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

Dil.



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

Analysis File Name 240502 data.uaf

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

File Name 6.D Sample Name 6 Acq. Method File 2405

 Acq. Method File
 240501 scan

 Acq. Date-Time
 5/1/2024 9:10:53 PM

**Instrument Name** GCMSD

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

 Sample Type
 Sample

 Acq. Method Path
 D:\MassHunter\GCMS\1\methods\RBEL\

Acq. Method Path D:\MassHunter\GCMS\1\methods\RE Acq. Operator

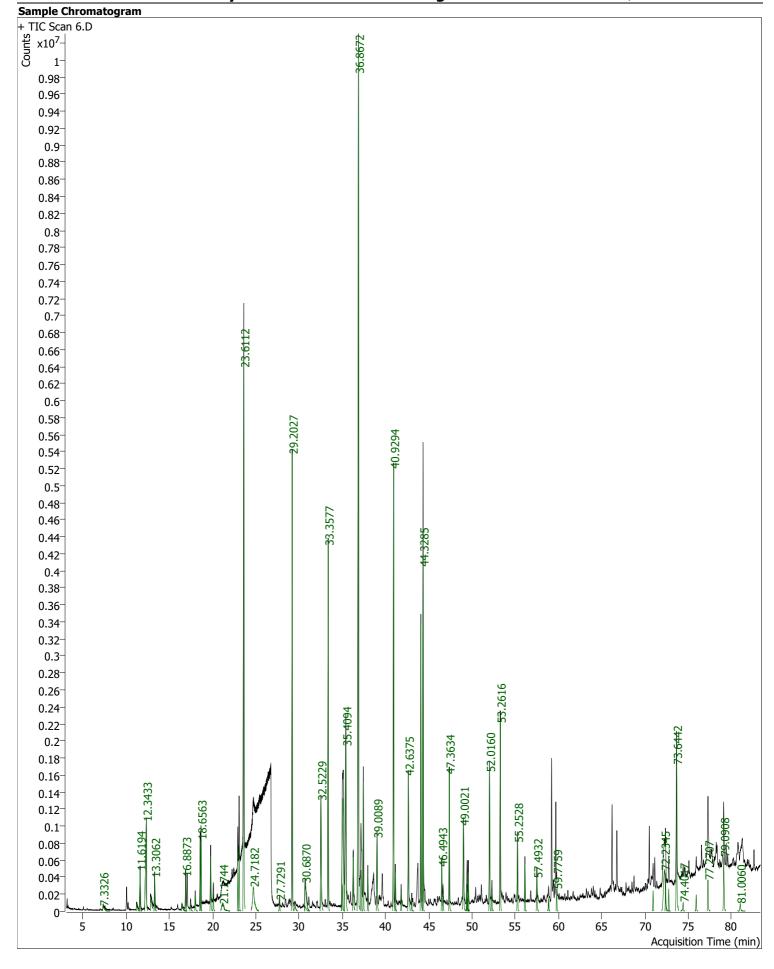
1

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Component R	Г Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
7.3326	1,3-Propanediol	504-63-2	C3H8O2	714818.8	91.9	
11.2158	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	563489.6	87.4	
11.6194	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	2247236.6	76.7	
11.6194	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	2243713.4	76.0	
12.3433	Butyrolactone	96-48-0	C4H6O2	8140677.7	97.5	
12.8266	Methyltartronic acid	595-98-2	C4H6O5	1577576.0	94.7	
13.3027	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	1297134.3	79.9	
13.3062	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	1883411.8	79.5	
16.4521	Glycerol triethyl ether	162614-45-1	C9H20O3	734568.5	77.3	
16.8873	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	1710064.4	85.0	
17.4456	Silane, diethoxydimethyl-	78-62-6	C6H16O2Si	526966.0	75.7	
17.9884	Phenol	108-95-2	C6H6O	866359.9	96.3	
18.5714	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	3553782.7	93.8	
18.6563	Diisoamyl ether	544-01-4	C10H22O	3120389.9	95.2	
19.7780	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2840962.6	94.8	
20.0885	1,2-Cyclopentanedione, 3-methyl-	765-70-8	C6H8O2	981151.7	93.8	
21.1744	1,3,5-Trioxane	110-88-3	C3H6O3	1720991.0	78.1	
22.9155	1-Propanol, 2-(2-hydroxypropoxy)-	106-62-7	C6H14O3	1692274.3	79.3	
23.0619	1-Octanol	111-87-5	C8H18O	3613372.9	98.2	
23.6112	Phenol, 2-methoxy-	90-05-1	C7H8O2	29247888.8	98.8	
24.7182	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	4468103.0	84.7	
27.7291	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	575552.3	82.0	
29.2027	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	21358387.2	99.4	
29.5243	Alpha-monopropionin	624-47-5	C6H12O4	550139.5	79.2	
30.6774	2-Propenenitrile	107-13-1	C3H3N	552831.9	76.7	
30.6870	Catechol	120-80-9	C6H6O2	3885535.5	97.6	
32.5229	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	7083077.6	98.6	
33.3577	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	16443804.0	97.3	
35.0048	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	1415607.5	90.7	
35.1003	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	14376090.0	78.7	
35.4094	Butanoic acid, anhydride	106-31-0	C8H14O3	13819611.4	81.9	
36.2609	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	3342384.4	83.3	
36.8672	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	51337962.3	99.0	
37.1504	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	1989128.4	86.2	
37.4339	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	5560185.8	95.1	
37.9466 39.0089	3,5-Dimethoxy-4-hydroxytoluene Vanillin	6638-05-7 121-33-5	C9H12O3 C8H8O3	1494192.0 3824794.5	89.1 97.6	
40.9294	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	21633743.3	94.9	
41.1262	trans-Isoeugenol	5932-68-3	C10H12O2	1733740.0	82.2	
41.7923		97-53-0	C10H12O2	823723.3	87.6	
42.6375	Eugenol Apocynin	498-02-2	C9H10O3	7279608.1	99.2	
43.0266	Benzene, 1,2,3-trimethoxy-5-methyl-	6443-69-2	C10H14O3	555999.9	76.4	
44.0803	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	12818195.4	98.9	
44.3285	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	19517366.6	94.6	
44.3369	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6866421.4	89.3	
46.4943	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	2308676.4	97.2	
46.6397	Butyrovanillone	64142-23-0	C11H14O3	722605.7	90.4	
47.3634	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	6150550.2	97.6	
49.0021	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	5666194.8	96.3	
49.3716	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	997348.6	89.1	
49.4217	2-Naphthalenol, 3-methoxy-	18515-11-2	C11H10O2	1437666.1	88.9	
49.4510	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	703839.4	85.8	
49.5619	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	1756204.0	83.7	
52.0160	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	6877453.8	98.2	
52.2970	.beta(4-Hydroxy-3-methoxyphenyl)propionic acid		C10H12O4	1012420.5	93.4	
53.2616	Syringylacetone	19037-58-2	C11H14O4	9081747.4	97.5	
55.2528	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5650-43-1	C11H14O4	3458786.7	95.3	
56.1115	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	2247489.4	83.9	
57.4932	Dihydrosyringenin	20736-25-8	C11H16O4	1741404.6	94.0	
58.8395	Asarone	2883-98-9	C12H16O3	673422.3	80.8	
58.8395	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-	487-11-6	C12H16O3	652475.8	79.6	
59.7759	8-Amino-6,7-dimethoxy-4-methylquinoline	1000213-07-2	C12H14N2O2	1071121.5	75.2	
70.9260	Methyl dehydroabietate	1235-74-1	C21H30O2	953706.2	87.3	
72.2345	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	7449482.9	79.8	
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## **Library Search Results - NonTarget Hits with Details**

Agilent Trus	ted Answers
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Component	: RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
72.3682	Methyl dehydroabietate	1235-74-1	C21H30O2	1779470.9	75.1	
72.7346	1-(2,4-Dihydroxyphenyl)-2-(3,4- dimethoxyphenyl)ethanone	24126-98-5	C16H16O5	1094225.5	83.7	
73.6442	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	9080573.5	94.0	
74.4017	N-(3-Amino-4-methoxyphenyl)-3,5- dimethoxybenzamide	1000435-48-0	C16H18N2O4	544902.8	80.0	
75.9096	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	862218.0	80.3	
77.2707	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	1791299.4	95.1	
79.0908	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	3638405.6	86.8	
81.0060	Phenol, 4,4'-methylenebis[2,6-dimethoxy-	15640-40-1	C17H20O6	611649.7	83.2	



#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 714818.8 504-63-2 C3H8O2 7.3326 1,3-Propanediol 91.9 Component RT: 7.3326 y x10<sup>2</sup> 0.9 57.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 45.0 0.2 0.1 40.0 55 15 25 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 75 5 10 15 20 25 30 35 40 45 50 65 80 Mass-to-Charge (m/z) + Scan (7.2972-7.7312 min, 73 scans) 6.D st x10<sup>2</sup> 0.9 57.0 0.8 0.7 31.0 0.6 0.5 $0.4^{-}$ 0.3 0.2 0.1 86.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 7.3326 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 57.0 Component 57.0 58.0 5 1.2 58.0 31.0 1 31.0 43.0 0.8

45.0

3

2

1

7.6

7.8

Acquisition Time (min)

45.0

43.0

0.6

0.4

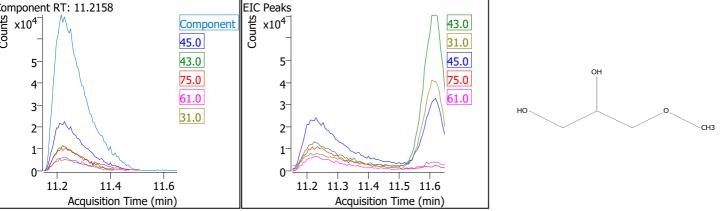
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7.4

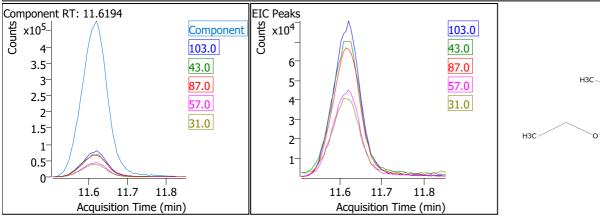
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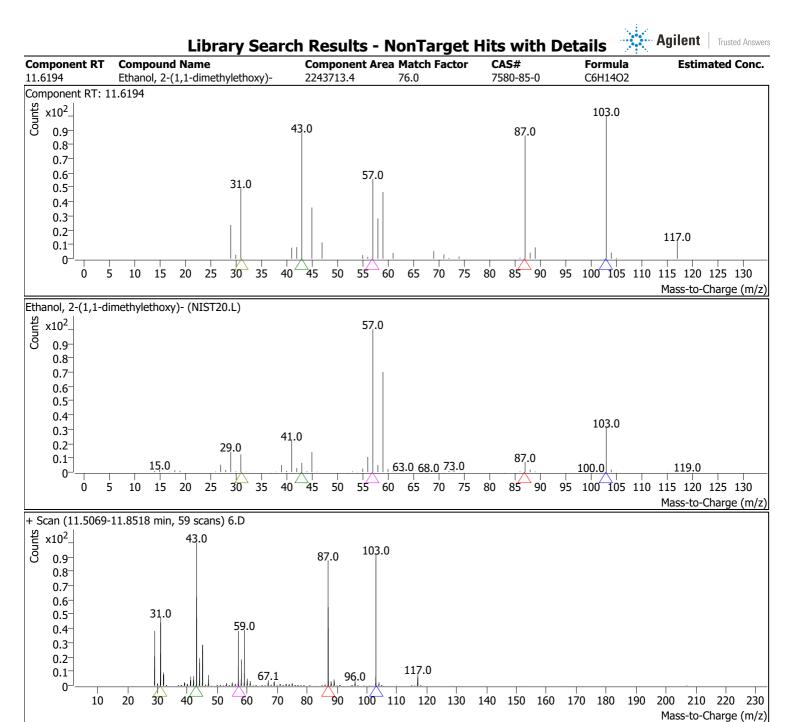
7.8

#### -- 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 11.2158 1,2-Propanediol, 3-methoxy-563489.6 87.4 C4H10O3 Component RT: 11.2158 v10<sup>2</sup> 0.9 45.0 0.8 $0.7^{-}$ 0.6 43.0 75.0 0.5 0.4 61.0 0.3 31.0 0.2 33.0 0.1 88.0 10 15 20 25 30 35 55 60 65 75 80 85 100 105 110 115 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 45.0 0.8 0.7 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 15.0 0.2 33.0 18.0 0.1 88.0 63.0 103.0 71.0 10 15 20 25 30 35 40 50 55 60 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (11.1601-11.5069 min, 59 scans) 6.D St x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 75.0 31.0 0.3 61.0 0.2 0.1 88.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.2158 **EIC Peaks** Counts Counts x10<sup>4</sup> Component 43.0 45.0 31.0



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 11.6194 Propane, 1,1-diethoxy-2247236.6 76.7 C7H16O2 Component RT: 11.6194 v10<sup>2</sup> 0.9 103.0 43.0 87.0 0.8 $0.7^{-}$ 0.6 57.0 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 90 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 131.0 130 0 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.5069-11.8518 min, 59 scans) 6.D St x10<sup>2</sup> 0.9 103.0 87.0 0.8 0.7 0.6 0.5 31.0 59.0 $0.4^{-}$ 0.3 0.2 117.0 0.1 96.0 67.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.6194 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>4</sup> 103.0 Component 103.0 43.0 6





103.0

EIC Peaks

Component

x10<sup>4</sup>

Component RT: 11.6194

#### -- 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 12.3433 Butyrolactone 8140677.7 97.5 C4H6O2 Component RT: 12.3433 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 0 25 55 75 85 20 30 35 40 45 50 65 70 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 0-20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (12.1315-12.4821 min, 59 scans) 6.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 29.0 0.3 86.0 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) Component RT: 12.3433 **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 29.0 86.0

12.3

12.4

Acquisition Time (min)

56.0

1.5

1

0.5

12.2

29.0

56.0

0.6

0.5  $0.4^{-}$ 

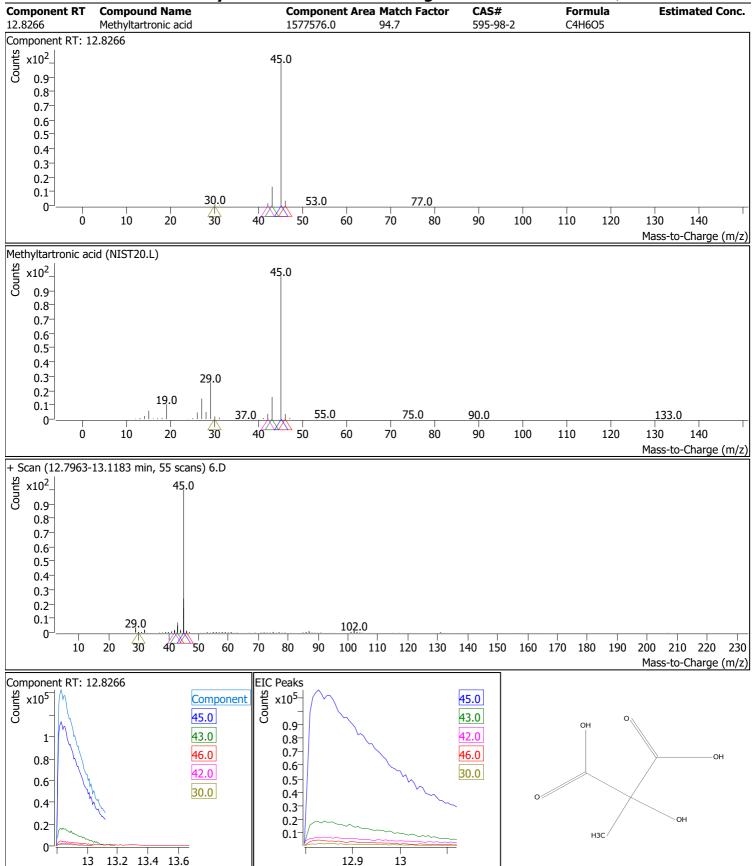
0.3 0.2-

0.1

12.2 12.3 12.4

# 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.** 2-(2-methoxyethoxy)propanoic acid, O-acetyl-79.9 13.3027 1297134.3 1000506-61-7 C8H14O5 Component RT: 13.3027 x10<sup>2</sup>\_ 103.0 0.9 8.0 59.0 0.7 0.6 0.5 43.0 31.0 0.4 0.3 $0.2^{-}$ 47.0 0.1 117.0 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) $x10^{2}$ 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 60 40 130 0 10 20 50 70 80 90 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (13.2081-13.5108 min, 51 scans) 6.D x10<sup>2</sup>. 0.9 103.0 0.8 0.7 0.6 0.5 87.0 57.0 0.4 31.0 0.3 0.2 0.1 117.1 0 30 60 190 200 210 220 230 10 20 40 50 70 80 90 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) EIC Peaks Component RT: 13.3027 Counts Counts x10<sup>4</sup> x10<sup>5</sup>-103.0 Component 103.0 2.25 43.0 59.0 31.0 5 1.75

13.3

13.4

Acquisition Time (min)

43.0

58.0

31.0

4

3

2

1.5

1

1.25

0.75

0.5

13.3

13.4

Acquisition Time (min)

59.0

58.0

нзс

#### --- 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 13.3062 Propane, 1,1-diethoxy-1883411.8 79.5 C7H16O2 Component RT: 13.3062 v10<sup>2</sup> 0.9 103.0 43.0 0.8 87.0 $0.7^{-}$ 0.6 57.0 0.5 31.0 0.4 0.3 0.2 0.1 0 40<sup>2</sup> 30 70 130 10 20 50 60 90 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 131.0 130 0 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (13.2087-13.4810 min, 46 scans) 6.D St x10<sup>2</sup> 0.9 103.0 0.8 0.7 0.6 0.5 87.0 57.0 $0.4^{-}$ 31.0 0.3 0.2 0.1 117.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 13.3062 EIC Peaks Counts Counts x10<sup>4</sup> 103.0 Component 103.0 43.0 3 43.0 87.0 5 2.5 Н3С < 87.0 57.0

13.3

13.4 Acquisition Time (min)

31.0

2

1.5

1 0.5

13.3

13.4

Acquisition Time (min)

57.0

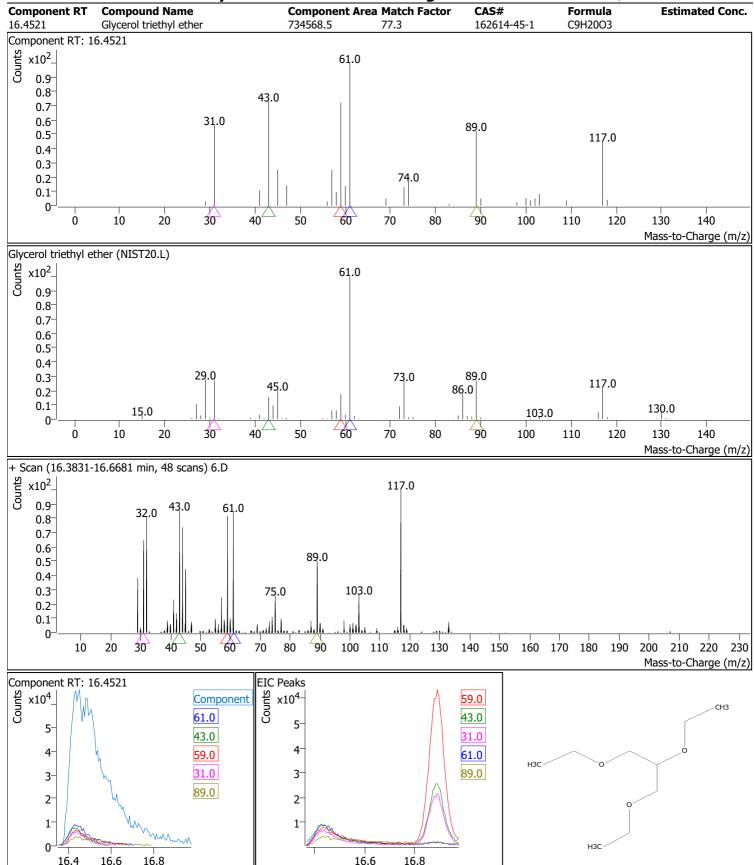
31.0

3

2

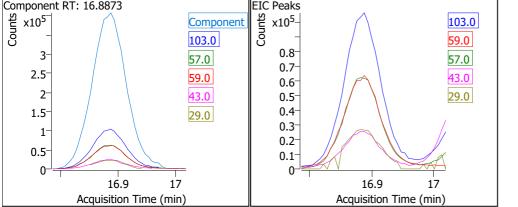






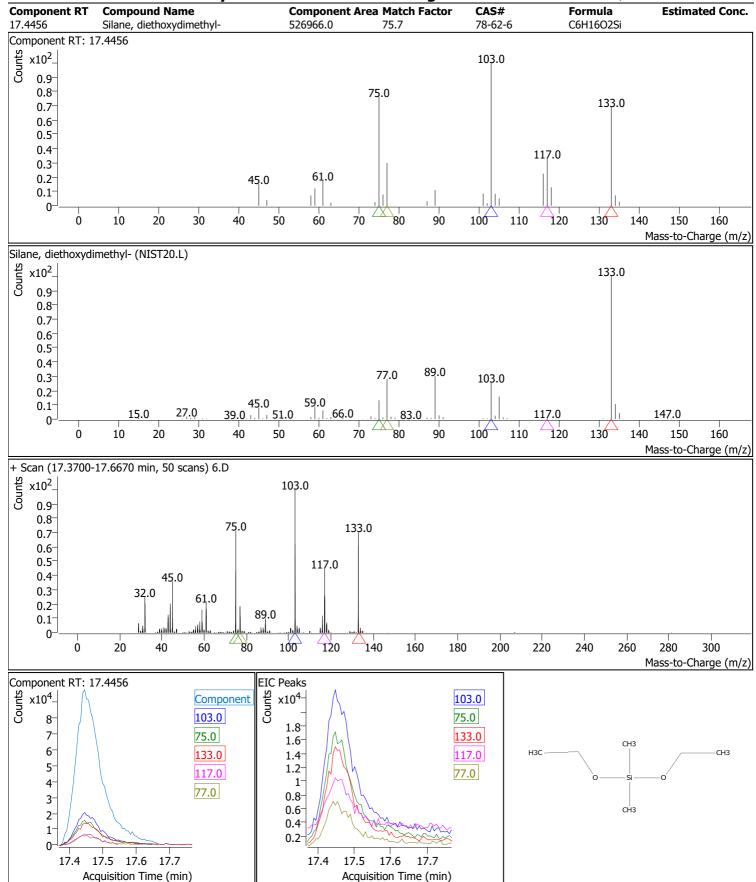
Acquisition Time (min)

#### --- 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 16.8873 1,3-Dioxolane-4-methanol, 2-ethyl-1710064.4 85.0 C6H12O3 Component RT: 16.8873 v10<sup>2</sup> 0.9 103.0 0.8 $0.7^{-}$ 57.0 0.6 0.5 0.4 0.3 43.0 29.0 131.0 0.2 0.1 30 100 130 Ó 10 20 40 50 60 70 80 90 110 120 140 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 30 0 10 20 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (16.7958-17.0189 min, 38 scans) 6.D St x10<sup>2</sup> 0.9 103.0 0.8 59.0 0.7 0.6 0.5 44.0 $0.4^{-}$ 0.3 29.0 0.2 131.0 0.1 117.0 88.0 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: 16.8873 x10<sup>5</sup>-103.0 Component 103.0 59.0



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





#### Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 108-95-2 C6H6O 17.9884 Phenol 866359.9 96.3 Component RT: 17.9884 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 63.0 55.0 50.0 25 40 55 75 85 90 95 20 30 35 45 50 60 65 70 80 100 Mass-to-Charge (m/z) Phenol (NIST20.L) S 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 (17.9197-18.2564 min, 57 scans) 6.D St x10<sup>2</sup> 0.9 94.0 0.8 0.7 0.6 0.5 0.4 61.0 0.3 32.0 43.0 0.2 0.1 103.0 117.0 133.0 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 17.9884 Counts Counts x10<sup>4</sup> 94.0 Component 94.0 66.0 6 1.4 66.0 65.0 1.2 5 39.0 65.0 1 4

18.1

Acquisition Time (min)

18.2

39.0

40.0

18.1

Acquisition Time (min)

18.2

3-

2-

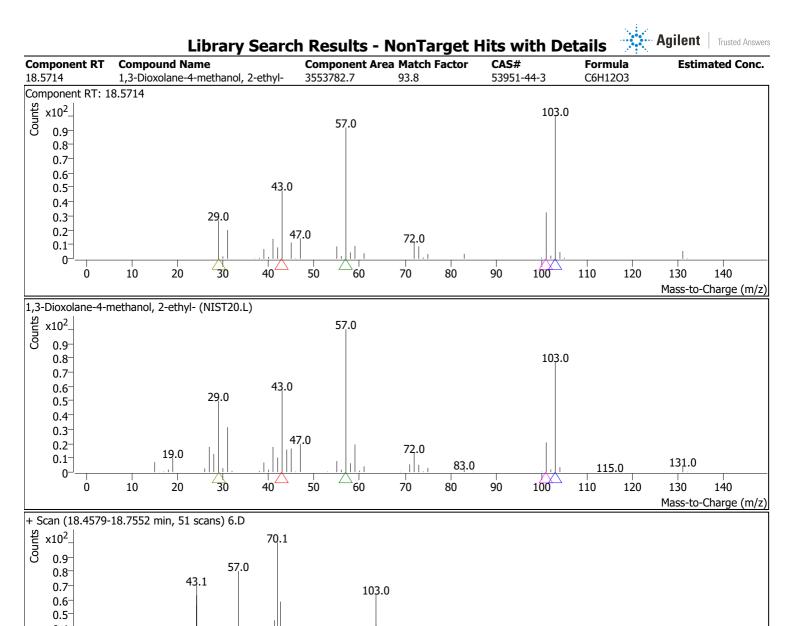
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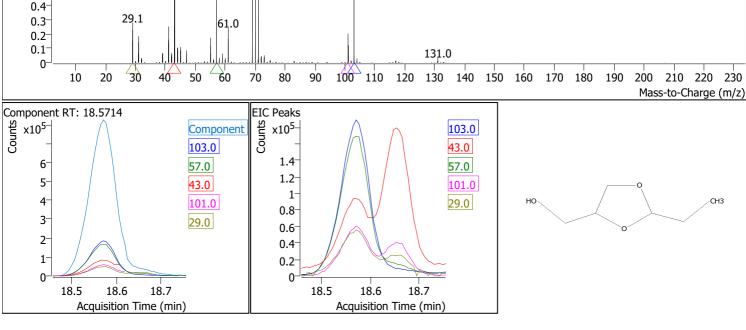
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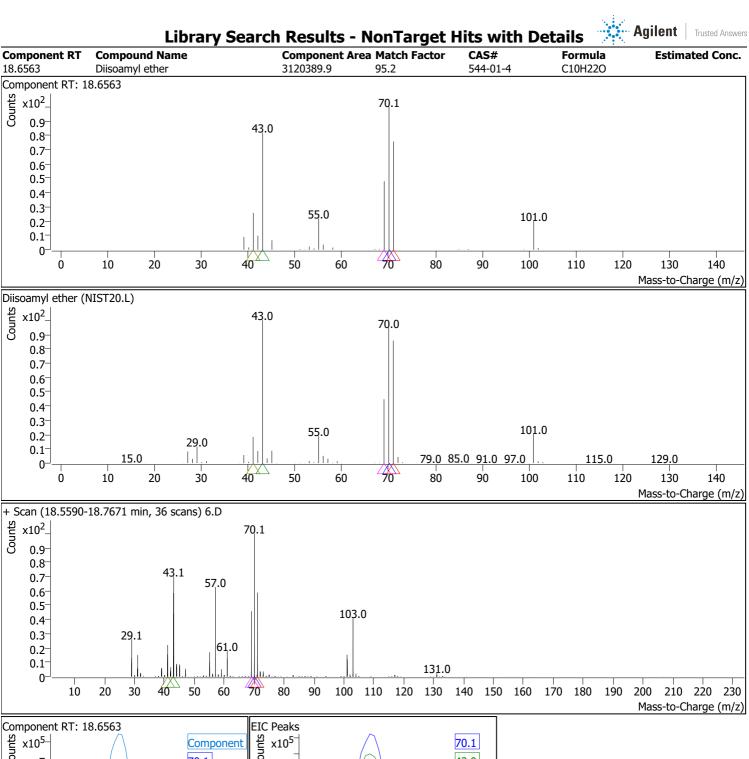
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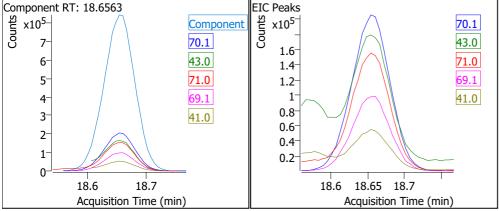
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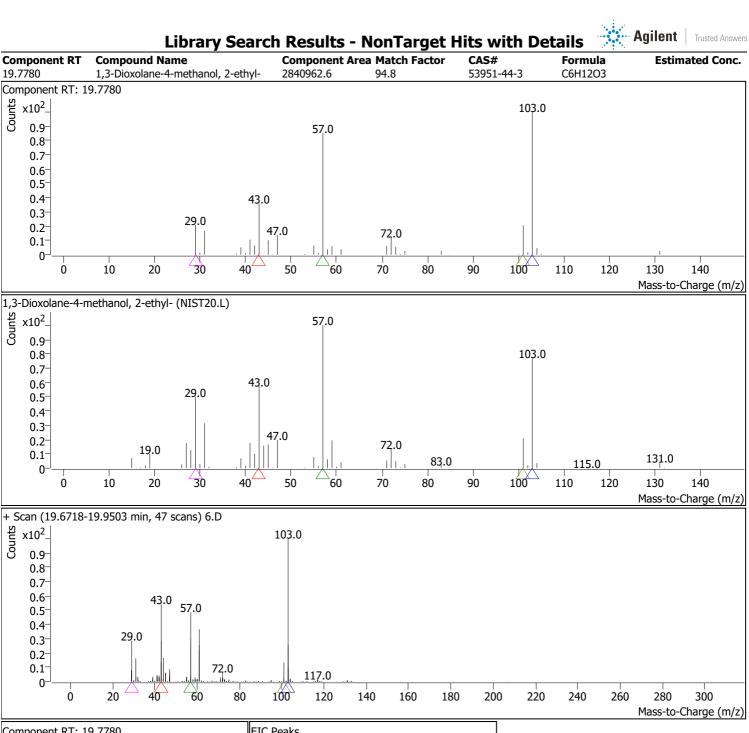
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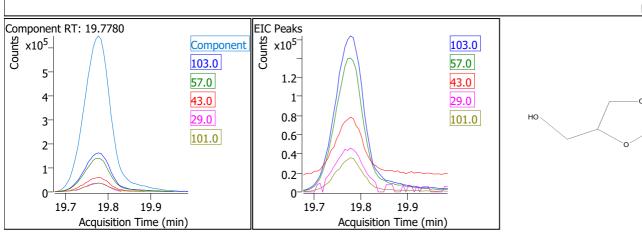




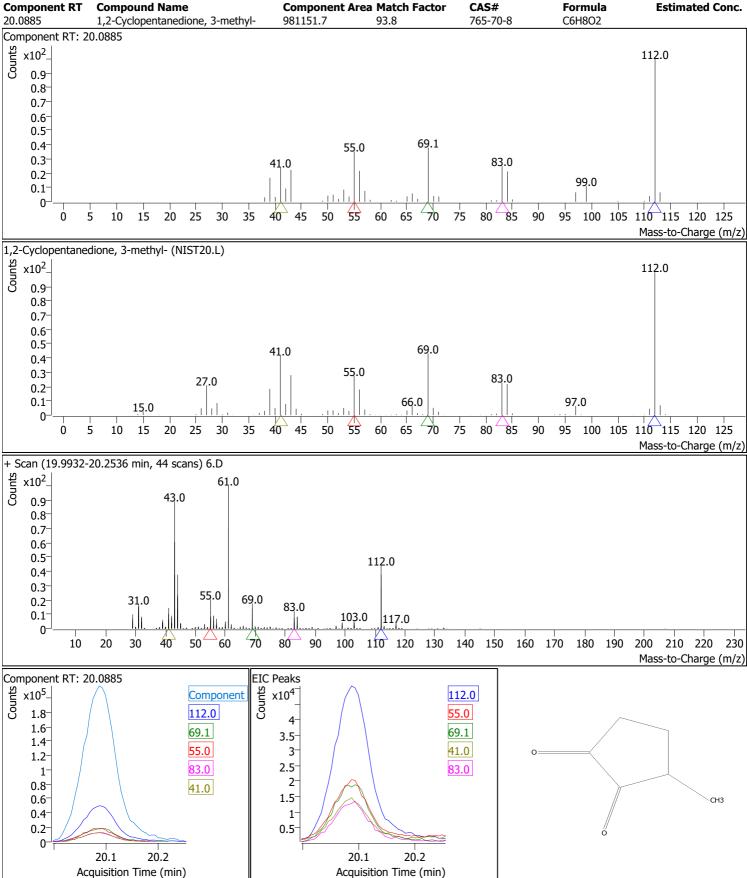












#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** Component Area Match Factor CAS# **Component RT Compound Name Formula Estimated Conc.** 1720991.0 110-88-3 21.1744 1,3,5-Trioxane 78.1 C3H6O3 Component RT: 21.1744 v10<sup>2</sup> 0.9 61.0 89.0 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 45.0 56.0 0 90 55 25 75 80 10 15 20 30 35 40 45 50 60 65 70 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 (20.9017-21.9958 min, 185 scans) 6.D st x10<sup>2</sup> 0.9 61.0 0.8 43.0 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 117.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.1744 **EIC Peaks** Counts x10<sup>4</sup> x10<sup>5</sup>-Component 61.0 43.0 0.9 7 0.8 6 89.0 0.7 5 43.0 89.0 0.6 31.0 60.0 4 0.5 3 60.0 0.4

21.2 21.4 21.6 21.8

Acquisition Time (min)

0.3

0.2

0.1

2

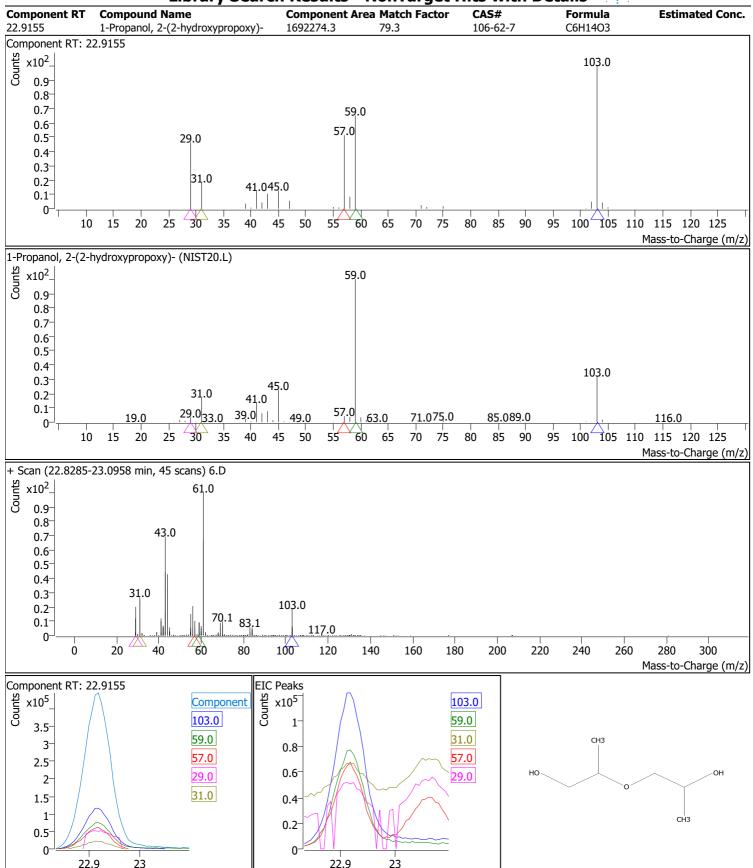
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21

21.5







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.** 23.0619 1-Octanol 3613372.9 98.2 111-87-5 C8H18O Component RT: 23.0619 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 50 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 55 20 25 35 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9671-23.1552 min, 32 scans) 6.D St x10<sup>2</sup>\_ 0.9 0.8 0.7 43.0 0.6 0.5 $0.4^{-}$ 31.0 56.1 0.3 0.2 70.1 84.1 0.1 103.0 117.0 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: 23.0619 EIC Peaks Counts Counts x10<sup>5</sup> 56.0 Component 56.0 55.0 0.8 6 55.0 41.0 0.7 5 41.0 0.6 69.0 4

23.1

23.2

Acquisition Time (min)

70.0

0.5

0.4

0.3

0.2

0.1

23

70.0

69.0

3

2

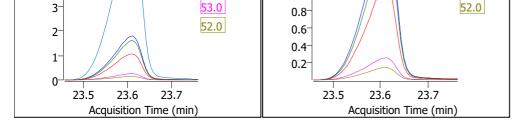
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23

23.1

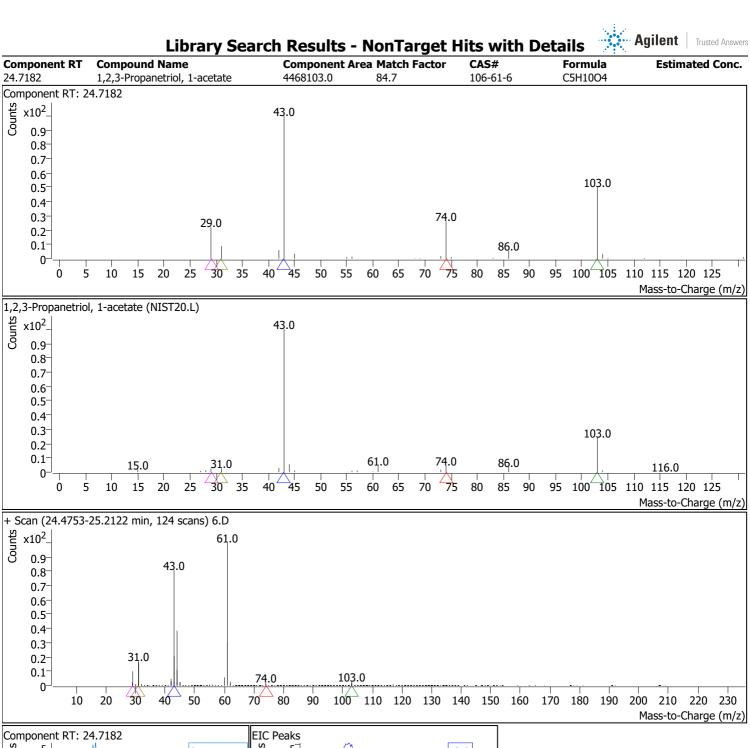
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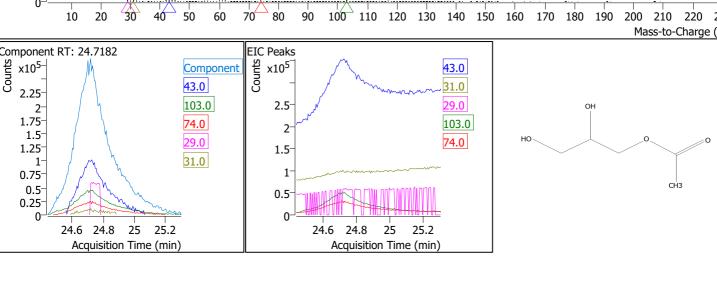
#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 29247888.8 90-05-1 23.6112 Phenol, 2-methoxy-98.8 C7H8O2 Component RT: 23.6112 v10<sup>2</sup> 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 0.1 39.0 63.0 80 110 120 10 20 30 40 70 90 100 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 109.0 124.0 0.8 81.0 0.7 0.6 0.5 0.4 0.3 53.0 0.2 39.0 63.0 0.1 27.0 77.0 95.0 15.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4585-23.7617 min, 52 scans) 6.D St x10<sup>2</sup>\_ 0.9 109.0 124.0 0.8 0.7 81.0 0.6 61.0 43.0 0.5 $0.4^{-}$ 0.3 0.2 31.0 53.0 0.1 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 10 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.6112 Counts Counts x10<sup>6</sup> 109.0 Component 109.0 124.0 5 1.4 124.0 81.0 1.2 4 81.0 53.0



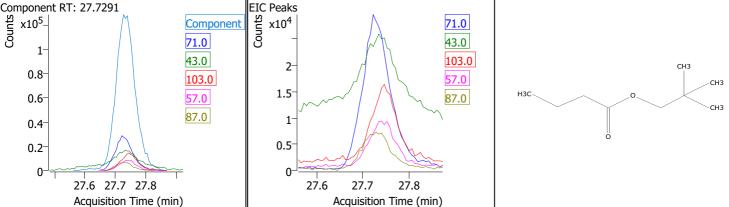
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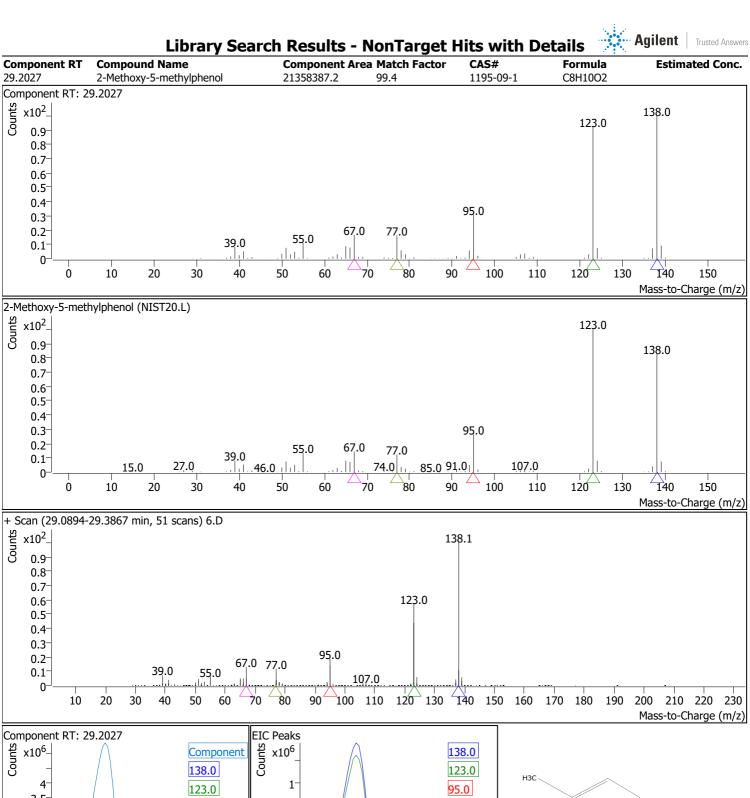
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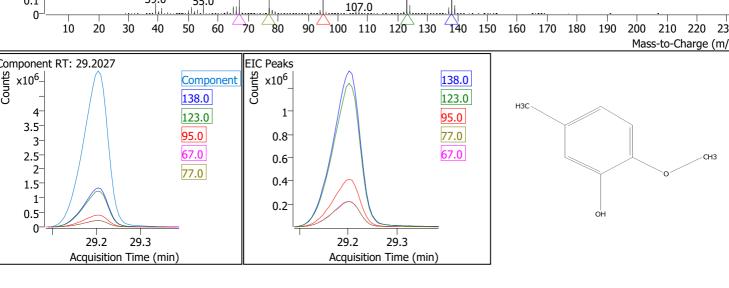




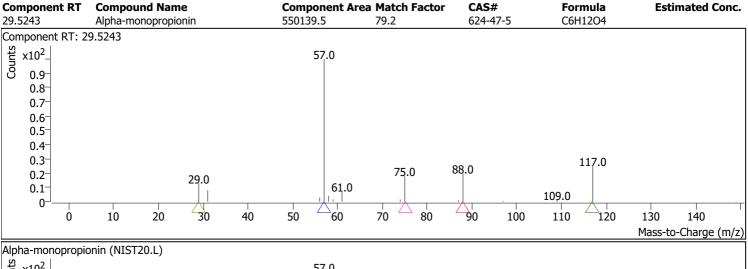
#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7291 Butanoic acid, 2,2-dimethylpropyl 575552.3 82.0 23361-69-5 C9H18O2 Component RT: 27.7291 x10<sup>2</sup>\_ 71.0 0.9 8.0 43.0 0.7 0.6 103.0 0.5 0.4 57.0 0.3 87.0 31.0 $0.2^{-}$ 0.1 0-70 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<sup>2</sup>. 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 10 20 30 40 50 60 70 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6575-27.8229 min, 28 scans) 6.D x10<sup>2</sup>. 0.9 0.8 0.7 71.1 0.6 0.5 0.4 61.0 103.0 0.3 31.0 57.0 0.2 87.0 0.1 151.0 117.0 165.9 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)

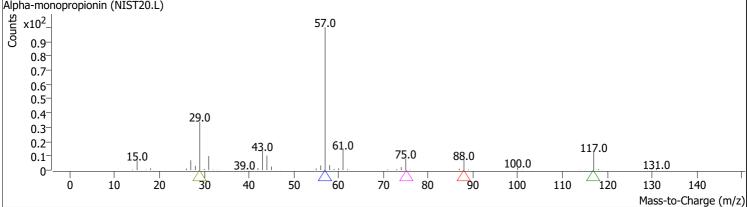


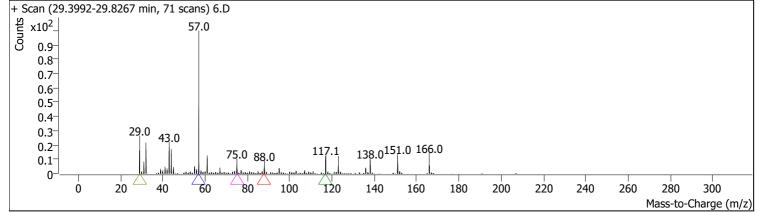


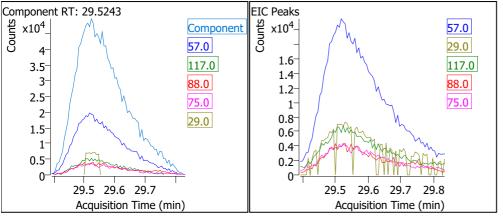


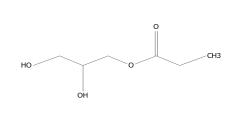


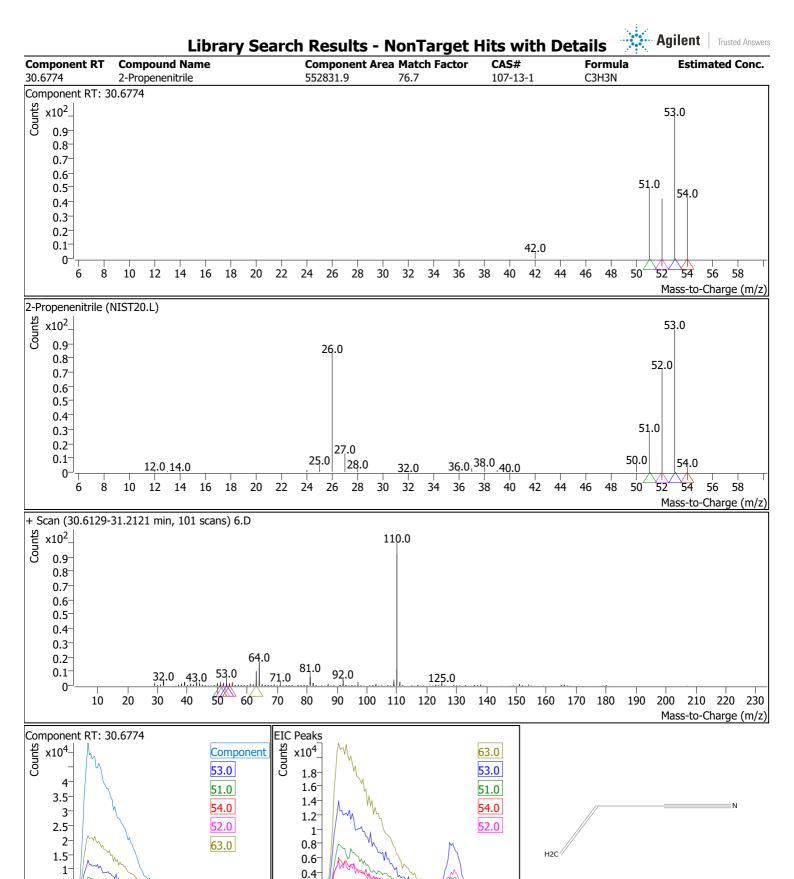












31

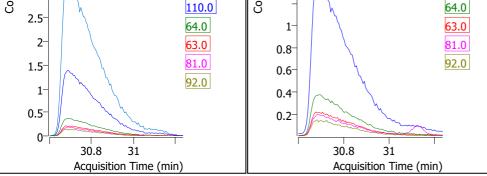
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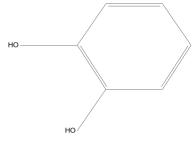
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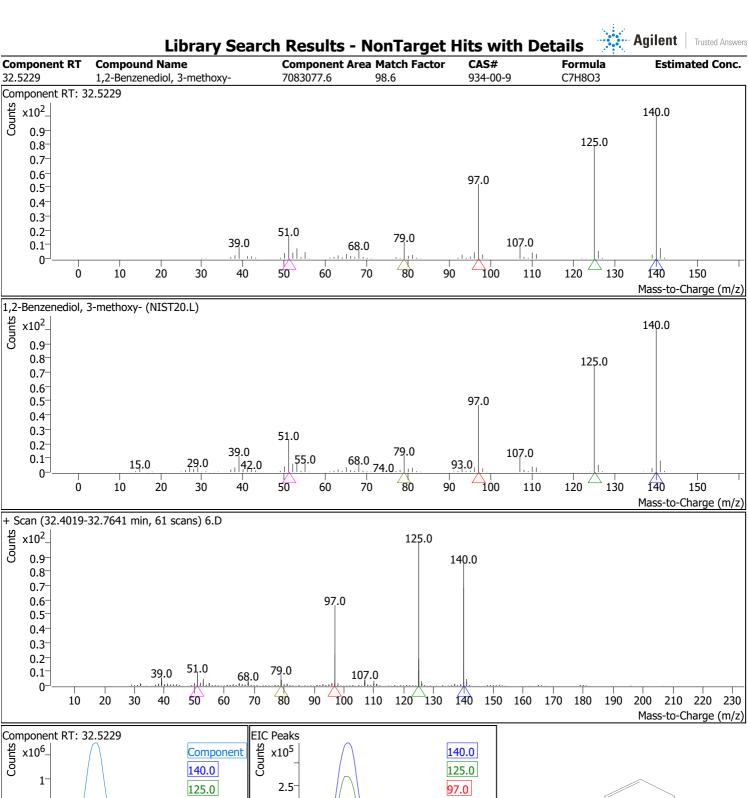
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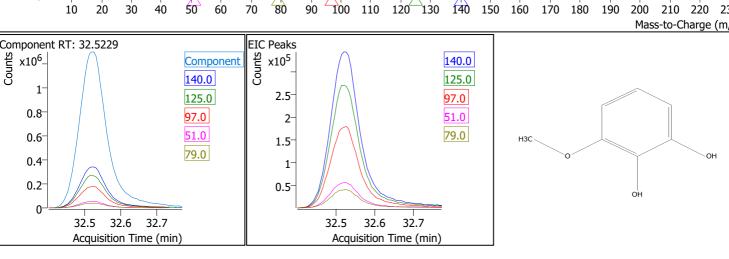
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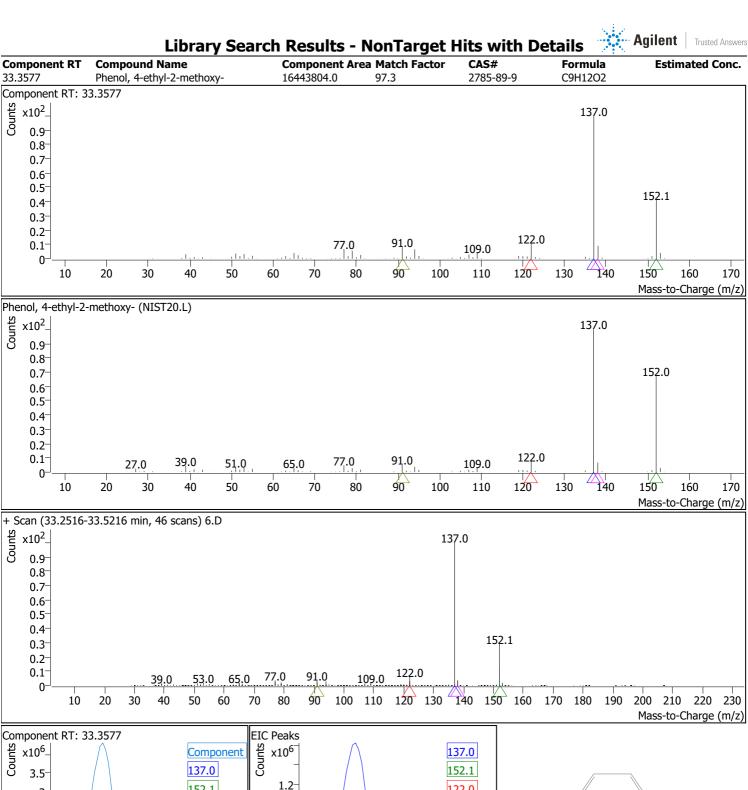
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.6870 Catechol 3885535.5 97.6 C6H6O2 Component RT: 30.6870 y x10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 81.0 92.0 53.0 0.1 110 115 120 125 10 15 35 50 55 75 80 85 90 95 100 105 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 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 (30.5997-31.2359 min, 108 scans) 6.D st x10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 81.0 92.0 0.1 32.0 125.0 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.6870 EIC Peaks Counts Counts x10<sup>5</sup> 110.0 Component 110.0 64.0 2.5 64.0 1 63.0

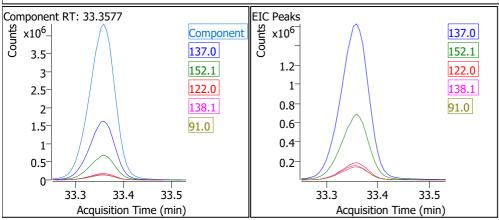


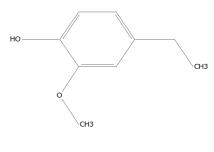












#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 452-86-8 35.0048 1,2-Benzenediol, 4-methyl-1415607.5 90.7 C7H8O2 Component RT: 35.0048 v10<sup>2</sup> 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 0.2 51.0 107.0 40.0 95.0 0.1 50 10 20 30 40 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 0.7 0.6 0.5 78.0 0.4 0.3 0.2 51.0 107.0 39.0 95.0 0.1 62.0 67.0 27.0 47.0 50 10 20 30 40 60 70 80 90 100 110 130 140 Mass-to-Charge (m/z) + Scan (34.9240-35.1484 min, 38 scans) 6.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 78.0<sup>89.0</sup>101.0 124.0 60 80 20 40 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0048 Counts stupo x10<sup>5-</sup> 2.5x10<sup>4</sup> 124.0 Component 124.0 123.0 2.5 123.0 6 78.0 2 78.0 5 77.0

35.1

Acquisition Time (min)

35.2

51.0

1.5

1

0.5

35.1

Acquisition Time (min)

35.2

77.0 51.0

3-

2

35

-СН3

#### -- 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 35.1003 2-Furanmethanol, tetrahydro-14376090.0 78.7 C5H10O2 Component RT: 35.1003 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 57.0 0.1 31.0 89.0 10 15 25 55 60 65 85 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 15.0 53.0,57.0 61.0 67.0 102.0 10 15 20 25 35 40 45 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (34.8392-35.2138 min, 64 scans) 6.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 78.0<sup>89.0</sup>101.0 124.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.1003 Counts Counts x10<sup>5</sup> 71.0 Component 71.0 43.0 1 43.0 5 41.0 0.8 42.0 41.0



42.0

31.0

3

2-

34.9

35

35.1

Acquisition Time (min)

35.2

0.6

0.4

0.2

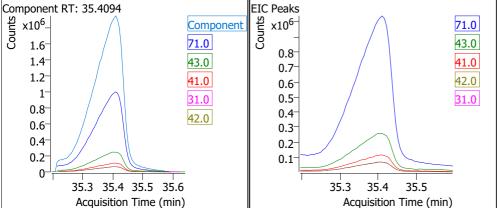
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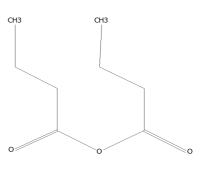
Acquisition Time (min)

35.1 35.2

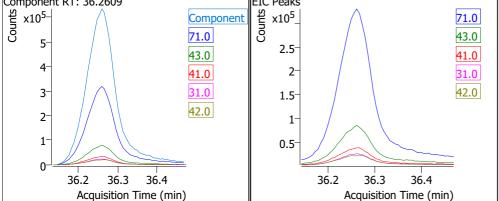
31.0

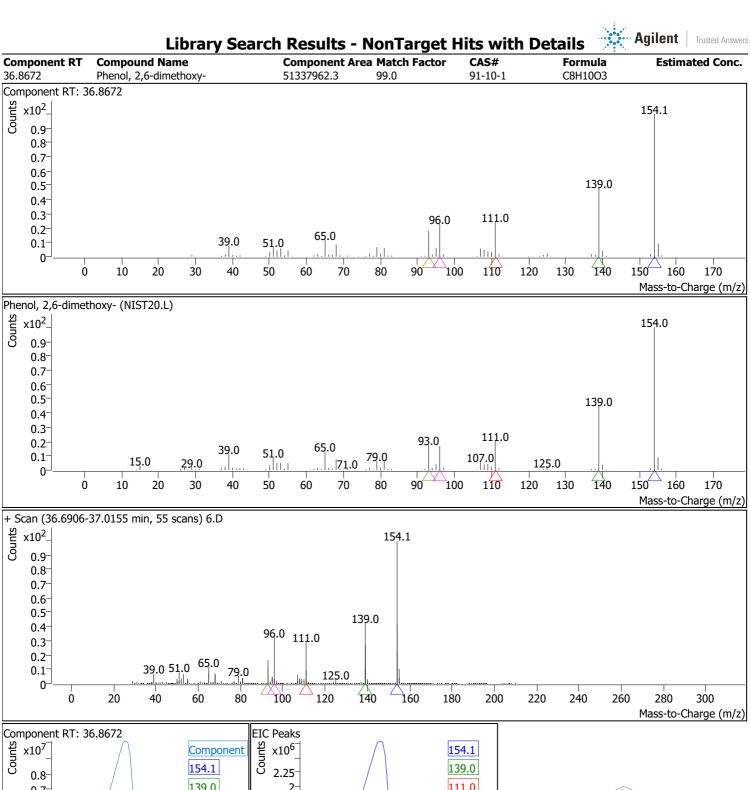
#### - Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.4094 Butanoic acid, anhydride 13819611.4 81.9 C8H14O3 Component RT: 35.4094 v10<sup>2</sup> 0.9 71.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 89.0 10 15 20 25 30 35 40 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) Butanoic acid, anhydride (NIST20.L) st x10<sup>2</sup>\_ 0.9-71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 41.0 0.1 55.0 29.0 15.0 60.0 85.0 89.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (35.2138-35.5944 min, 65 scans) 6.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<sub>101.1114.0</sub> 131.1 40 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.4094 Counts x10<sup>6</sup>x10<sup>6</sup> 71.0 Component CH3 CH3 71.0 43.0 1.6 0.8 1.4 43.0 41.0 0.7

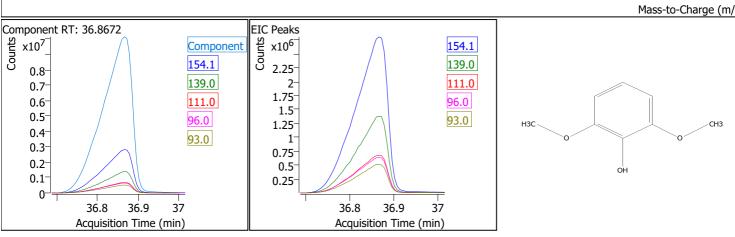




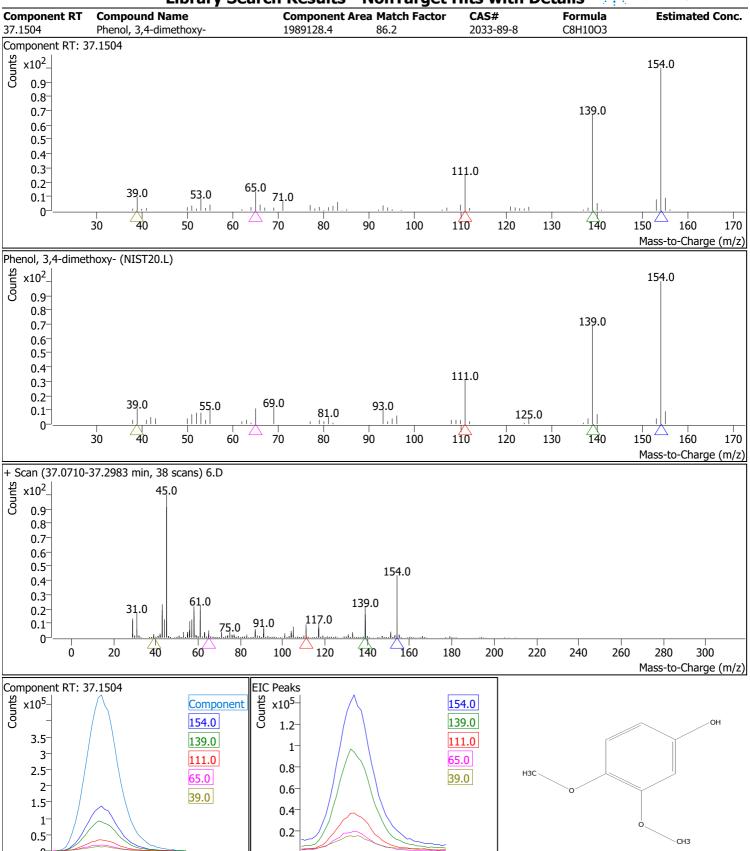
#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.2609 2-Furanmethanol, tetrahydro-3342384.4 83.3 C5H10O2 Component RT: 36.2609 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 57.0 100 105 110 10 15 25 30 35 55 60 65 90 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 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.1434-36.4684 min, 55 scans) 6.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 57.0 131.0 154.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 36.2609 Counts Counts x10<sup>5</sup> x10<sup>5</sup> 71.0 Component 71.0 43.0 5 2.5 43.0 41.0 4











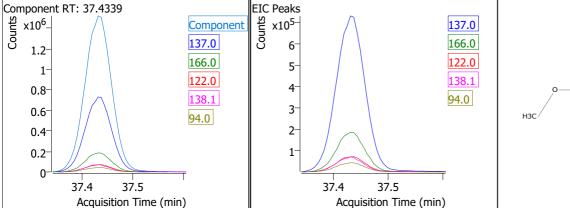
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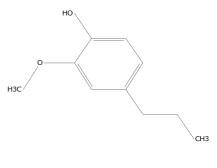
37.1

37.1

37.2

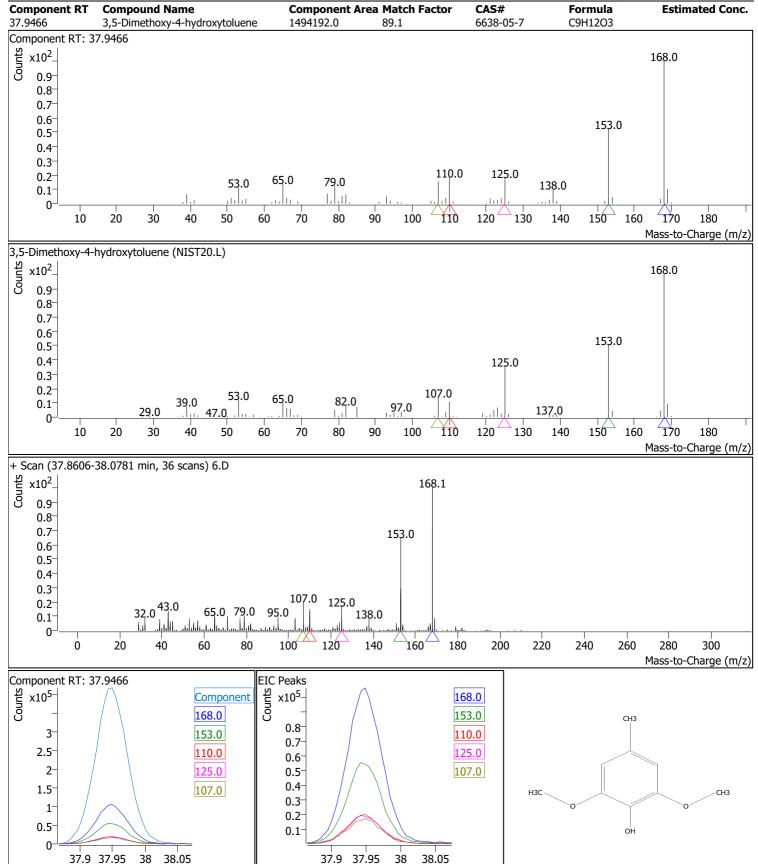
# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4339 Phenol, 2-methoxy-4-propyl-5560185.8 95.1 C10H14O2 Component RT: 37.4339 v10<sup>2</sup> 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 103.0 0.1 77.0 51.0 65.0 160 - 170 50 100 120 10 20 30 40 60 70 80 110 130 180 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 (37.3425-37.6041 min, 45 scans) 6.D st x10<sup>2</sup> 0.9 137.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 166.1 0.2 122.0 0.1 94.0 103.0 57.0 29.0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 37.4339 x10<sup>6</sup>-Counts x10<sup>5</sup> 137.0 Component 137.0 166.0 6 1.2 166.0 122.0 5 1

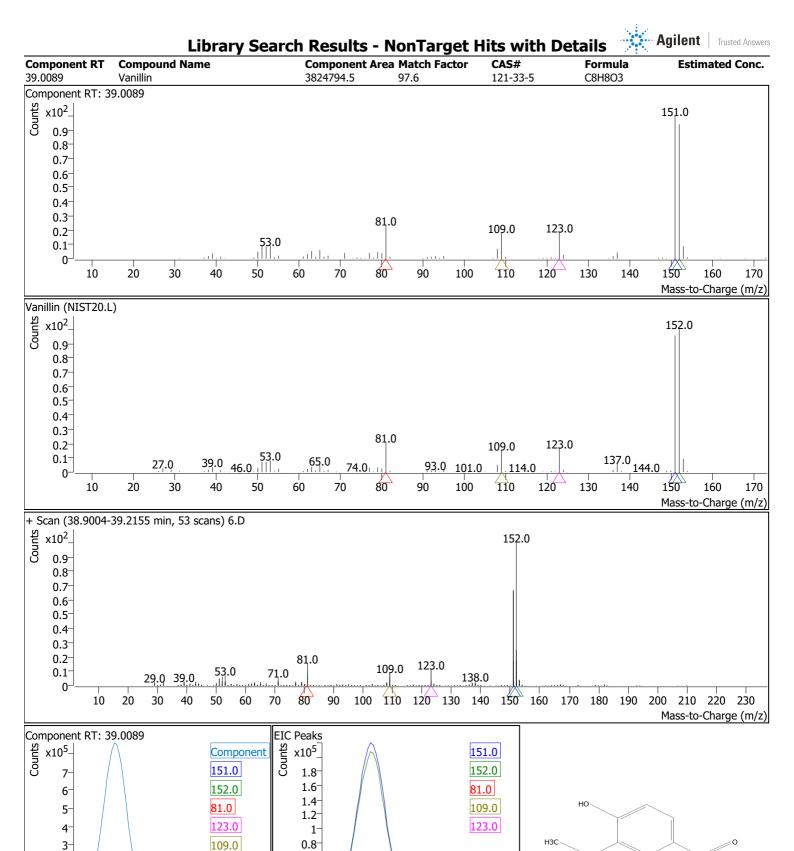












Acquisition Time (min)

0.6

0.4

2

1

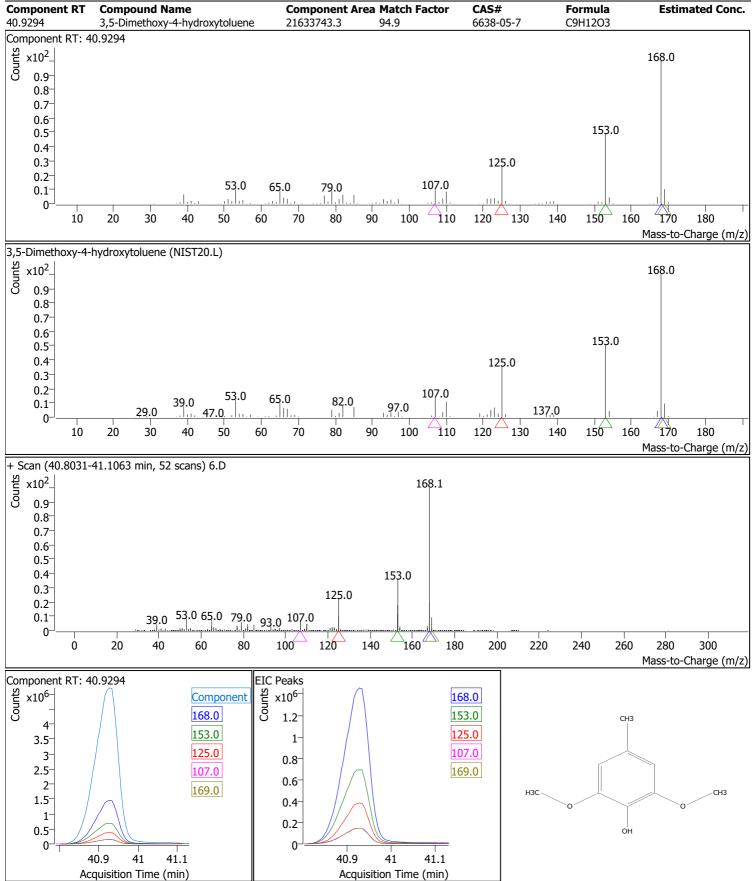
39.1

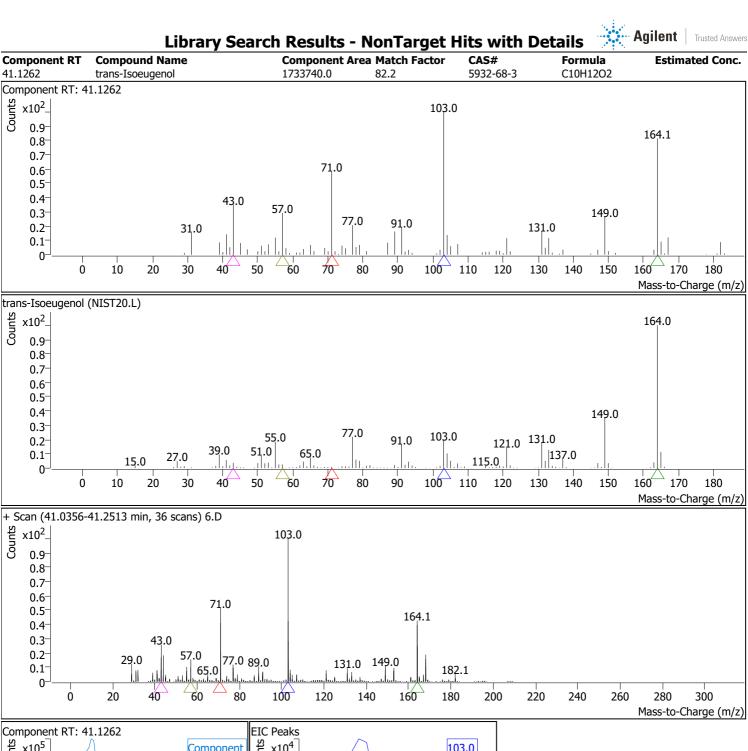
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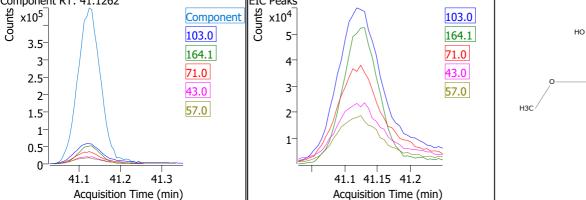
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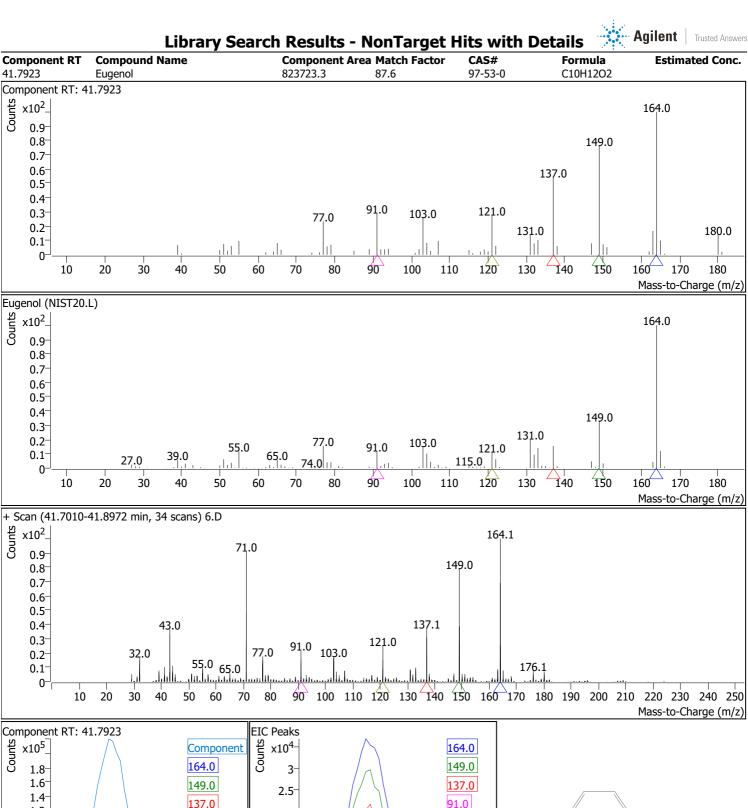


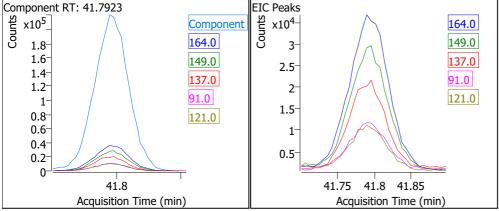






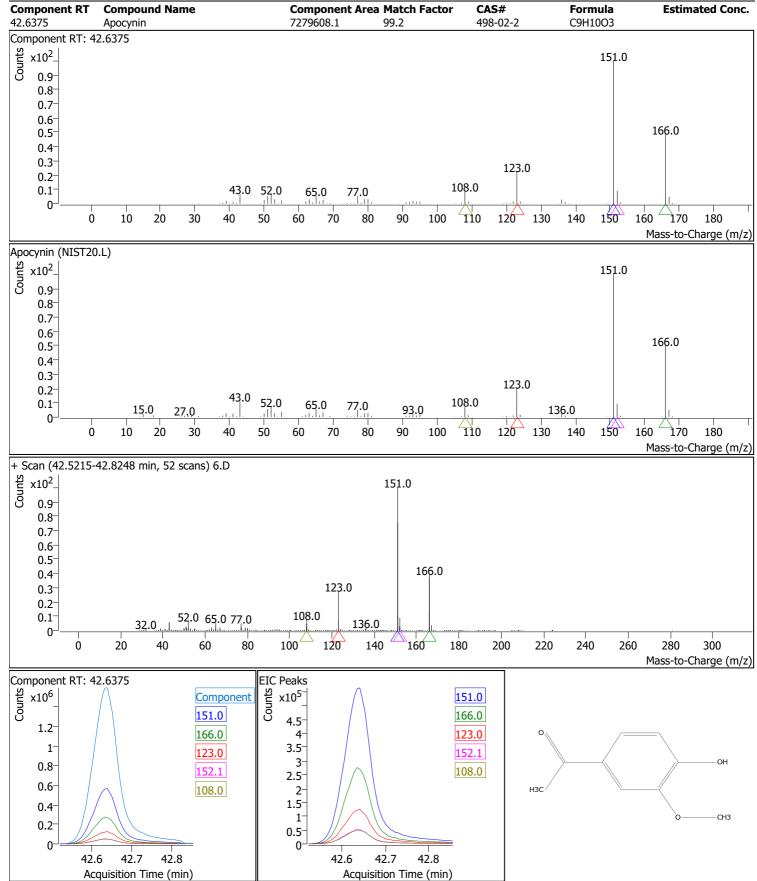






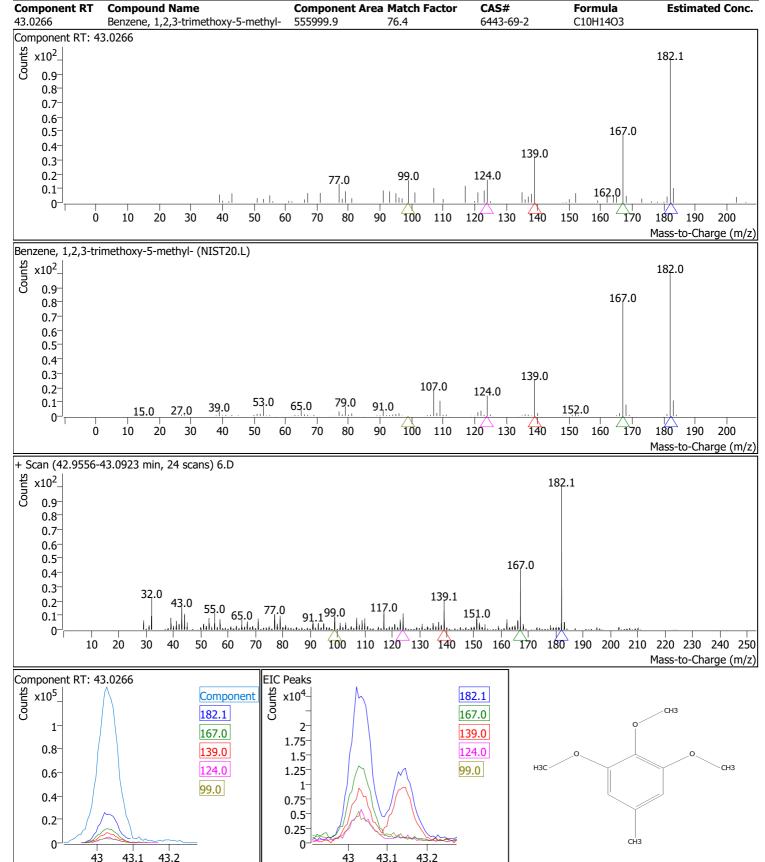






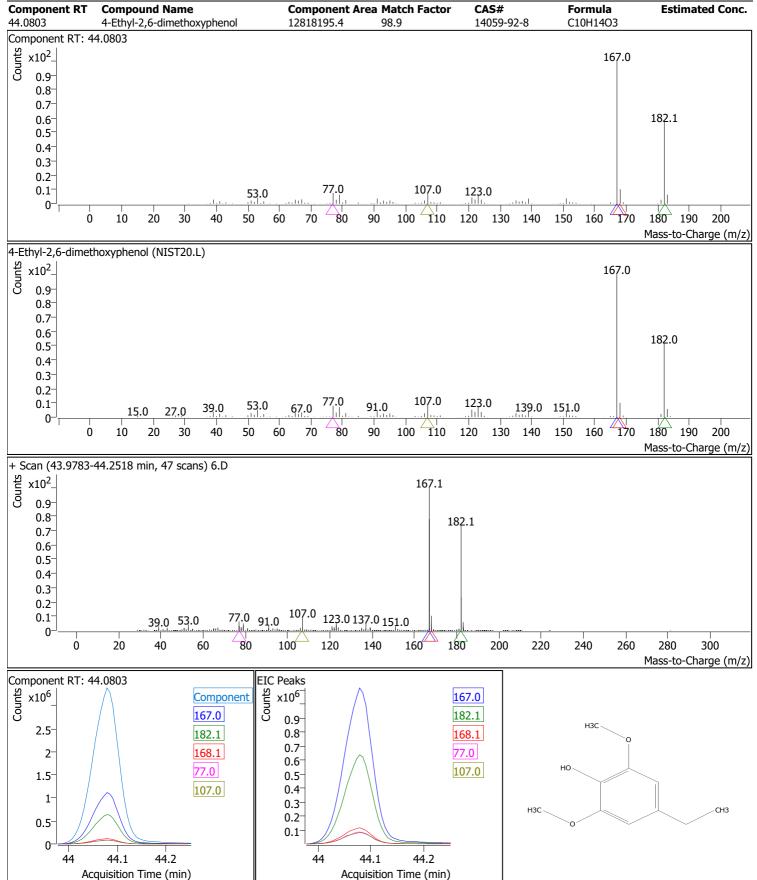












# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-44.3285 19517366.6 94.6 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3285 Counts x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2 122.0 0.1 66.0 0-120 180 20 30 50 60 100 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2042-44.5134 min, 53 scans) 6.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 180.1 74.0 87.0 122.0 43.0 55.066.0 0.1 0 60 100 120 140 180 Ó 20 40 80 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3285 **EIC Peaks** Counts Counts x10<sup>6</sup> x10<sup>6</sup> 137.0 Component 180.0 137.0 3 1.2 180.0 122.0 2.5 1 138.0 122.0

44.3

44.4

Acquisition Time (min)

94.0

0.8

0.6

0.4

0.2

138.0

94.0

2

1

44.3

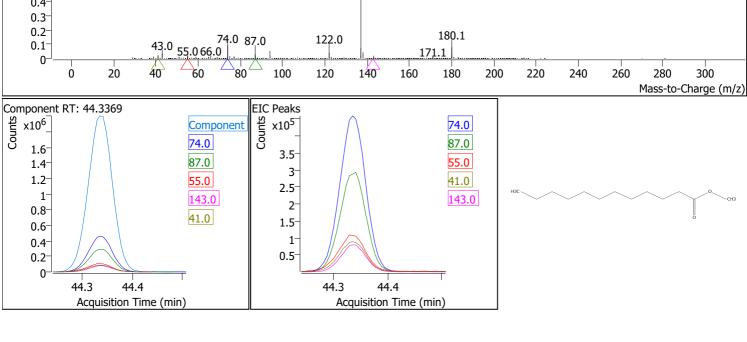
44.4

Acquisition Time (min)

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.** 44.3369 Dodecanoic acid, methyl ester 6866421.4 89.3 111-82-0 C13H26O2 Component RT: 44.3369 Counts $x10^{2}$ 74.0 0.9 0.8 0.7 87.0 0.6 0.5 0.4 0.3 55.0 41.0 143.0 0.2 69.0 0.1 70 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts 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 40 50 60 70 80 Mass-to-Charge (m/z) + Scan (44.2459-44.5075 min, 45 scans) 6.D st x10<sup>2</sup> 0.9 137.0 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1-Propanone, 1-(4-hydroxy-3-1835-14-9 46.4943 2308676.4 C10H12O3 methoxyphenyl)-Component RT: 46.4943 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 180.1 0.3 123.0 $0.2^{-}$ 108.0 0.1 52.0 65.0 77.0 0-110 150 180 10 20 30 40 50 60 70 80 90 100 120 130 140 160 170 190 200 Mass-to-Charge (m/z) 1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 180.0 123.0 0.2 108.0 77.0 93.0 0.1 52.0 65.0 39.0 29.0 136.0 164.0 0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (46.4153-46.5886 min, 30 scans) 6.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 180.1 0.2 123.0 0.1 52.0 65.0 77.0 108.0 93.0 29.0 0 120 180 260 0 20 40 60 80 100 140 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 46.4943 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup>-151.0 Component СНЗ 180.1 151.0 1.8 4 180.1 123.0 1.6 3.5 1.4 123.0 152.1 3 1.2

46.5

Acquisition Time (min)

46.55

108.0

2.5

1.5

0.5

2

1

46.5

46.6

Acquisition Time (min)

46.7

152.1

108.0

1

0.8

0.6

0.4

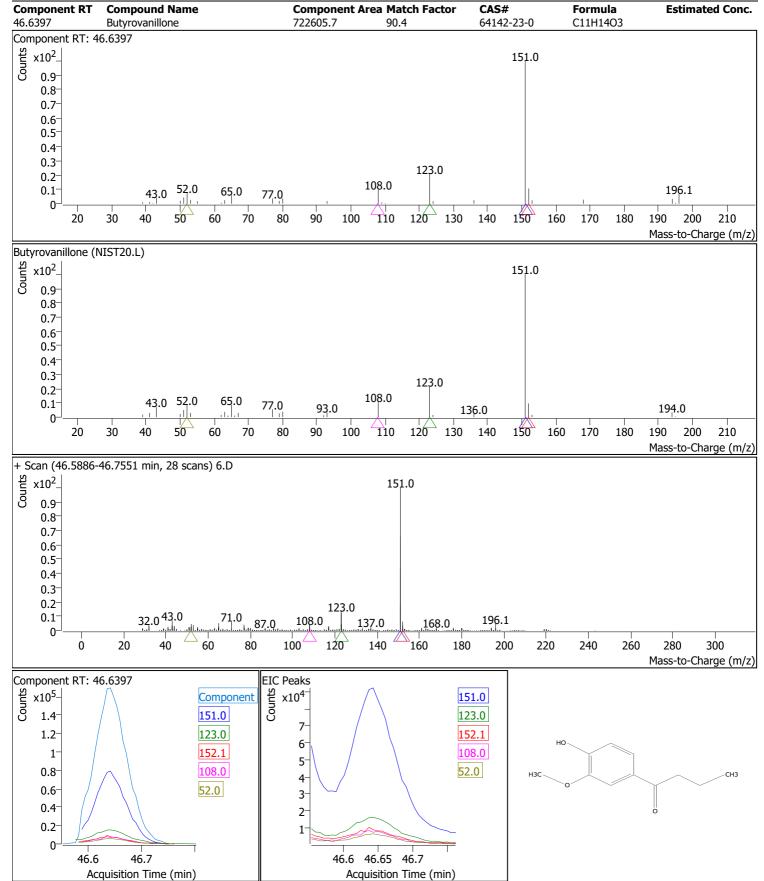
0.2

46.45

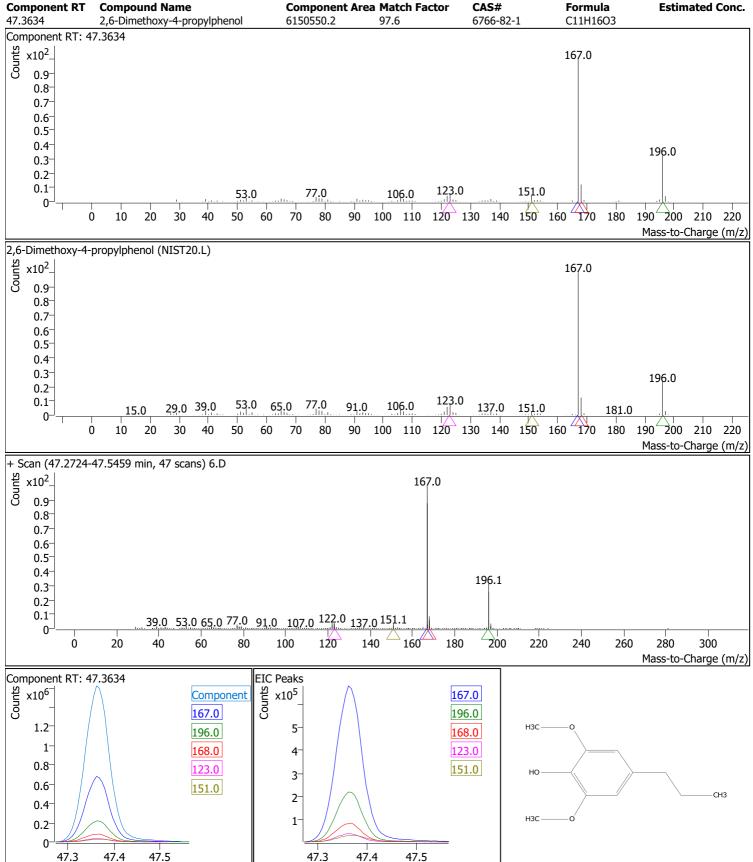
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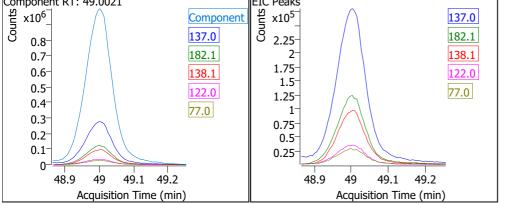








### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 49.0021 Benzenepropanol, 4-hydroxy-3-5666194.8 96.3 C10H14O3 methoxy-Component RT: 49.0021 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 182.1 0.4 0.3 $0.2^{-}$ 122.0 91.0 77.0 107.0 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) Counts $x10^{2}$ 137.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 182.0 0.4 0.3 122.0 0.2 77.0 91.0 106.0 65.0 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 (48.8659-49.2524 min, 66 scans) 6.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 182.1 0.4 0.3 0.2 65.0 77.0 91.0 106.0 122.0 0.1 149.0 164.0 0 40 80 100 120 180 200 220 Ó 20 60 140 160 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.0021 **EIC Peaks** Counts Counts x10<sup>6</sup> x10<sup>5</sup> 137.0 Component 182.1 137.0 2.25 0.8 182.1 2 138.1 0.7 1.75 $0.6^{-}$ 122.0 138.1



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.3716 Benzaldehyde, 4-hydroxy-3,5-997348.6 89.1 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3716 x10<sup>2</sup>\_ 182.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 111.0 96.0 167.0 65.0 0.1 51.0 103.0 0-160 170 0 10 20 30 50 60 70 80 90 100 110 120 130 140 150 180 190 200 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 0.3 111.0 0.2 167.0 93.0 139.0 39.0 65.0 51.0 79.0 0.1 29.0 153.0 15.0 123.0 0 160 170 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2822-49.6151 min, 57 scans) 6.D x10<sup>2</sup>. 174.1 194.1 131.0 0.9 0.8 0.7 0.6 182.0 0.5 0.4 0.3 77.0 155.0 91.0 0.2 119.0 39.0 51.0 69.0 0.1 0 180 0 20 40 60 80 100 120 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3716 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>5</sup> 182.0 Component 0 181.0 182.0 1.6 4.5 181.0 111.0 1.4 4 3.5 167.0 1.2 111.0 3 1 96.0 96.0

49.4

49.5

Acquisition Time (min)

2.5

2

1

1.5

0.5

167.0

8.0

0.6

0.4

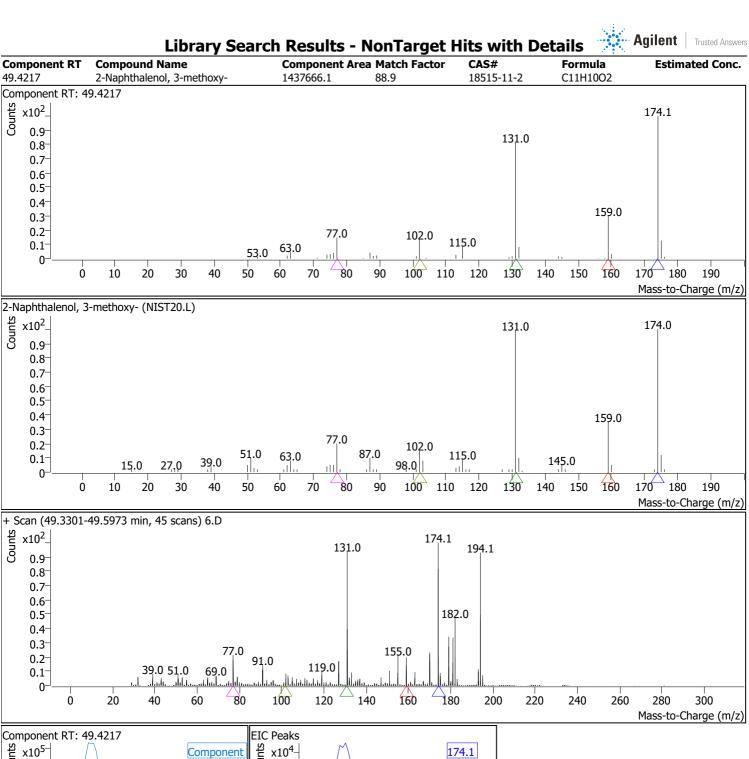
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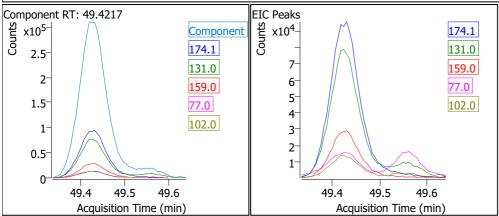
49.4

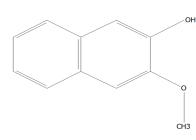
49.5

Acquisition Time (min)

ОΉ

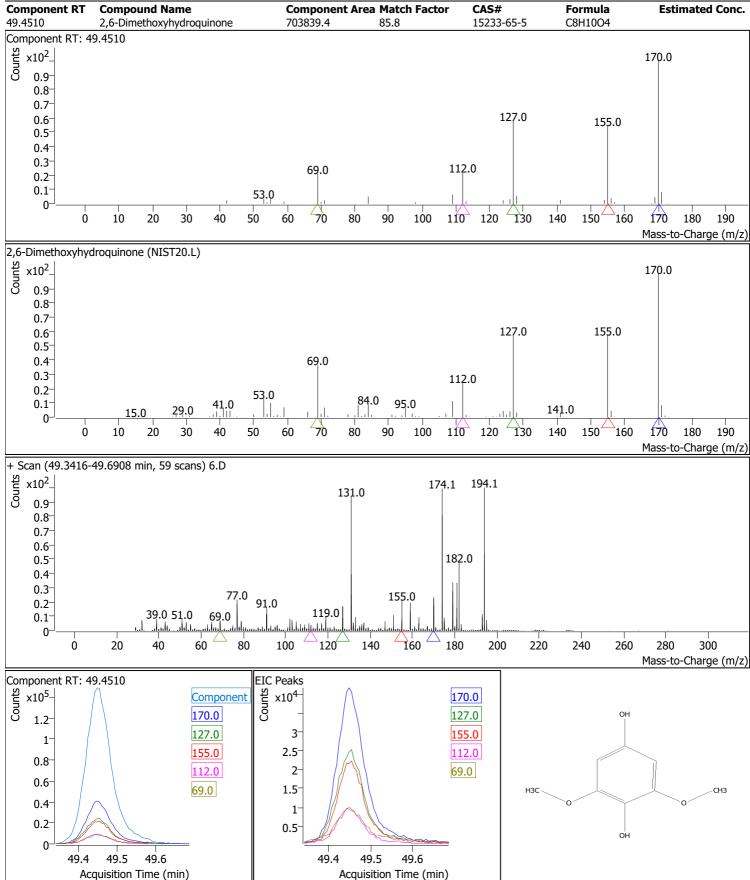












## --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 49.5619 (E)-2,6-Dimethoxy-4-(prop-1-en-1-1756204.0 83.7 C11H14O3 yl)phenol Component RT: 49.5619 x10<sup>2</sup>\_ 194.1 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 91.0 $0.2^{-}$ 77.0 119.0 133.0 151.0 163.0 0.1 0-10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 200 210 220 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 ا 97.0 27.0 85.0 0 90 180 10 20 40 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4605-49.7192 min, 44 scans) 6.D x10<sup>2</sup>. 194.1 0.9 0.8 0.7 0.6 0.5 0.4 179.1 0.3 0.2 91.0 131.0 155.0 77.0 105.0 0.1 32.043.0 65.0 0 120 180 200 Ó 20 40 60 80 100 140 160 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.5619 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup> 194.1 Component 179.0 194.1 0.9 3.5 **Н3С** 179.0 0.8 91.0 3 0.7 91.0 193.0 2.5 0.6 193.0 119.0 НО 2 $0.5^{-}$ 119.0 0.4 1.5 0.3

49.6

Acquisition Time (min)

0.2

0.1

49.5

1

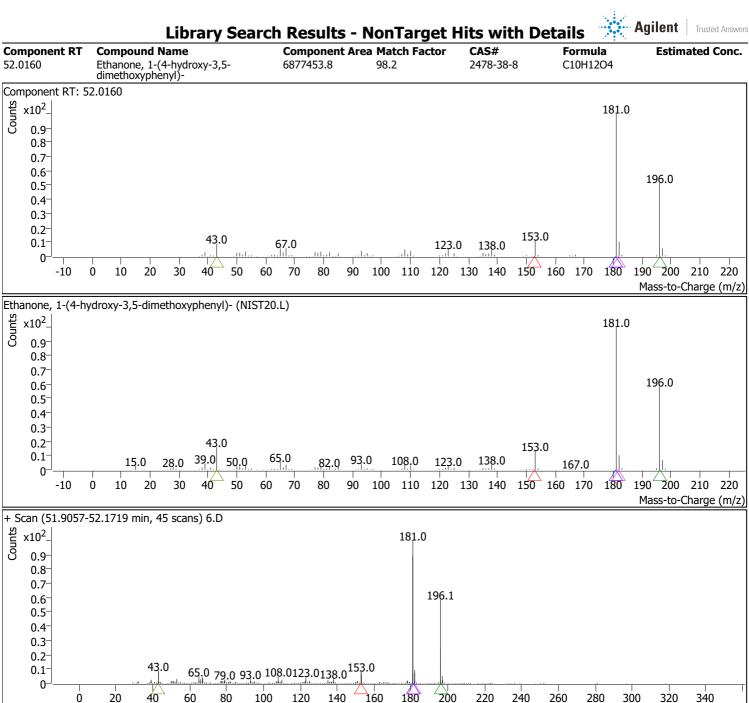
49.5

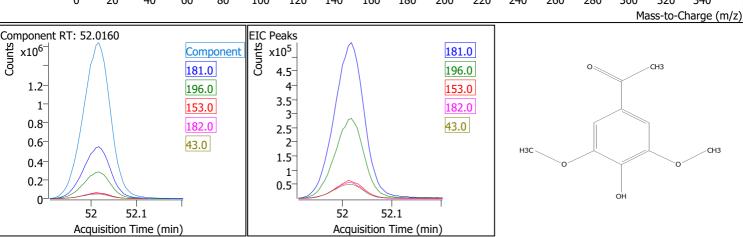
49.6

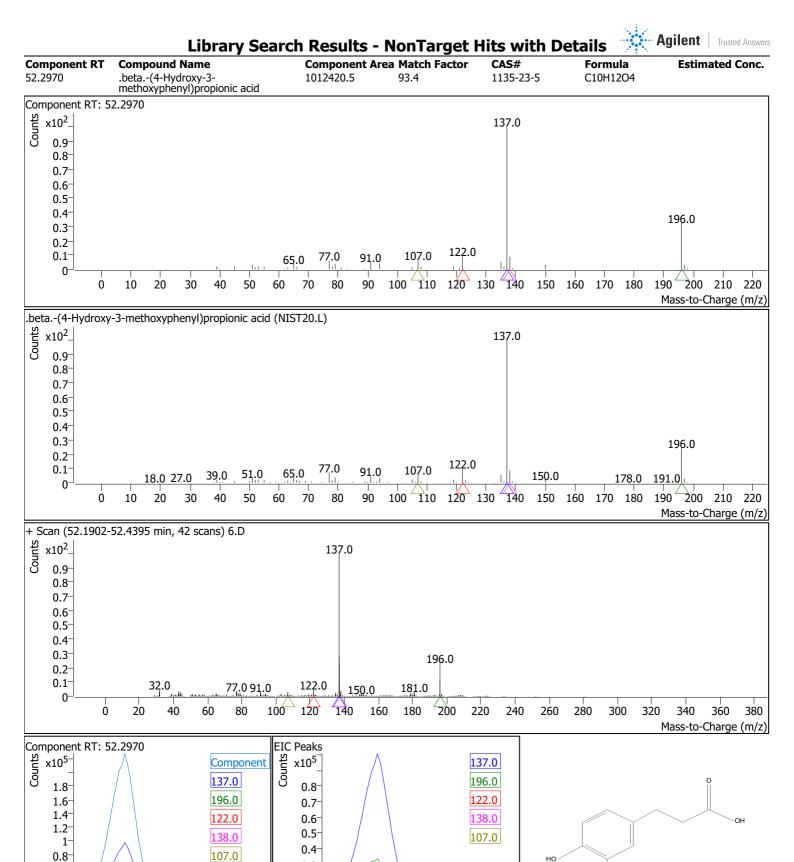
Acquisition Time (min)

0.5

НЗС







52.4

Acquisition Time (min)

0.3

 $0.2^{-}$ 

0.1

0.6

0.4

0.2

52.3

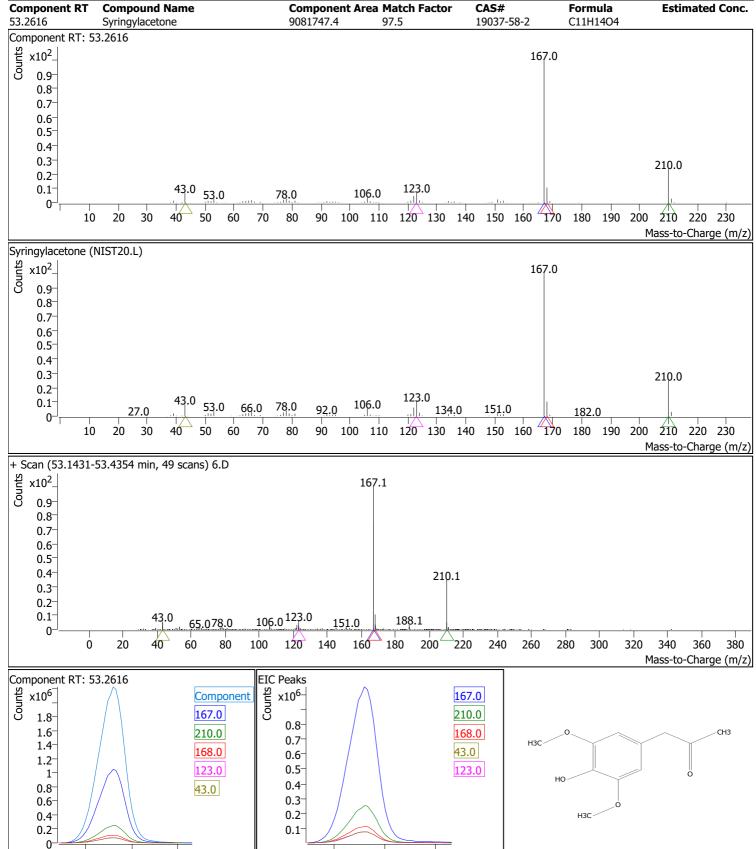
52.4

Acquisition Time (min)

СНЗ







Acquisition Time (min)

53.4

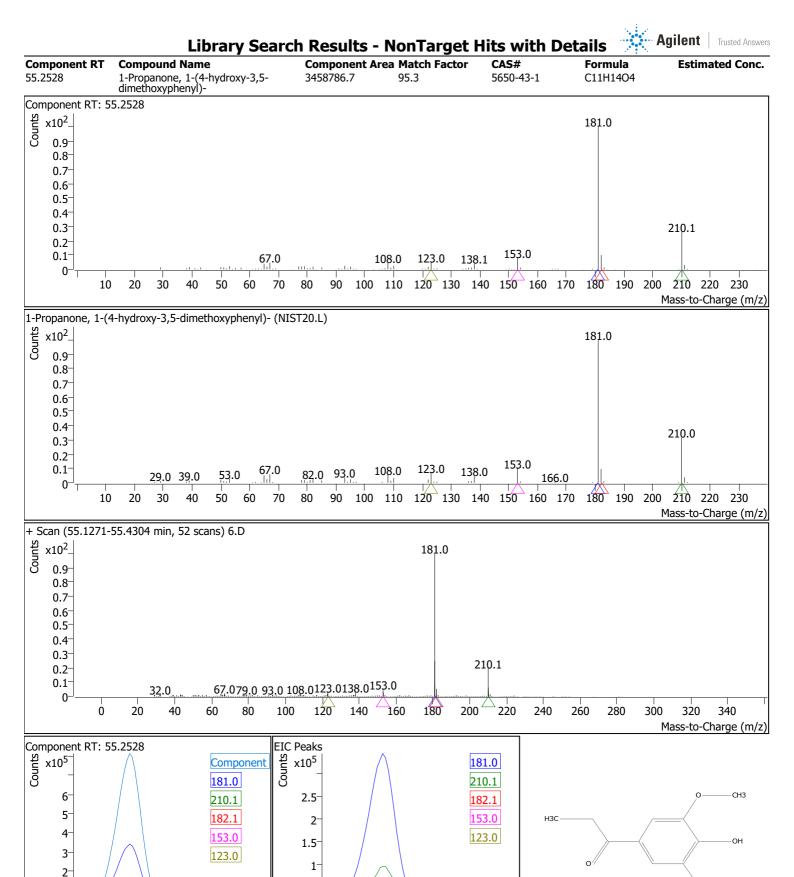
53.2

53.2

53.3

Acquisition Time (min)

53.4



Acquisition Time (min)

55.4

0.5

55.2

1

55.2

55.3

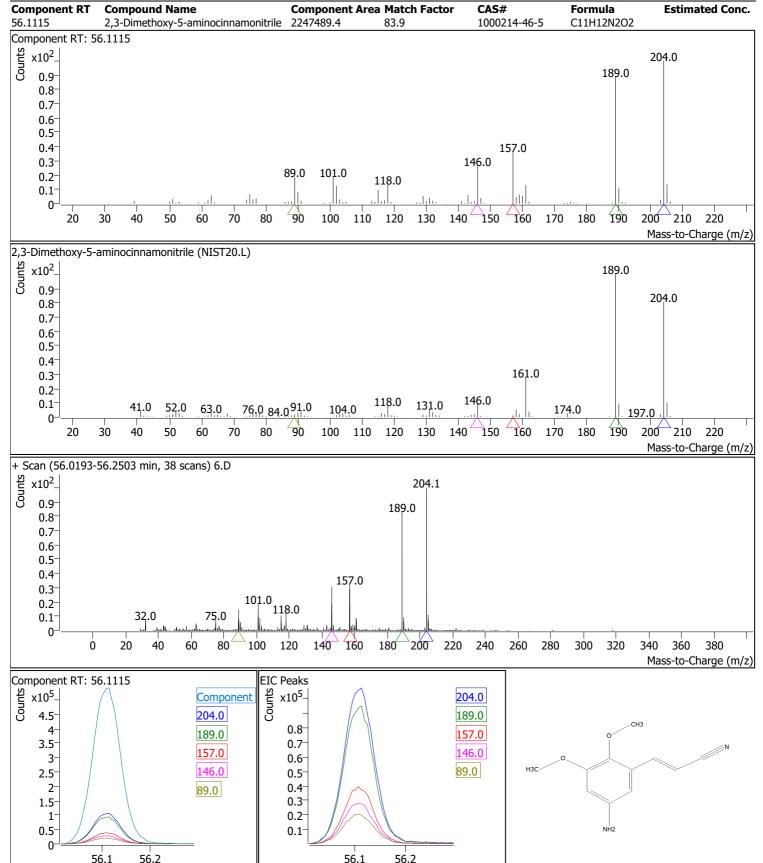
Acquisition Time (min)

55.4

-CH3

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

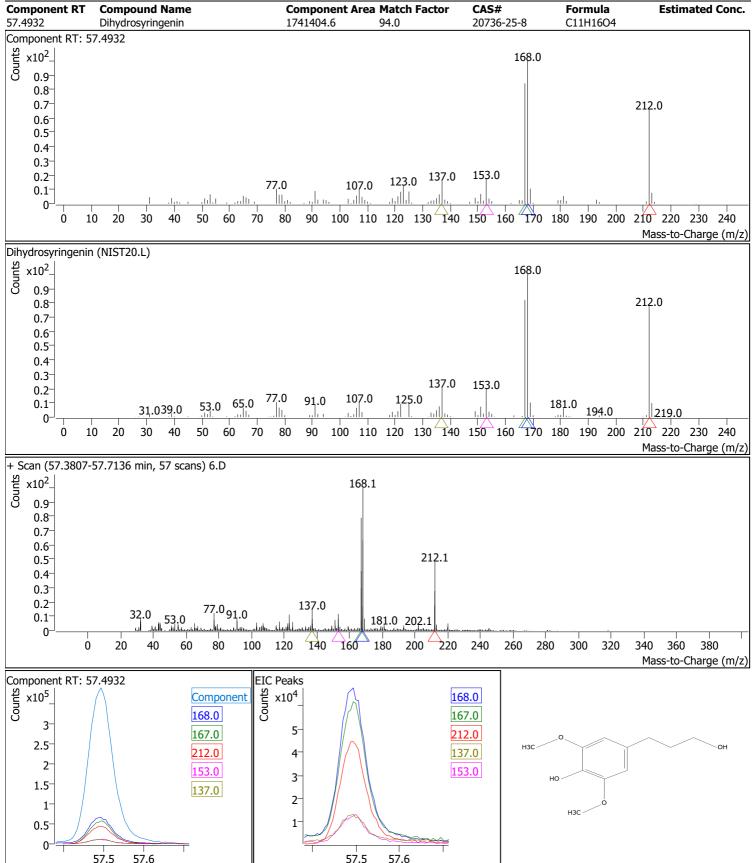




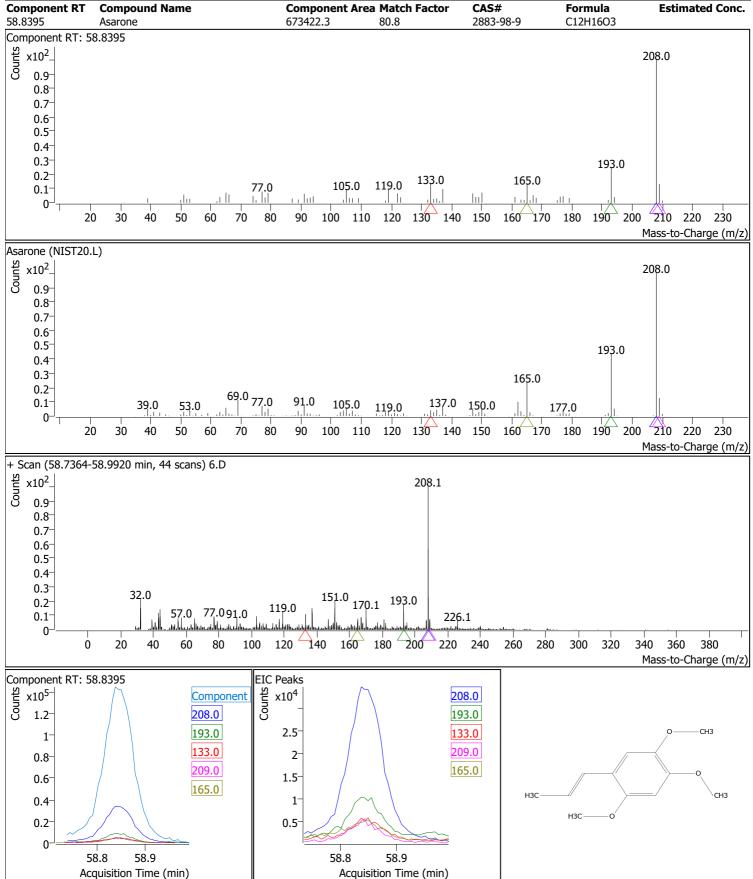
Acquisition Time (min)

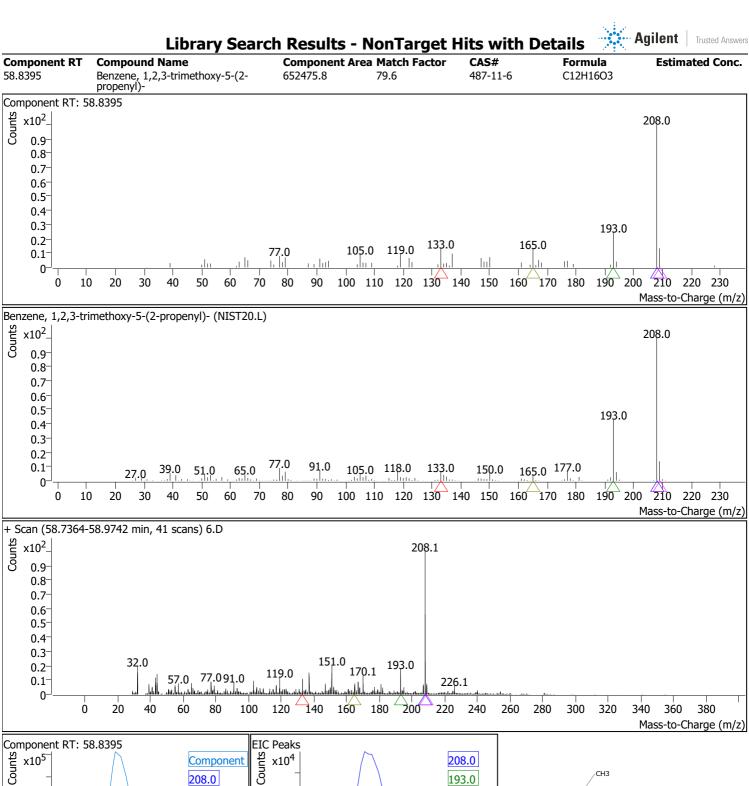


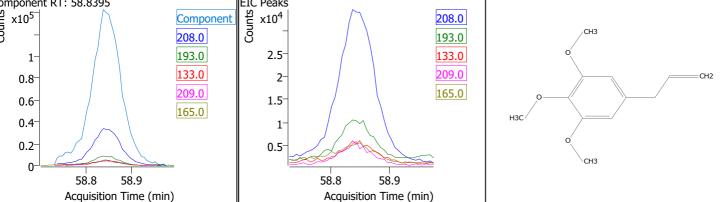






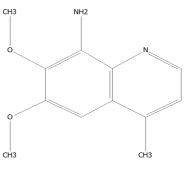






#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 59.7759 8-Amino-6,7-dimethoxy-4-1071121.5 75.2 1000213-07-2 C12H14N2O2 methylquinoline Component RT: 59.7759 x10<sup>2</sup>\_ 218.0 0.9 203.0 8.0 0.7 0.6 0.5 0.4 160.0 171.0 0.3 115.0 0.2-103.0 132.0 0.1 <u>.ul II</u> 0-200 220 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 230 Mass-to-Charge (m/z) 8-Amino-6,7-dimethoxy-4-methylquinoline (NIST20.L) x10<sup>2</sup>. 218.0 203.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 160.0 132.0 145.0 0.2 104.0 175.0 187.0 0.1 77.0 51.0 117.0 63.0 89.0 0 200 210 220 230 240 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) + Scan (59.6758-59.8780 min, 35 scans) 6.D x10<sup>2</sup>. 117.0 0.9 0.8 $0.7^{-}$ 0.6 0.5 0.4 43.0 0.3 57.0 218.1 137.0 0.2 77.0 94.0 0.1 151.0 171.0 0 120 180 200 220 320 20 40 80 100 140 160 240 260 280 300 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 59.7759 Counts Counts x10<sup>4</sup>-218.0 x10<sup>5</sup> Component NH2 СНЗ 218.0 203.0 5 2

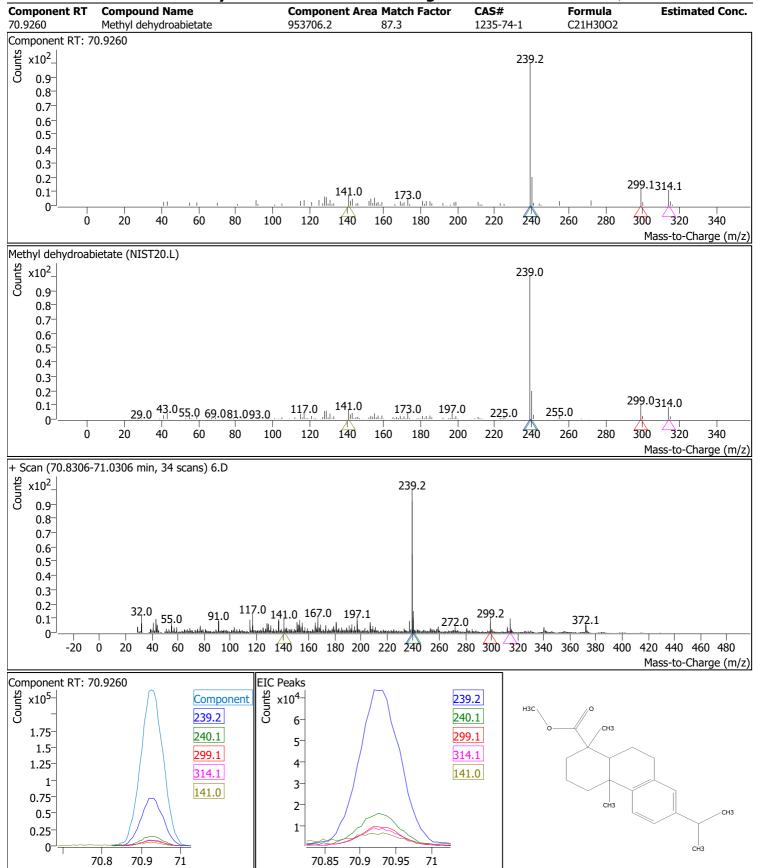
203.0



171.0

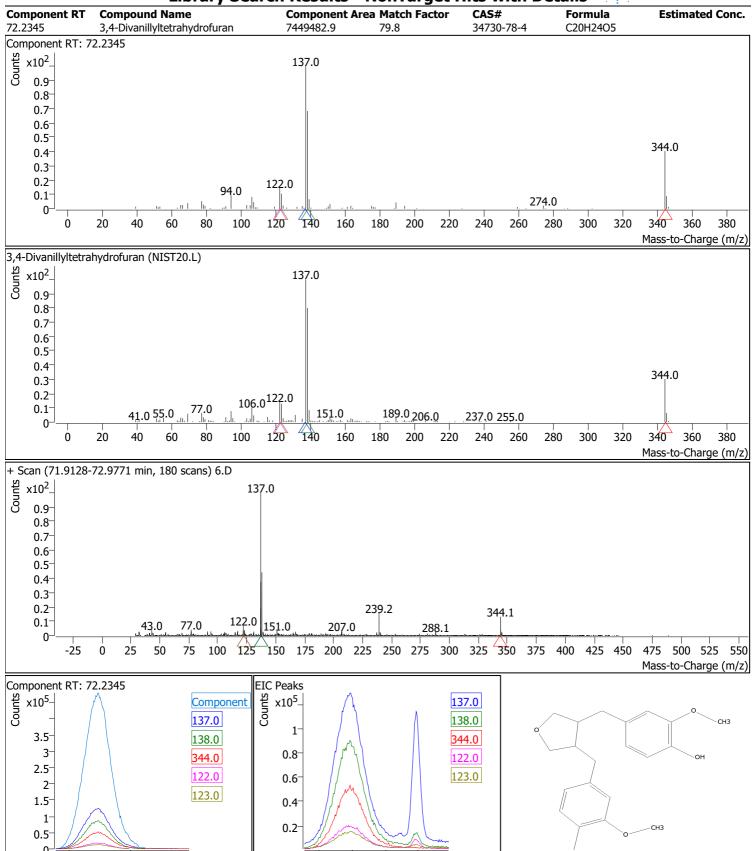












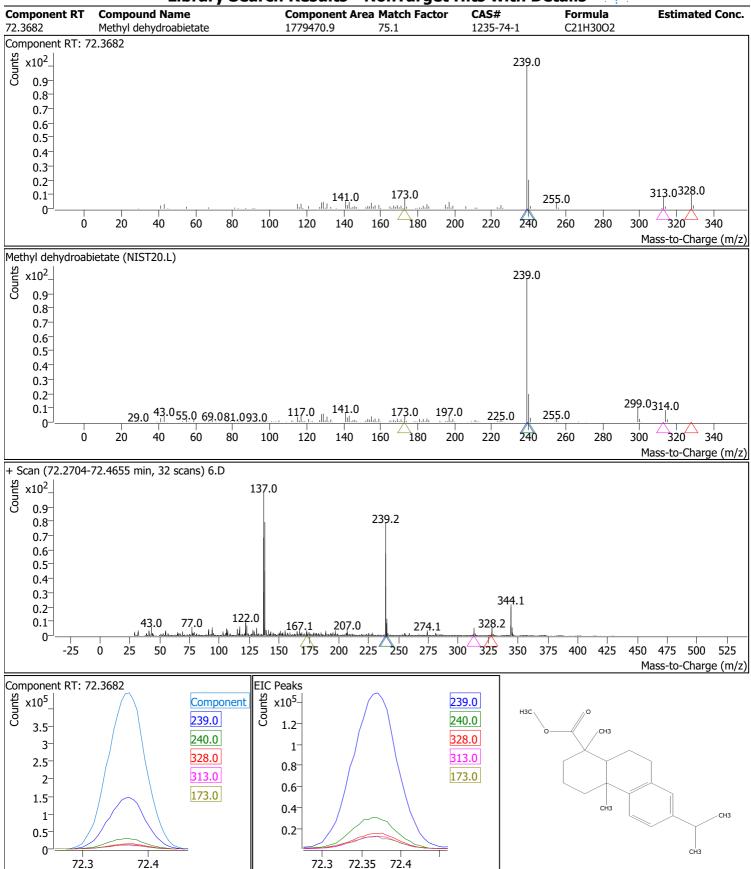
72.25 72.5 72.75

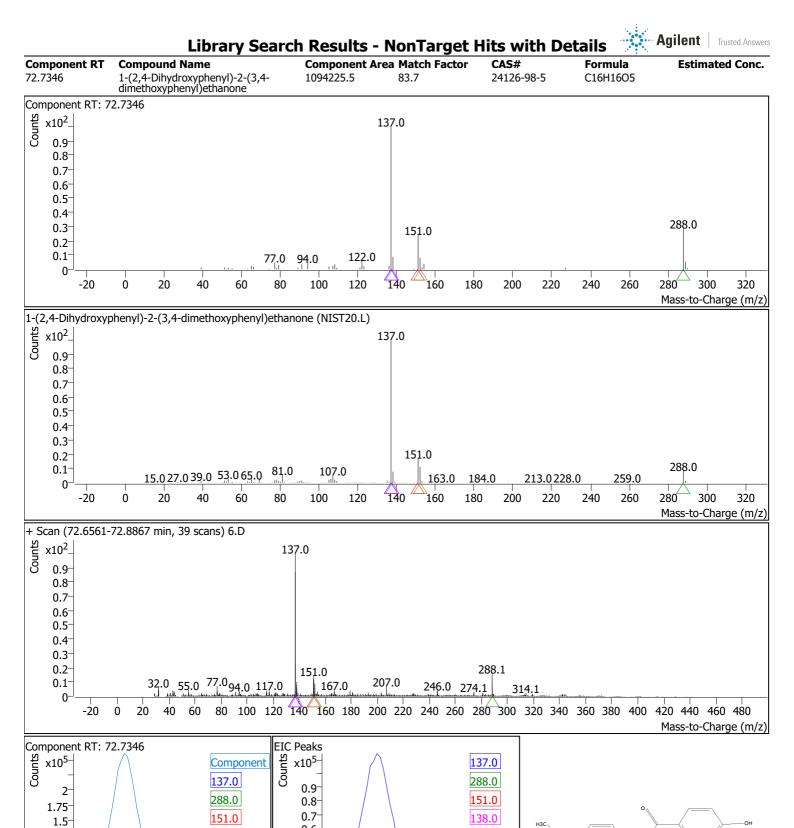
Acquisition Time (min)

72

72.5







Acquisition Time (min)

152.0

0.6

0.5

0.4

0.3

0.2

0.1

72.7

138.0

152.0

1.25

0.75

0.25

72.7

72.8

Acquisition Time (min)

0.5

1

73.7

Acquisition Time (min)

73.8

0.8

0.6

0.4

0.2

141.0

0.6

0.4

0.2

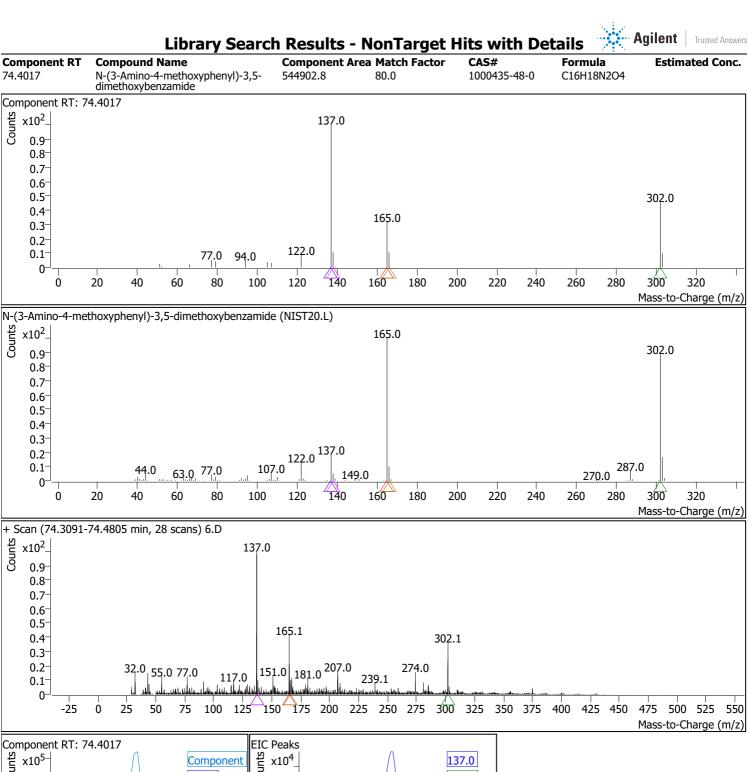
73.6

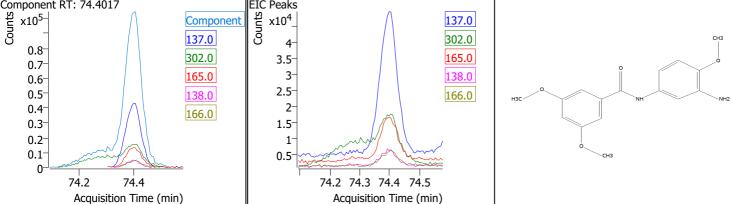
73.7

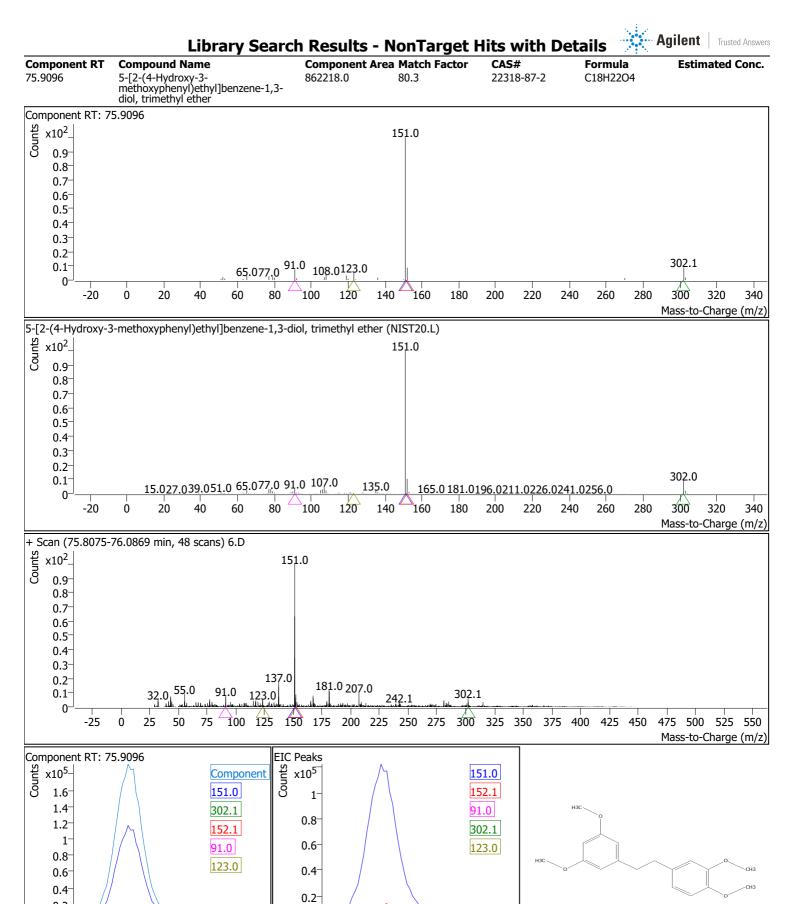
Acquisition Time (min)

73.8

СНЗ







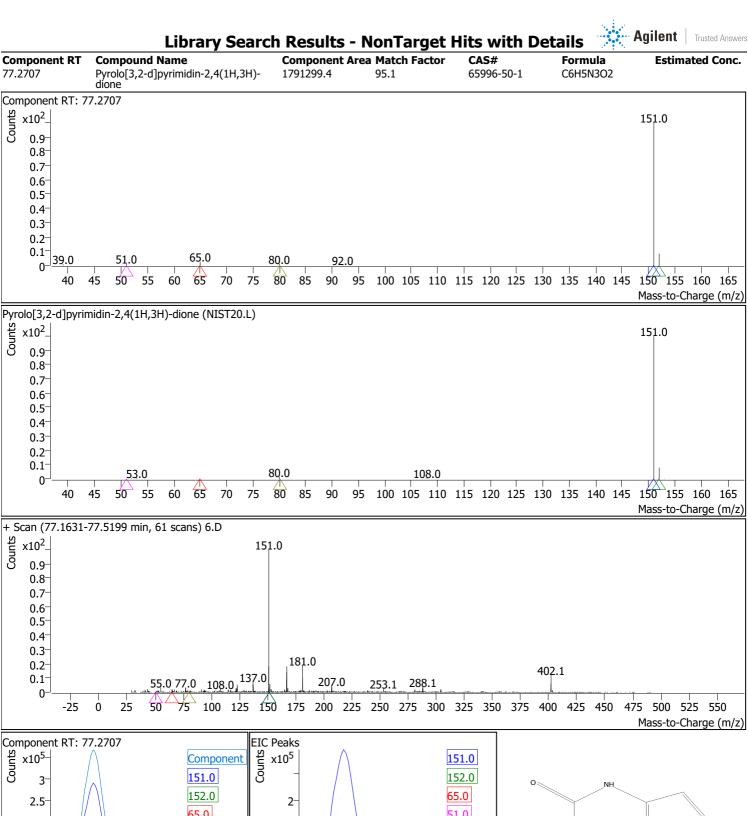
76

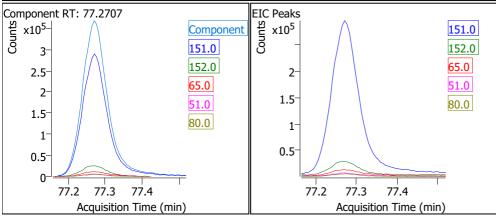
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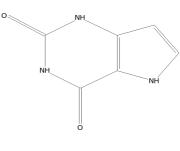
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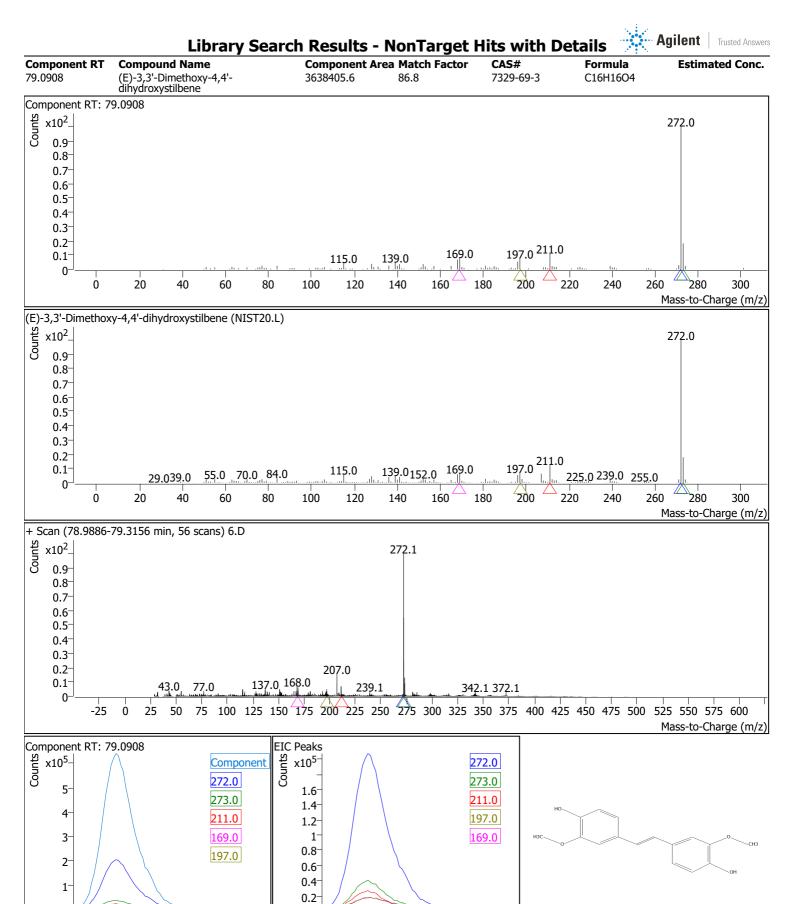
75.9

76









79.2

Acquisition Time (min)

79.1

79.2

