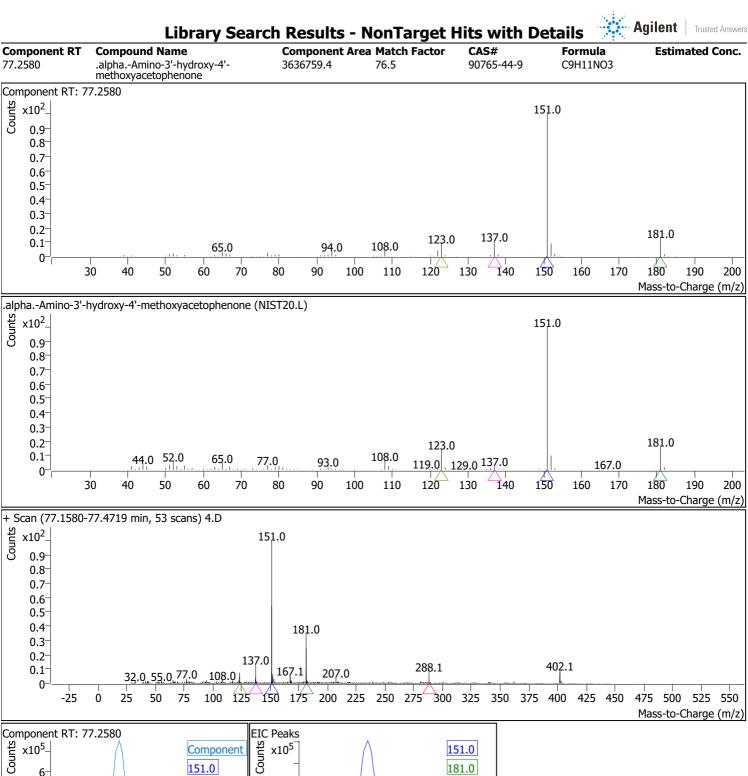
76.5

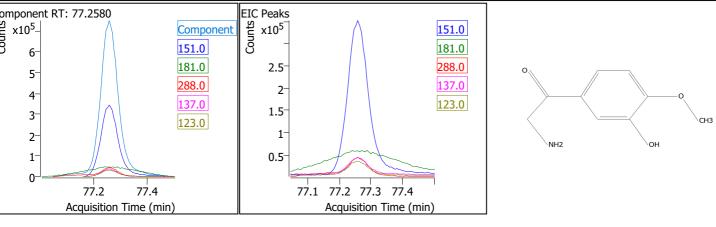
0.6

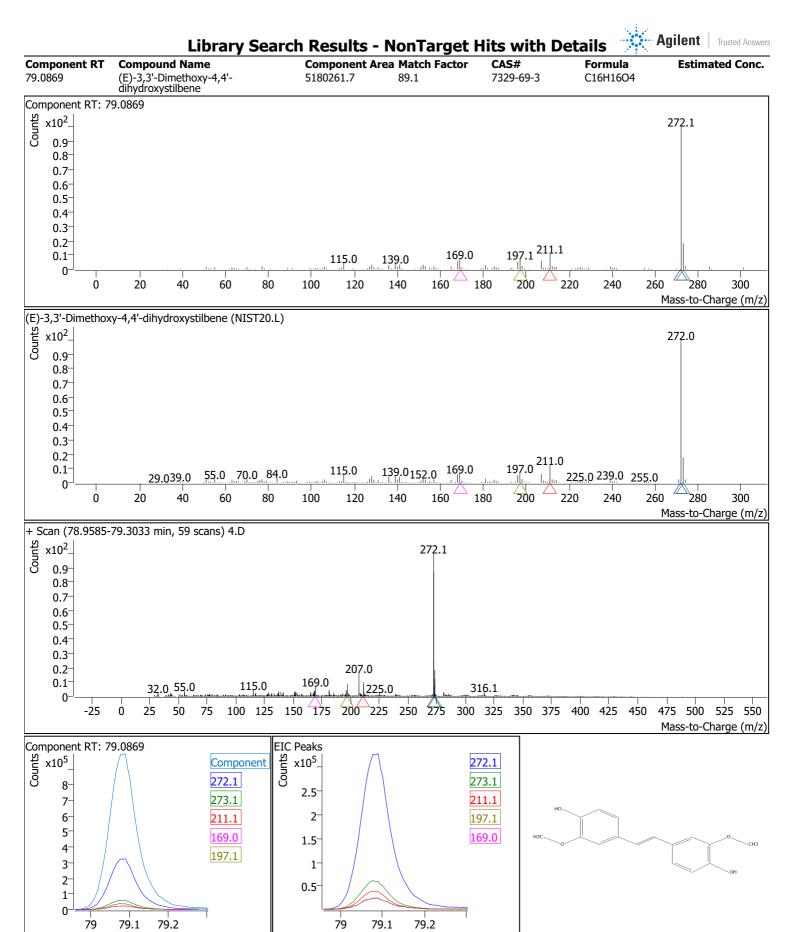
77

76.5

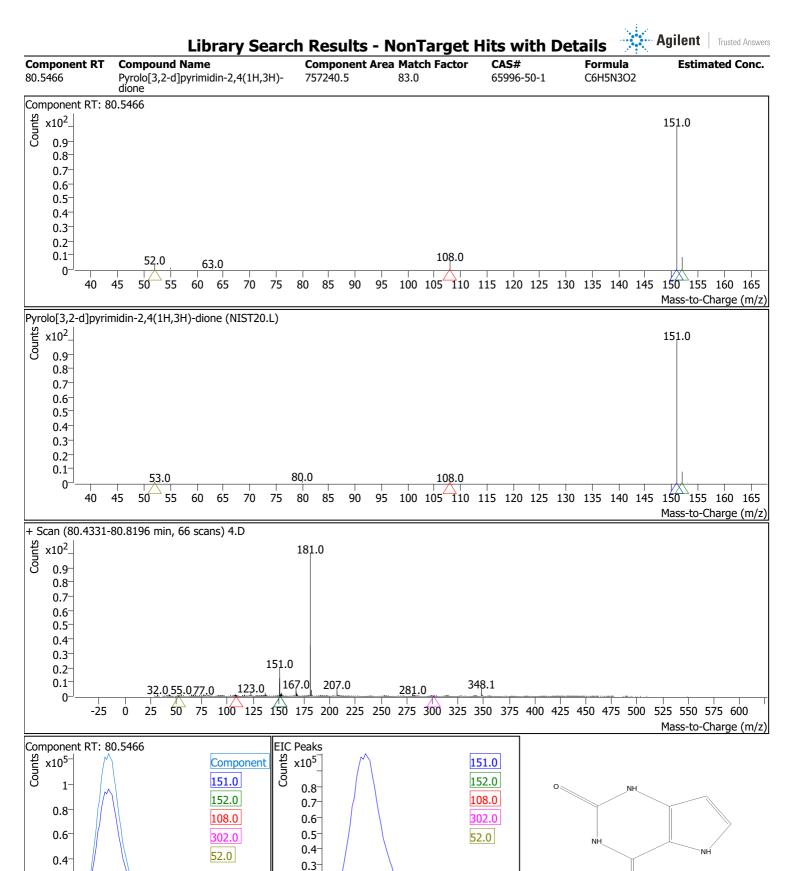
77.5







Acquisition Time (min)



80.7

Acquisition Time (min)

80.6

 $0.2^{-}$ 

0.1

80.5

0.2

80.5 80.6 80.7 80.8