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



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

5/1/2024 3:07:36 PM

240502 data.uaf **Analysis File Name** 

Acq. Date-Time

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

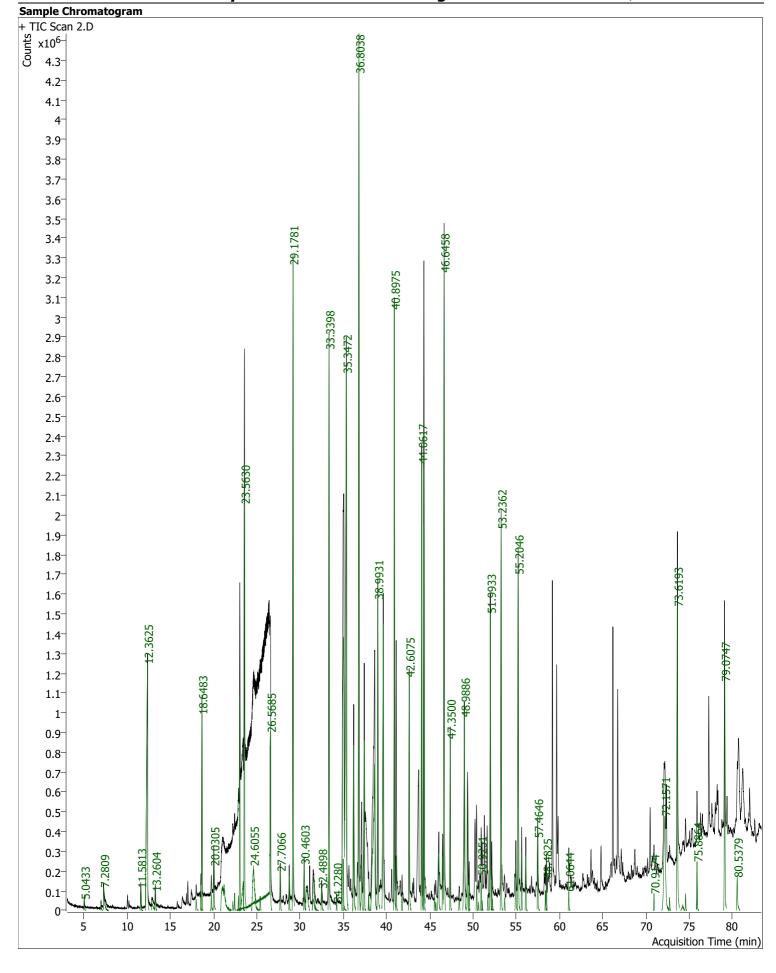
2.D D:\MassHunter\GCMS\1\data\RBEL\240501 scan **File Name Path Name Sample Name Sample Type** 2 Sample Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

**Instrument Name** GCMSD Dil. 1

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
5.0433	2-Furanol, tetrahydro-	5371-52-8	C4H8O2	188882.7	88.5	
6.9807	Furfural	98-01-1	C5H4O2	150585.4	92.5	
7.2809	1,3-Propanediol	504-63-2	C3H8O2	925296.6	95.9	
11.5804	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	431566.3	77.3	
11.5813	2-[2-[2-(2- Methoxyethoxy)ethoxy]ethoxy]ethyl acetate	1000351-91-3	C13H26O7	538229.9	78.0	
12.3625	Butyrolactone	96-48-0	C4H6O2	11047770.1	97.9	
12.8681	Methyltartronic acid	595-98-2	C4H6O5	415567.6	88.5	
13.2604	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	458979.5	76.1	
17.9856	Phenol	108-95-2	C6H6O	274586.0	93.4	
18.5390	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	409631.9	92.0	
18.6483	Diisoamyl ether	544-01-4	C10H22O	3686697.4	98.2	
19.7362	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	384492.3	90.8	
20.0305	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	1098758.3	96.9	
21.2046	1,3,5-Trioxane	110-88-3	C3H6O3	3417826.6	79.0	
22.2327	p-Cresol	106-44-5	C7H8O	180089.9	84.9	
22.4353	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	330106.3	93.6	
22.8690	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	311820.8	75.6	
23.0308	1-Octanol	111-87-5	C8H18O	4445035.6	98.8	
23.4297	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	1531121.4	93.6	
23.5630	Phenol, 2-methoxy-	90-05-1	C7H8O2	8765662.5	98.5	
24.6055	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	3524648.5	91.3	
25.3846	2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-	21835-00-7	C7H10O1	304943.5	77.1	
26.5685	Glycerin	56-81-5	C3H8O3	13670144.5	75.8	
27.7066	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	872463.8	82.0	
28.7415	Naphthalene	91-20-3	C10H8	699608.4	97.6	
29.1781	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	13244044.4	99.3	
30.4603	1,3-Dioxolane, 2-butyl-4-methyl-	74094-60-3	C8H16O2	1051989.4	78.6	
30.7588	Catechol	120-80-9	C6H6O2	1651884.3	86.5	
31.5313	5-Hydroxymethylfurfural	67-47-0	C6H6O3	2002808.7	95.4	
31.5315	l-Alanine, n-propargyloxycarbonyl-, ethyl ester	1000322-67-3	C9H13NO4	678504.3	79.5	
	, , , , , , , , ,				79.5 95.5	
32.4898 33.3398	1,2-Benzenediol, 3-methoxy-	934-00-9 2785-89-9	C7H8O3 C9H12O2	578478.4 11135894.7	95.5 97.6	
34.2280	Phenol, 4-ethyl-2-methoxy- Naphthalene, 2-methyl-	91-57-6	C11H10	155737.7	78.2	
34.9811	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	1051855.9	90.5	
35.0488		97-72-3	C8H14O3	16256114.2	83.6	
35.0793	Propanoic acid, 2-methyl-, anhydride	212762-88-4	C15H20O4	145009.1	78.6	
35.3472	Pentandioic acid, (p-t-butylphenyl) ester Ethylene glycol Formate Isobutyrate	1000458-48-0	C7H12O4	21982689.0	78.6	
36.2009	Propanoic acid, 2-methyl-, anhydride	97-72-3	C8H14O3	4141813.2	85.6	
36.2009	2-Furanmethanol, tetrahydro-	97-72-3 97-99-4	C5H10O2	4289960.8	84.5	
36.8038	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O2	17769986.3	99.1	
37.1195	5-Fluoro-2-hydroxyacetophenone	394-32-1	C8H7FO2	1569677.8	80.4	
37.4136	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	3164872.0	93.8	
				260785.3		
37.9287 37.9290	3,5-Dimethoxy-4-hydroxytoluene 1,2,3-Trimethoxybenzene	6638-05-7 634-36-6	C9H12O3 C9H12O3	294957.5	81.6 80.1	
38.6225	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	10832043.7	79.1	
	Sulfurous acid, isobutyl pentyl ester				79.1 76.4	
38.6228 38.9931	Vanillin	1000309-13-8 121-33-5	C9H20O3S C8H8O3	10952627.8	97.4	
				6992601.5	75.0	
39.6191	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	8252841.2		
40.8975	3,5-Dimethoxy-4-hydroxytoluene Phenol, 2-methoxy-4-(2-propenyl)-, acetate	6638-05-7	C9H12O3	11548388.6	95.3	
41.1106	, , , , , , , , , , , , , , , , , , , ,	93-28-7 97-53-0	C12H14O3	1040935.6	79.8 81.0	
41.7787	Eugenol Apocynin	498-02-2	C10H12O2	341215.3		
42.6075 44.0617	• •	14059-92-8	C9H10O3 C10H14O3	4963040.2 8373385.5	98.9	
	4-Ethyl-2,6-dimethoxyphenol				98.6 93.8	
44.2931	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	8338048.4		
44.3284	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	7789517.6	95.1 77.7	
45.5429 45.7045	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	322435.3 194537.2	77.7 81.2	
45.7045	Phenol, 4-ethenyl-2,6-dimethoxy-	28343-22-8	C10H12O3			
46.0382	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	1844358.2	95.2	
46.4793 46.6458	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9 64142-23-0	C10H12O3	1111484.7	91.9 94.4	
46.6458	Butyrovanillone	64142-23-0	C11H14O3	13832172.3		
47.3500	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	3228213.5	97.2	
48.3929	Benzeneacetic acid, .alpha.,4-dihydroxy-3-methoxy-, methyl ester		C10H12O5	316596.3	75.5	
48.9886	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	5862365.1	95.6	



Component R1	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
49.3563	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2524757.3	95.2	
49.5437	N,N-Diethyl-p-nitroaniline	2216-15-1	C10H14N2O2	553483.1	79.2	
50.4168	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	615087.7	86.3	
50.6302	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	1081-71-6	C10H10O5	155122.2	78.6	
50.9251	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	6627-88-9	C11H14O3	847290.5	82.0	
51.0508	2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]-	1000131-52-4	C8H11NO2	210089.8	79.8	
51.7086	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	4899-74-5	C10H12O4	336745.6	87.8	
51.9933	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	6384267.2	98.1	
52.1482	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	871583.9	78.5	
52.2249	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	4899-74-5	C10H12O4	292272.3	83.7	
53.2362	Syringylacetone	19037-58-2	C11H14O4	7738114.4	97.2	
53.6457	9H-Fluorene, 9-methylene-	4425-82-5	C14H10	257391.0	82.5	
54.9472	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	1132096.9	88.5	
55.2046	Butylsyringone	69271-91-6	C12H16O4	7797717.8	92.7	
55.6143	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	1032702.5	90.2	
56.0909	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	1105112.6	81.2	
57.4646	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	1608727.9	93.6	
58.3576	.betaHydroxypropiosyringone	136196-47-9	C11H14O5	429712.0	78.6	
58.4825	Ethyl (E)-ferulate	28028-62-8	C12H14O4	616261.0	87.6	
61.0644	Hexadecanoic acid, ethyl ester	628-97-7	C18H36O2	385114.9	77.2	
70.9174	Methyl dehydroabietate	1235-74-1	C21H30O2	315352.9	78.5	
72.1571	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6755335.1	83.1	
72.7132	1-(2,4-Dihydroxyphenyl)-2-(3,4-dimethoxyphenyl)ethanone	24126-98-5	C16H16O5	310167.7	75.7	
73.6193	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	7974946.1	93.1	
74.2321	1H-isoindole-1,3(2H)-dione, 2-(5-methoxy-8-nitro-1-naphthalenyl)-	1000398-30-5	C19H12N2O5	270961.6	77.7	
74.5711	Silane, diethylnonyloxypropoxy-	1010363-08-5	C16H36O2Si	354036.6	75.2	
75.8864	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	1091277.6	79.3	
75.8864	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	857506.2	88.3	
79.0747	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	6146817.1	93.3	
80.5379	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	1084953.1	97.3	



### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5.0433 2-Furanol, tetrahydro-188882.7 88.5 5371-52-8 C4H8O2 Component RT: 5.0433 v10<sup>2</sup> 0.9 42.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 57.0 0.3 31.0 39.0 0.2 47.0 87.0 0.1 0 30 40 85 20 25 35 50 55 65 70 75 80 90 95 Mass-to-Charge (m/z) 2-Furanol, tetrahydro- (NIST20.L) st x10<sup>2</sup> 0.9 42.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 27.0 57.0 39.0 0.2 71.0 47.0 84.0 87.0 0.1 55.0 25.0 33.0 50.0 20 25 30 35 40 45 55 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (5.0077-5.0968 min, 16 scans) 2.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 57.0 $0.4^{-}$ 32.0 0.3 0.2 87.0 0.1 71.0 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: 5.0433 **EIC Peaks** Counts x10<sup>4</sup>. x10<sup>4</sup> 42.0 Component 42.0 41.0 1.4 4 41.0 57.0 3.5 1.2 43.0 57.0

31.0

1

0.8

0.6

0.4

 $0.2^{-}$ 

5.05

5.1

5.15

Acquisition Time (min)

5.2

43.0

31.0

5.2

3

2

2.5

1.5

0.5

5.05 5.1 5.15

### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 98-01-1 6.9807 **Furfural** 150585.4 92.5 C5H4O2 Component RT: 6.9807 y x10<sup>2</sup> 0.9 95.0 0.8 0.7 0.6 39.0 0.5 0.4 0.3 0.2 67.0 0.1 82.0 100 10 15 20 25 30 35 55 60 65 75 80 85 90 105 Mass-to-Charge (m/z) Furfural (NIST20.L) St x10<sup>2</sup>\_ 0.9 96.0 0.8 0.7 39.0 0.6 0.5 0.4 0.3 29.0 0.2 67.0 0.1 42.0 51.0 26.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 105 Mass-to-Charge (m/z) + Scan (6.9286-7.1775 min, 41 scans) 2.D St x10<sup>2</sup> 0.9 95,0 0.8 32.0 0.7 0.6 44.0 0.5 $0.4^{-}$ 0.3 0.2 67.0 0.1 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 70 Mass-to-Charge (m/z) EIC Peaks Component RT: 6.9807 Counts x10<sup>4</sup> x10<sup>4</sup> 96.0 Component 95.0 95.0 2.5 96.0 39.0 0.8 2 38.0 39.0

7.1

Acquisition Time (min)

67.0

7.2

0.6

0.4

 $0.2^{-}$ 

0-

38.0 67.0

7.2

7.1

Acquisition Time (min)

1.5

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.** 504-63-2 7.2809 1,3-Propanediol 925296.6 95.9 C3H8O2 Component RT: 7.2809 v10<sup>2</sup> 0.9 58.0 31.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 43.0 0.2 0.1 39.0 55 5 15 25 70 75 10 20 30 35 40 80 85 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 28.0 58.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 45.0 0.2 0.1 15.0 18.0 41.0 55.0 68.0 73.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (7.2440-7.8499 min, 102 scans) 2.D st x10<sup>2</sup> 0.9 58.0 31.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 43.0 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: 7.2809 **EIC Peaks** Counts Counts x10<sup>4</sup> Component 57.0 58.0 58.0 0.9 2.25 57.0 31.0 0.8 2 0.7 1.75 31.0 43.0 0.6 1.5 43.0 45.0 0.5 1.25

7.3 7.4 7.5 7.6 7.7 7.8 Acquisition Time (min)

45.0

7.8

1-

 $0.75^{-}$ 

0.5

0.4

0.3

0.2

0

7.4

7.6

### --- 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 11.5804 Propane, 1,1-diethoxy-431566.3 C7H16O2 Component RT: 11.5804 v10<sup>2</sup> 0.9 103.0 87.0 0.8 $0.7^{-}$ 57.0 0.6 31.0 0.5 59.0 45.0 0.4 0.3 0.2 47.0 0.1 29.0 100 105 10 15 20 25 30 35 40 45 50 55 60 65 75 90 110 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 0.6 103.0 0.5 29.0 75.0 0.4 31.0 0.3 57.0 0.2 41.0 45.0 0.1 15.0 19.0 39.0 78.0 105 10 15 20 25 30 35 40 45 50 55 60 65 70 75 85 90 95 100 110 115 Mass-to-Charge (m/z) + Scan (11.4973-11.7557 min, 43 scans) 2.D St x10<sup>2</sup> 0.9 103.0 0.8 87.0 0.7 0.6 31.0 0.5 $0.4^{-}$ 57.0 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: 11.5804 **EIC Peaks** Counts Counts x10<sup>4</sup> 103.0 Component 103.0 87.0 1.6 7 87.0 1.4 57.0 6 Н3С < 1.2 57.0 31.0 5

11.6

11.7

Acquisition Time (min)

11.8

59.0

1

0.8

0.6

0.4

31.0

59.0

4

3

2-

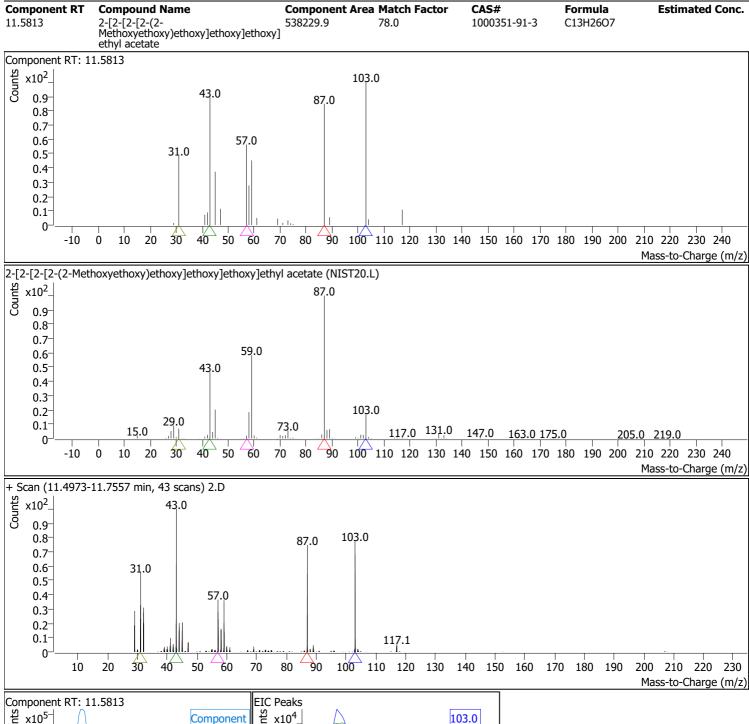
11.6

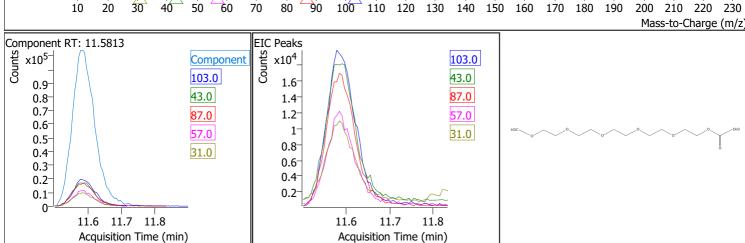
11.7

Acquisition Time (min)

11.8

### **Library Search Results - NonTarget Hits with Details** --- Agilent | Trusted Answers **Compound Name Component Area Match Factor** CAS# **Formula** 2-[2-[2-(2-538229.9 78.0 1000351-91-3 C13H26O7 Methoxyethoxy)ethoxy]ethoxy] ethyl acetate





### -- 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 12.3625 Butyrolactone 11047770.1 97.9 C4H6O2 Component RT: 12.3625 v10<sup>2</sup> 0.9 42.1 0.8 0.7 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 0.1 0 25 55 75 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 (12.1094-12.5116 min, 68 scans) 2.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 29.0 86.0 0.3 56.0 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 12.3625 Counts Counts x10<sup>6</sup> x10<sup>5</sup>\_ 42.1 Component 42.1 41.1 3 1 41.1 86.0 2.5 0.8 29.0 86.0



12.3

12.4

Acquisition Time (min)

12.5

56.0

2

1

1.5

0.5

29.0

56.0

12.2 12.3 12.4 12.5

Acquisition Time (min)

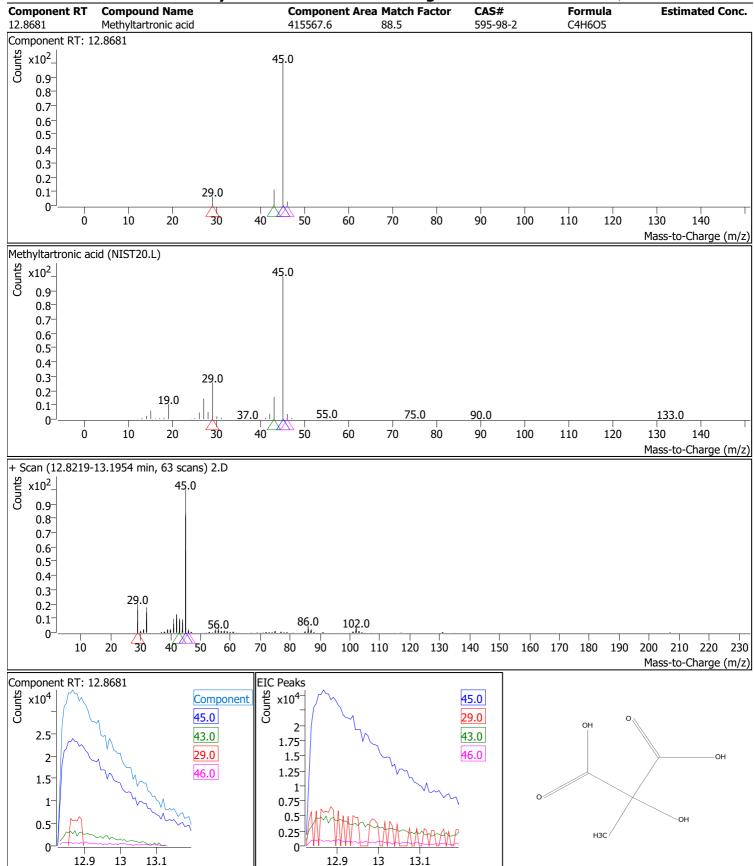
0.6

0.4

0.2

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

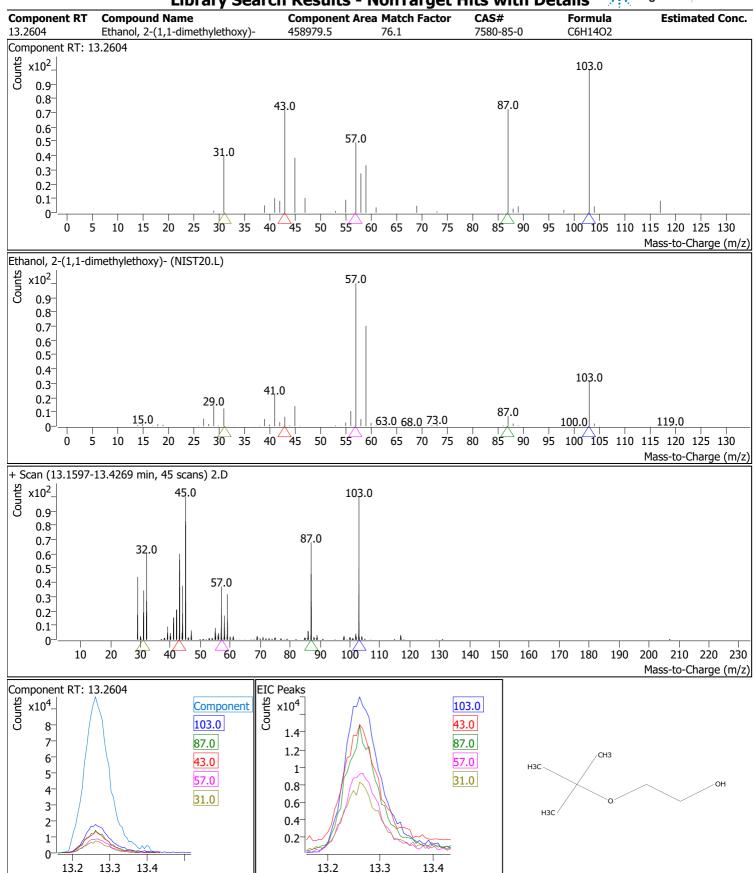




Acquisition Time (min)







Acquisition Time (min)

### Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 108-95-2 274586.0 C6H6O 17.9856 Phenol 93.4 Component RT: 17.9856 v10<sup>2</sup> 0.9 94.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 66.0 0.2 39.0 0.1 63.0 50.0 55.0 25 40 55 65 75 85 90 95 20 30 35 45 50 60 70 80 100 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10<sup>2</sup>\_0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 39.0 0.2 0.1 55.0 47.050.0 63.0 27.0 74.0 40 95 20 25 30 35 45 50 55 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) + Scan (17.9046-18.2376 min, 57 scans) 2.D St x10<sup>2</sup> 0.9 61.0 0.8 0.7 43.0 94.0 0.6 0.5 0.4 0.3 32.0 0.2 103.0 117.0 0.1 75.0 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: 17.9856 Counts x10<sup>4</sup>. x10<sup>4</sup>-94.0 Component 94.0 66.0 2 66.0 65.0 3.5 1.75 39.0 65.0 1.5 3

18

18.1

Acquisition Time (min)

18.2

40.0

39.0

40.0

1.25

0.75

0.5

0.25

2.5

1.5

2

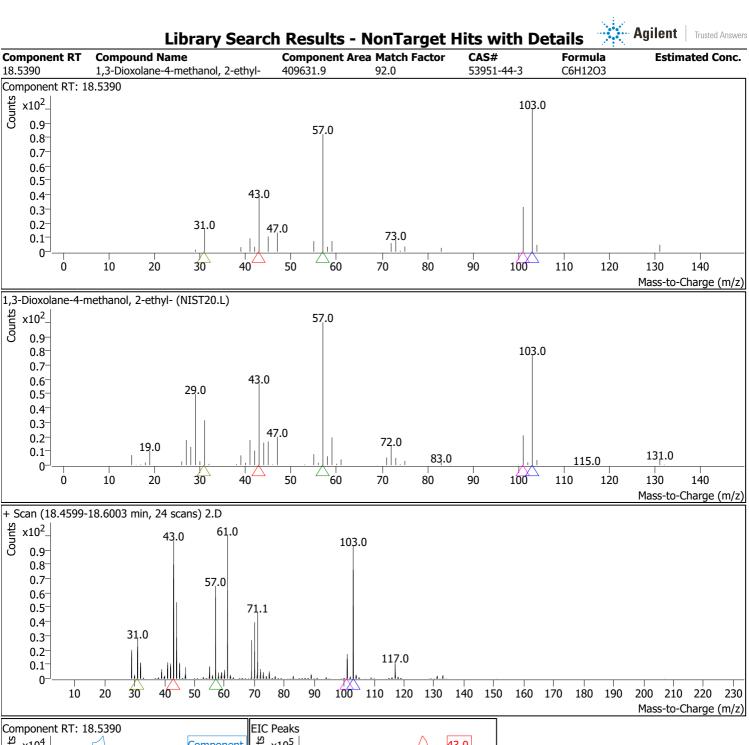
1. 0.5

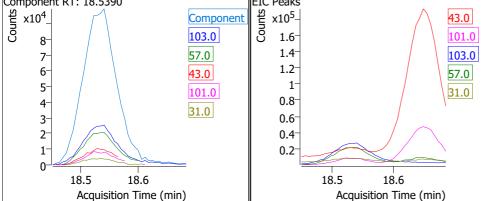
18

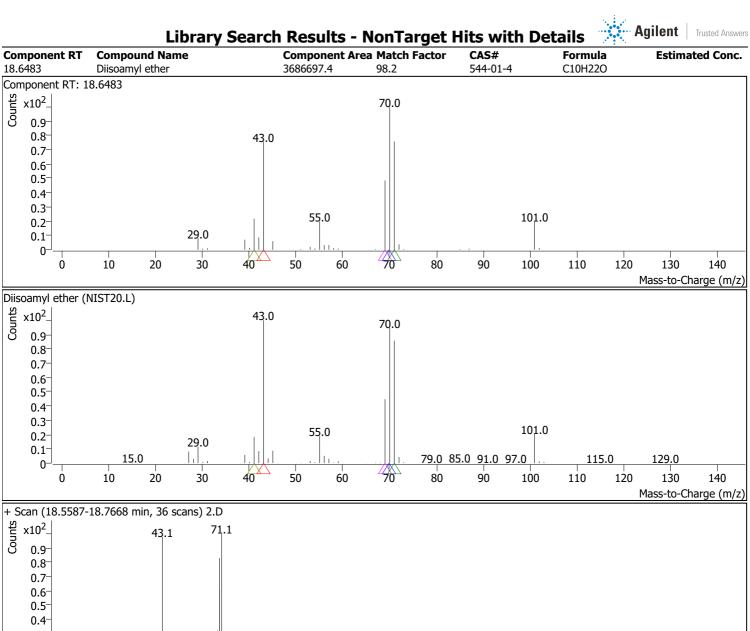
18.1

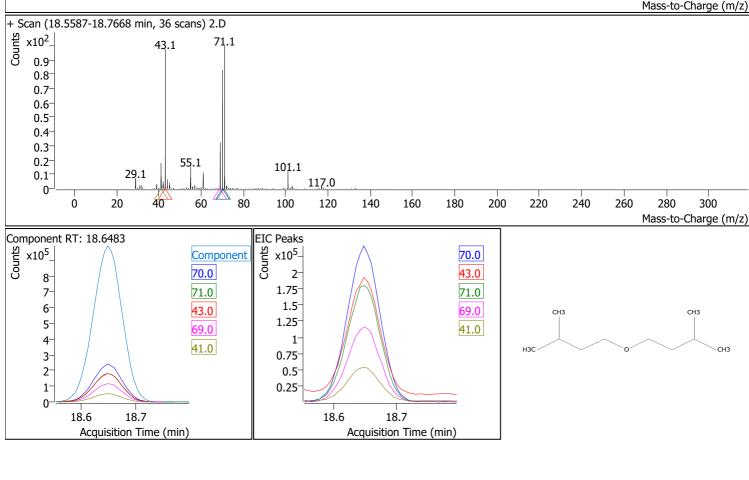
Acquisition Time (min)

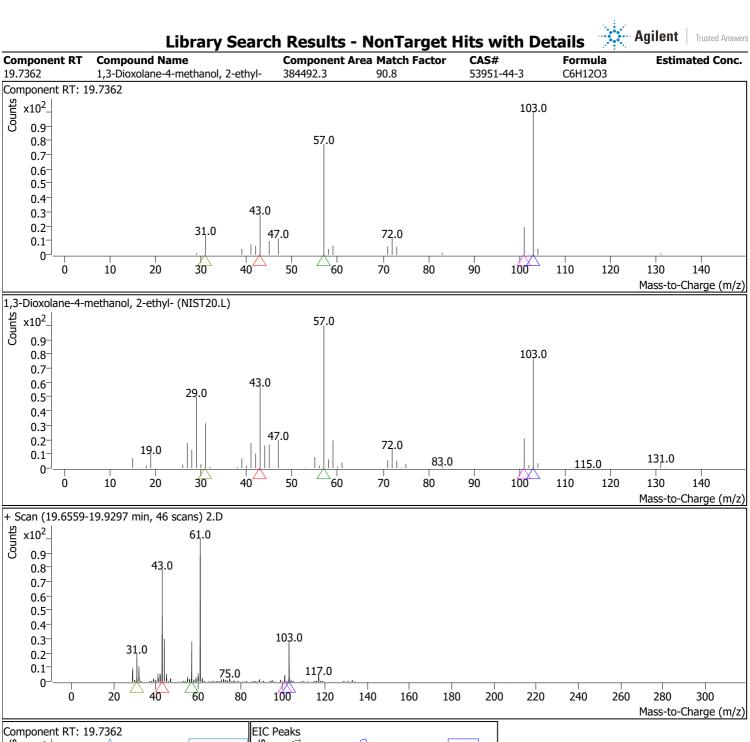
18.2

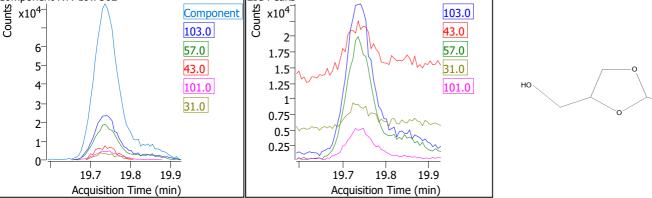












### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 80-71-7 20.0305 2-Cyclopenten-1-one, 2-hydroxy-3-1098758.3 96.9 C6H8O2 methyl-Component RT: 20.0305 x10<sup>2</sup>. 112.0 0.9 8.0 0.7 0.6 0.5 0.4 69.0 55.0 0.3 83.0 41.0 $0.2^{-}$ 0.1 0-55 30 35 45 50 60 65 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2-hydroxy-3-methyl- (NIST20.L) $x10^{2}$ 112.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 69.0 41.0 55.0 0.2 43.0 83.0 39.0 0.1 53.0 97.0 66.0 0 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (19.9266-20.2176 min, 49 scans) 2.D $x10^{2}$ 0.9 0.8 0.7 43.0 0.6 0.5 112.0 0.4 0.3 0.2 69.0 31.0 83.0 0.1 0 Ó 20 40 80 100 200 220 260 60 120 140 160 180 240 280 300 Mass-to-Charge (m/z) Component RT: 20.0305 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>5</sup> 112.0 Component 112.0 69.0 5 1.8 69.0 55.0 1.6 1.4 55.0 83.0 1.2 3-83.0 41.0 нзс 0.8 41.0 2-

20.1

Acquisition Time (min)

1

0.6 0.4

0.2

20

20.1

Acquisition Time (min)

ОН

### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 110-88-3 21.2046 1,3,5-Trioxane 3417826.6 79.0 C3H6O3 Component RT: 21.2046 v10<sup>2</sup> 0.9 89.0 0.8 61.0 0.7 0.6 0.5 0.4 31.0 0.3 43.0 0.2 0.1 29.0 45.0 98.0 70.1 0 <del>9</del>0 25 70 95 10 15 20 30 35 40 45 50 55 65 75 80 85 100 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 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 (20.8360-21.3236 min, 83 scans) 2.D st x10<sup>2</sup> 0.9 0.8 0.7 43.0 0.6 0.5 0.4 0.3 0.2 31.0 89.0 0.1 117.0 60 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.2046 **EIC Peaks** Counts Counts x10<sup>5</sup> Component 89.0 0.9 61.0 31.0 0.8 8.0 31.0 0.7 89.0 0.6 43.0 60.0 0.6

21.5

Acquisition Time (min)

 $0.5^{-}$ 

0.4

0.3

0.1

21

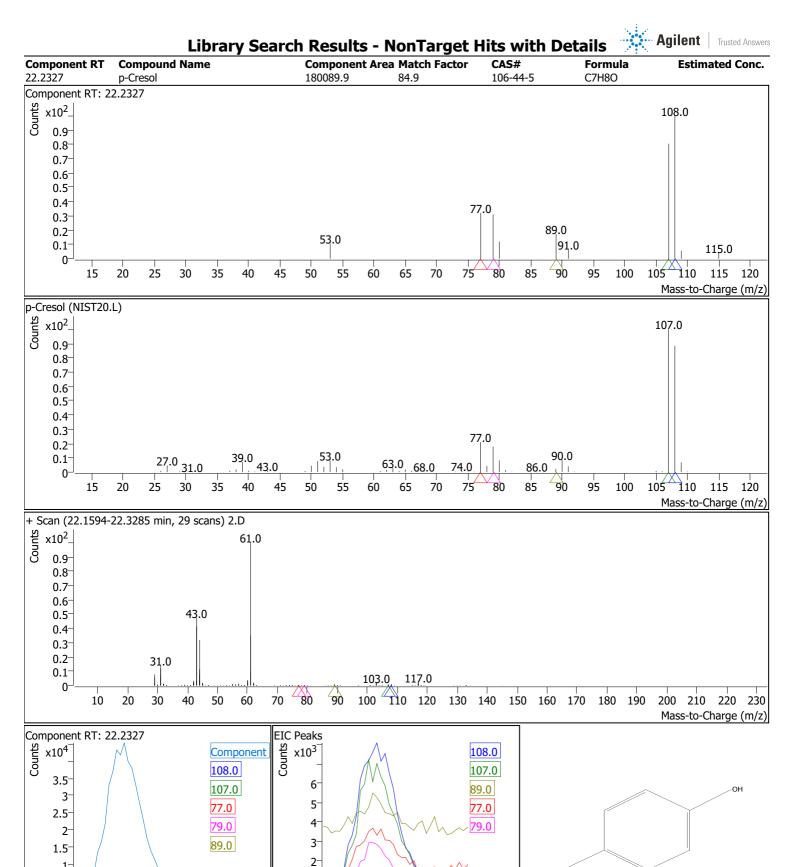
60.0

0.4

0.2

21

21.5



22.2 22.25 22.3

Acquisition Time (min)

1

1

22.2

22.3

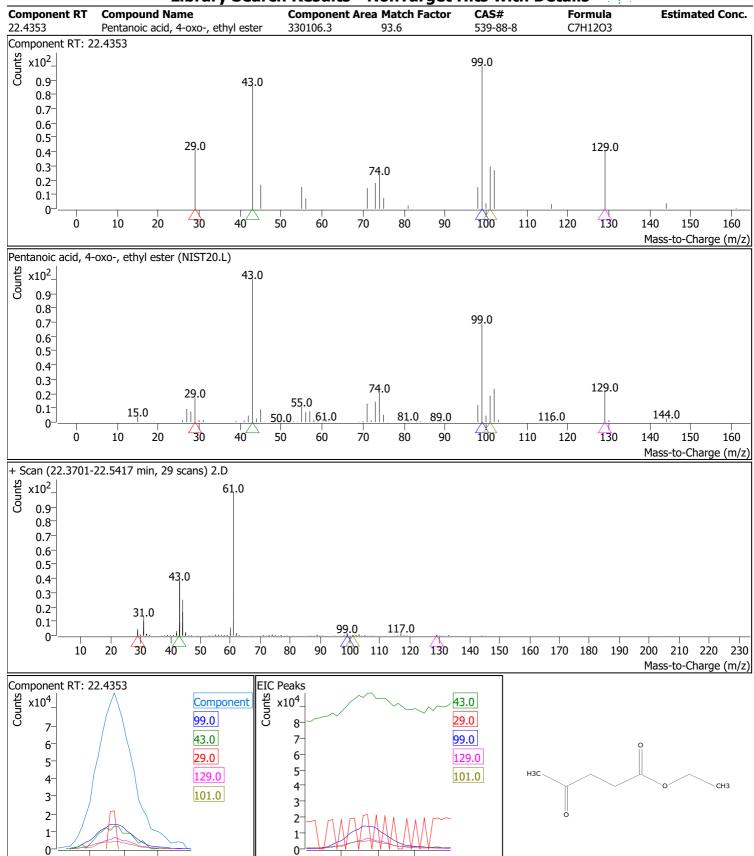
Acquisition Time (min)

0.5

**Н3С** 

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





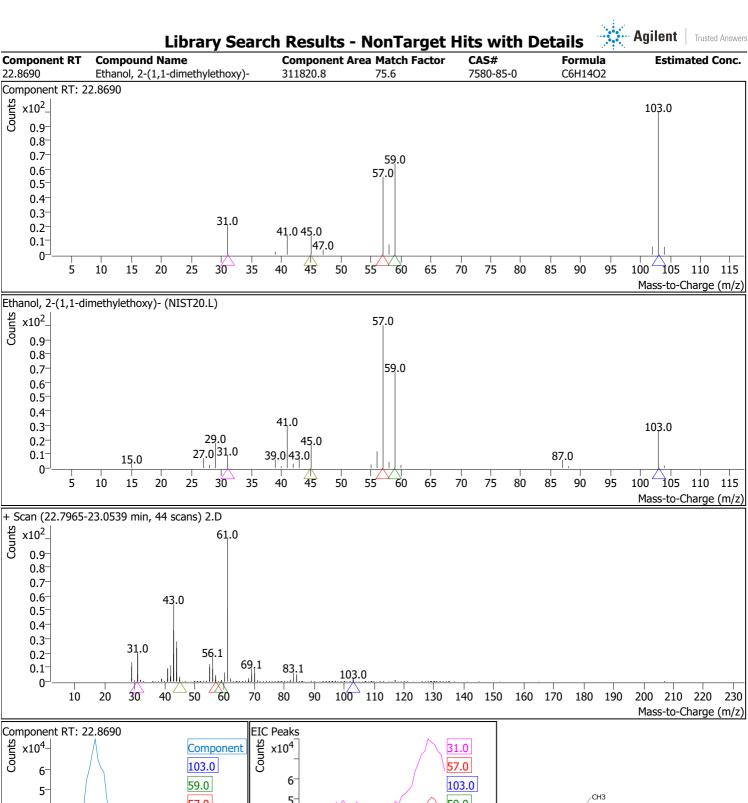
22.5

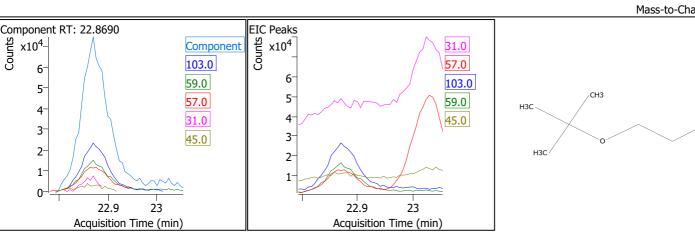
22.45

Acquisition Time (min)

22.4

22.45 22.5





### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0308 1-Octanol 4445035.6 98.8 111-87-5 C8H18O Component RT: 23.0308 y x10<sup>2</sup> 0.9 56.0 41.0 0.8 70.0 $0.7^{-}$ 84.0 29.0 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 (22.9418-23.2191 min, 46 scans) 2.D St x10<sup>2</sup>\_ 0.9 0.8 0.7 43.0 0.6 0.5 $0.4^{-}$ 0.3 31.0 0.2 56.1 70.1 83.1 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: 23.0308 Counts Counts x10<sup>5</sup> 56.0 Component 56.0 55.0 0.8 55.0 41.0 $0.7^{-}$ 0.8 41.0 69.0 0.6

23.1

Acquisition Time (min)

23.2

70.0

70.0

69.0

23.2

 $0.6^{-}$ 

0.4

0.2

0.5

0.4

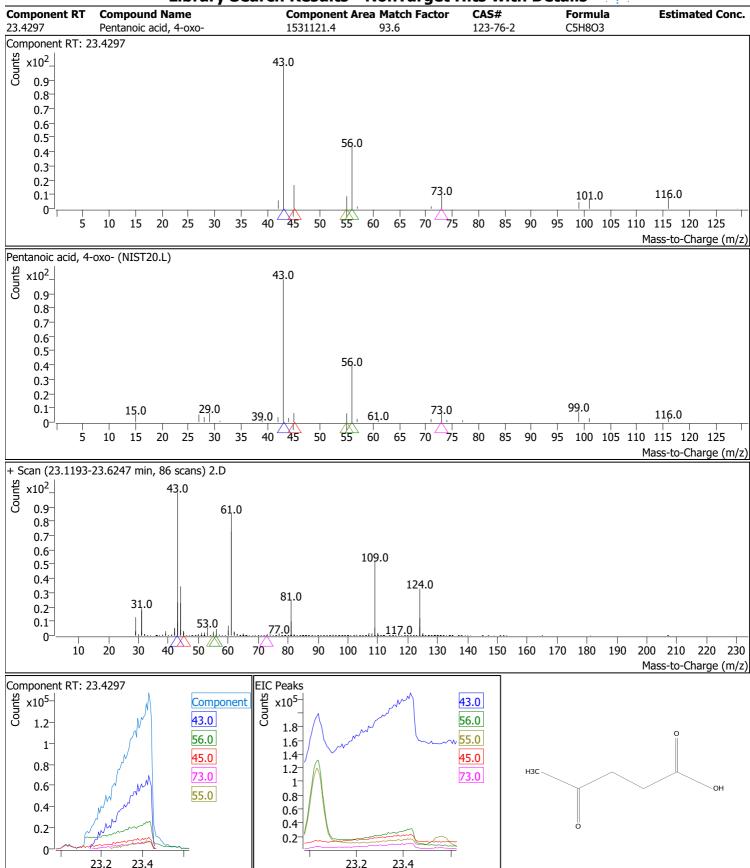
0.3 0.2

0.1

23

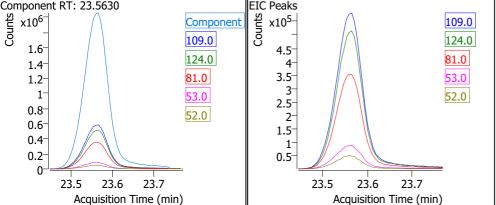


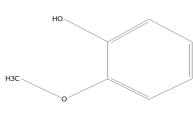




Acquisition Time (min)

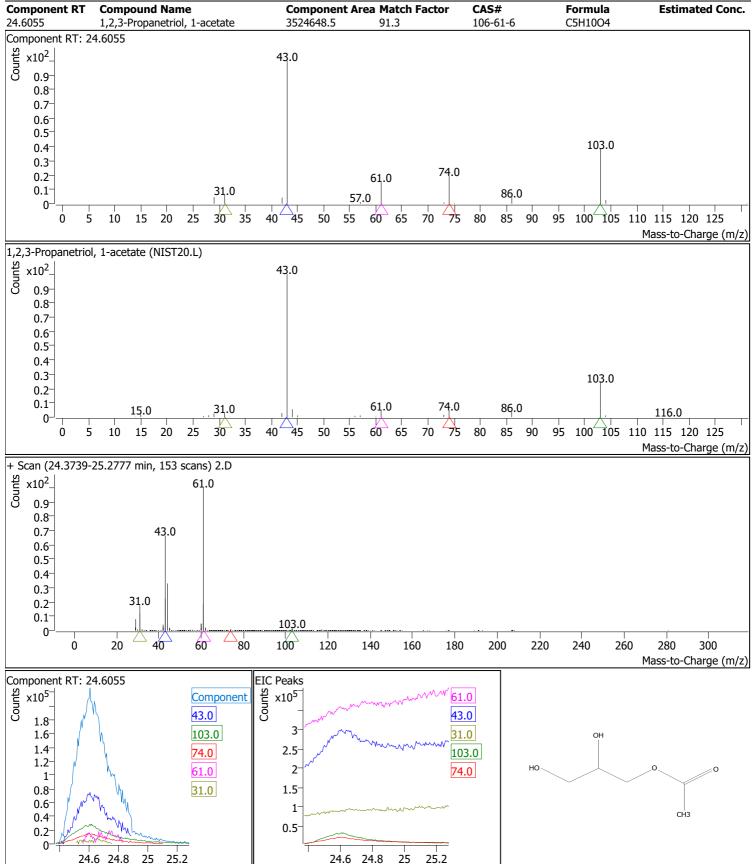
### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.5630 Phenol, 2-methoxy-8765662.5 98.5 C7H8O2 Component RT: 23.5630 v10<sup>2</sup> 0.9 109.0 124.0 0.8 $0.7^{-}$ 81.0 0.6 0.5 0.4 0.3 0.2 53.0 0.1 39.0 63.0 80 110 10 20 30 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 50 10 20 30 40 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4523-23.7317 min, 48 scans) 2.D st x10<sup>2</sup> 0.9 109.0 43.0 61.0 0.8 0.7 124.0 0.6 0.5 81.0 $0.4^{-}$ 0.3 31.0 0.2 53.0 0.1 77.0 117.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 23.5630 **EIC Peaks** Counts Counts x10<sup>5</sup> 109.0 Component 109.0 124.0 1.6 4.5 124.0 81.0 1.4





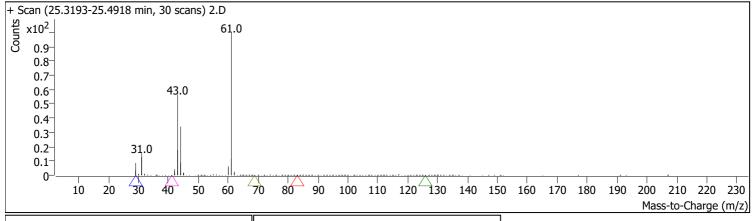






Acquisition Time (min)

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 25.3846 2-Cyclopenten-1-one, 2-hydroxy-3,4-304943.5 21835-00-7 C7H10O2 dimethyl-Component RT: 25.3846 $x10^{2}$ 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2 0.1 126.0 83.0 41.0 69.0 111.0 0 <del>7</del>0 110 35 40 45 50 55 60 65 75 80 85 90 95 100 105 115 120 125 130 135 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl- (NIST20.L) $x10^{2}$ 126.0 0.9 0.8 0.7 0.6 0.5 111.0 0.4 69.0 83.0 0.3 41.0 55.0 0.2 98.0 0.1



80

85

90

95

100

105

110

115

120

125

130 Mass-to-Charge (m/z)

70

75

65

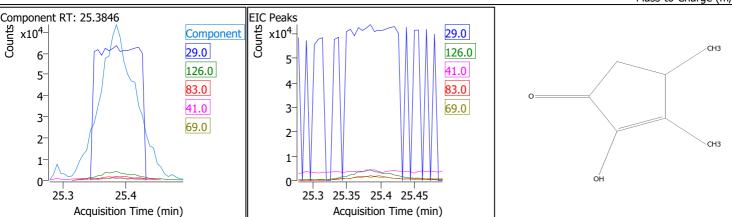
40

45

50

55

60



### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 26.5685 Glycerin 13670144.5 75.8 56-81-5 C3H8O3 Component RT: 26.5685 v10<sup>2</sup> 0.9 61.0 0.8 $0.7^{-}$ 0.6 43.0 0.5 0.4 0.3 0.2 31.0 0.1 55.0 74.0 55 75 10 15 20 25 30 35 50 65 70 85 90 95 100 Mass-to-Charge (m/z) Glycerin (NIST20.L) x10<sup>2</sup>\_ 0.9 61.0 0.8 0.7 43.0 0.6 0.5 0.4 0.3 31.0 15.0 0.2 29.0 18.0 0.1 <sup>\_</sup>45 85 5 10 15 20 25 30 35 40 50 55 60 65 70 75 80 90 95 100 Mass-to-Charge (m/z) + Scan (26.5145-26.7458 min, 39 scans) 2.D st x10<sup>2</sup> 0.9 61.0 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 31.0 0.3 0.2 0.1 117.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 26.5685 **EIC Peaks** Counts Counts x10<sup>5</sup> 61.0 Component 61.0 43.0 43.0 31.0 6 3.5 60.0 60.0

62.0

3

2

2.5

1.5

0.5

23

24

25

Acquisition Time (min)

26

31.0

62.0

5

4

3

2

1

23

24

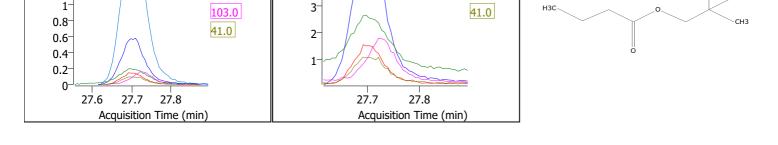
25

Acquisition Time (min)

26

ОН

### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7066 Butanoic acid, 2,2-dimethylpropyl 872463.8 82.0 23361-69-5 C9H18O2 Component RT: 27.7066 x10<sup>2</sup>\_ 71.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 0.3 87.0 103.0 57.0 $0.2^{-}$ 31.0 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) $x10^{2}$ 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 10 20 30 50 60 70 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6173-27.8741 min, 43 scans) 2.D x10<sup>2</sup>. 71.0 0.9 0.8 0.7 0.6 43.0 0.5 0.4 0.3 87.0 31.0 103.0 0.2 61.0 0.1 90 190 200 210 220 230 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z)



71.0

43.0

103.0

87.0

**EIC Peaks** 

St x10<sup>4</sup>

Component 71.0

43.0

87.0

Component RT: 27.7066

Counts

x10<sup>5</sup>.

1.6

1.4

1.2

СНЗ

-CH3

### --- 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 28.7415 Naphthalene 699608.4 97.6 C10H8 Component RT: 28.7415 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 51.0 64.0 50 75 45 55 65 70 85 100 105 110 115 120 Mass-to-Charge (m/z) Naphthalene (NIST20.L) 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 51.0 63.0 75.0 87.0 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 135 140 Mass-to-Charge (m/z) + Scan (28.6512-28.9524 min, 51 scans) 2.D st x10<sup>2</sup> 0.9 128.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 103.0 0.2 43.0 57.0 0.1 77.0 117.0 138.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 190 200 210 220 230 160 Mass-to-Charge (m/z) EIC Peaks Component RT: 28.7415 Counts st x10<sup>5</sup>x10<sup>4</sup>\_ 128.0 Component 128.0 127.0 1.4 127.0 129.0 1.2 6 129.0 102.0 1 5 102.0 126.0 0.8

28.8

Acquisition Time (min)

28.9

4

3-

2

1

28.7

126.0

0.6

0.4

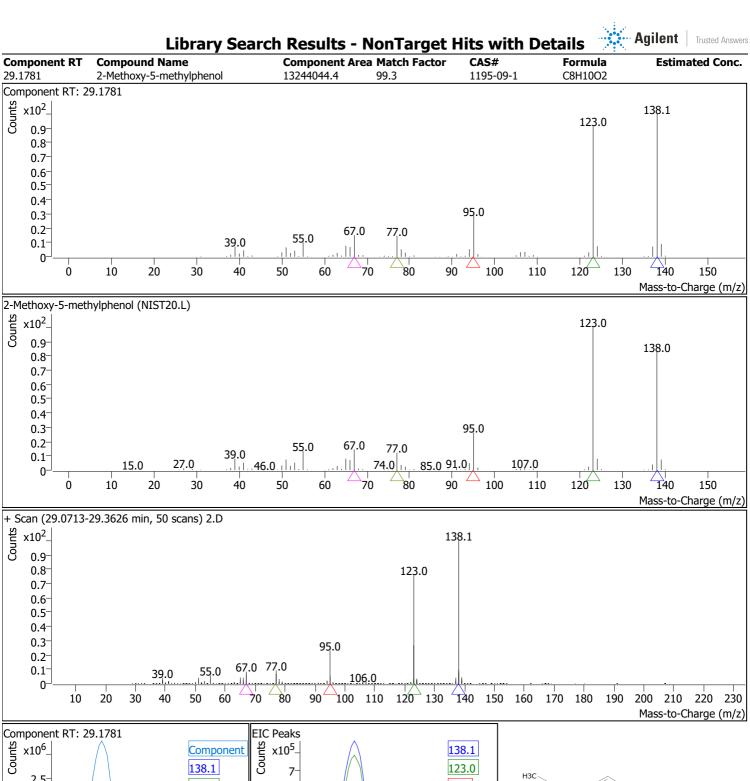
0.2

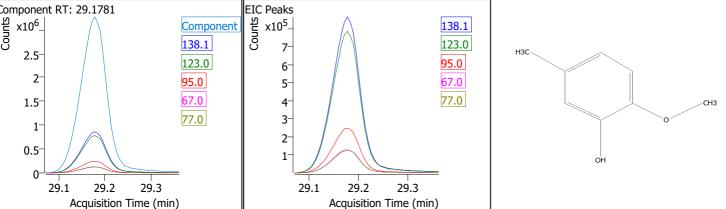
28.7

28.8

Acquisition Time (min)

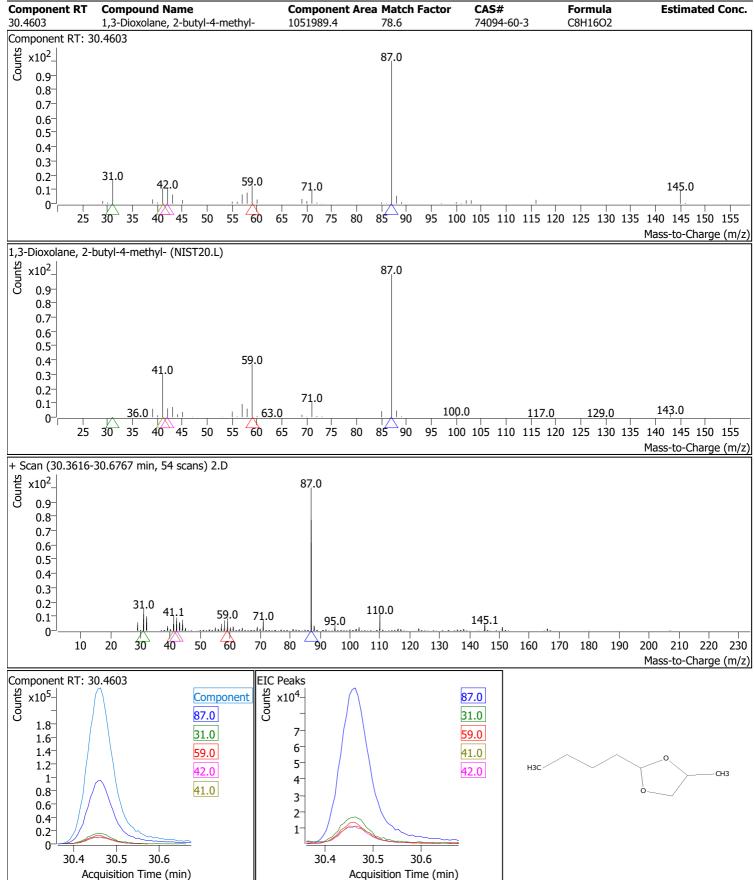
28.9





# **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.** 120-80-9 30.7588 Catechol 1651884.3 86.5 C6H6O2 Component RT: 30.7588 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 0.1 123.0 103.0 100 105 110 115 120 125 10 50 55 75 80 85 Mass-to-Charge (m/z) Catechol (NIST20.L) st x10<sup>2</sup> 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 <del>∠</del>65 10 15 25 30 35 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.6030-31.1167 min, 87 scans) 2.D St x10<sup>2</sup>\_ 0.9 110.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 64.0 0.2 125.0 81.0 32.0 44.0 53.1 97.0 0.1 154.1 69.0 0 90 100 10 20 40 50 60 80 110 120 130 140 150 170 180 190 200 210 220 230 160 Mass-to-Charge (m/z) EIC Peaks Component RT: 30.7588 Counts Counts x10<sup>4</sup> 110.0 Component 110.0 81.0 3 0.8 64.0 64.0 0.7 2.5 63.0 63.0 0.6



30.8

31

Acquisition Time (min)

92.0

2-

1-

1.5

0.5

81.0

92.0

0.5

 $0.4^{-}$ 

0.3

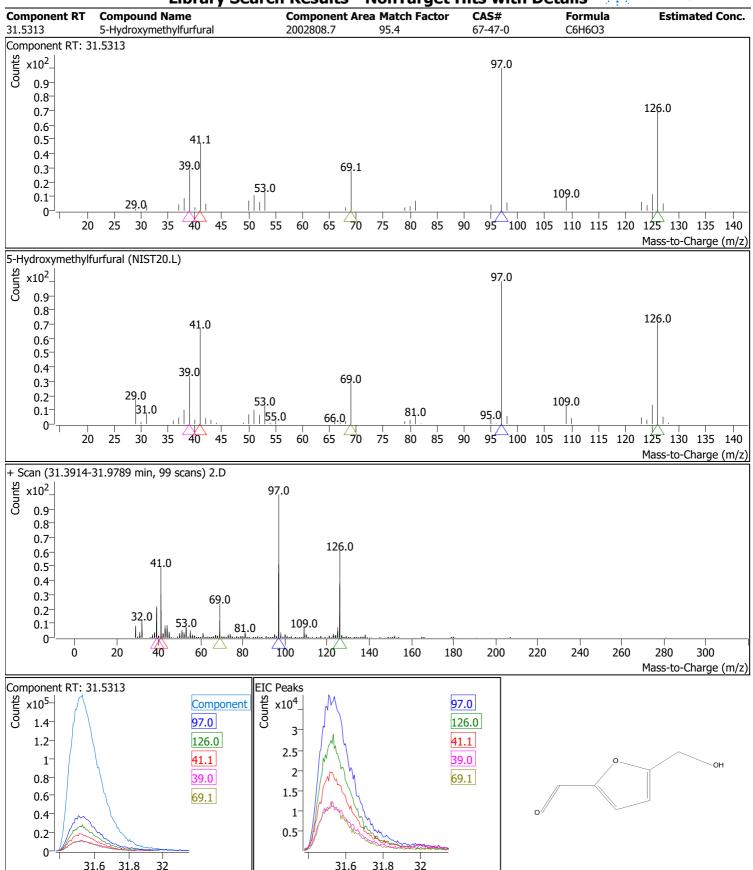
0.2-

0.1

30.8







Acquisition Time (min)

### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1000322-67-3 31.5315 I-Alanine, n-propargyloxycarbonyl-, 678504.3 79.5 C9H13NO4 ethyl ester Component RT: 31.5315 x10<sup>2</sup>\_ 126.0 0.9 8.0 0.7 0.6 29.0 39.0 0.5 0.4 0.3 $0.2^{-}$ 0.1 79.0 0 80 30 40 140 20 50 60 70 90 100 110 120 130 150 160 170 Mass-to-Charge (m/z) I-Alanine, n-propargyloxycarbonyl-, ethyl ester (NIST20.L) $x10^{2}$ 126.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 39.0 0.2 82.0 88.0 0.1 42.0 29.0 67.0 116.0 53.0 0 30 80 20 40 50 60 70 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (31.3914-31.9789 min, 99 scans) 2.D x10<sup>2</sup>\_ 97.0 0.9 0.8 0.7 126.0 0.6 41.0 0.5 0.4 0.3 69.0 0.2 32.0 53.0 109.0 0.1 81.0 0 Ó 40 80 220 260 280 300 20 60 100 120 140 160 180 200 240 Mass-to-Charge (m/z) Component RT: 31.5315 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup>-126.0 Component 126.0 39.0 5 2.25 29.0 29.0 1.75 39.0 38.0

Acquisition Time (min)

79.0

1.5

1.25

 $0.75^{-}$ 0.5

0.25

38.0

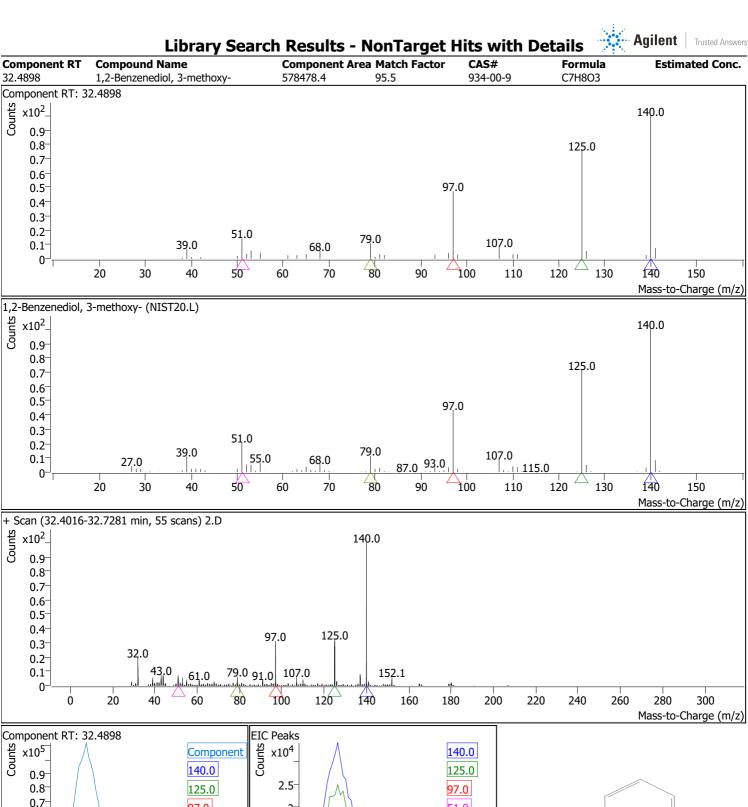
79.0

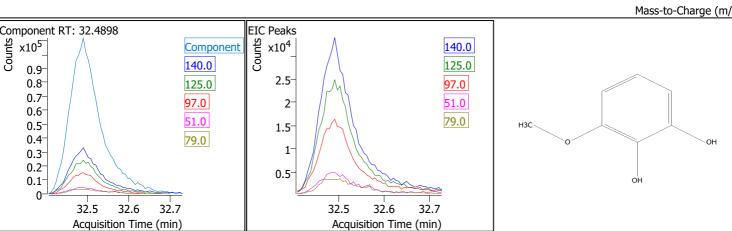
3

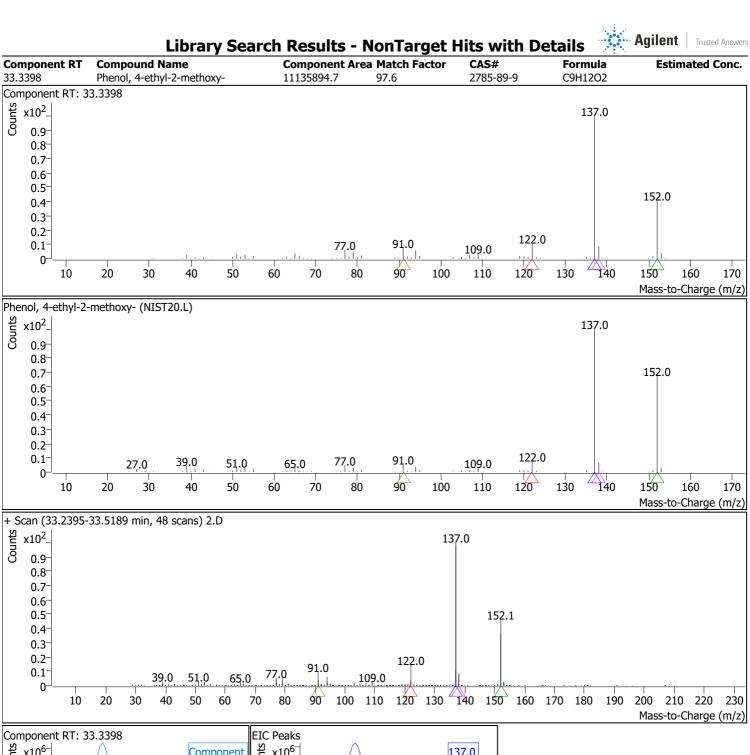
2

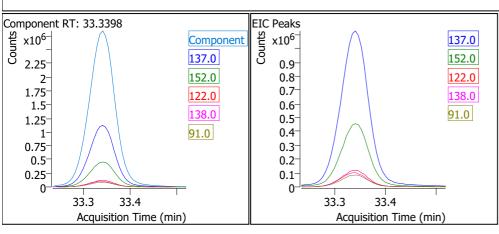
1

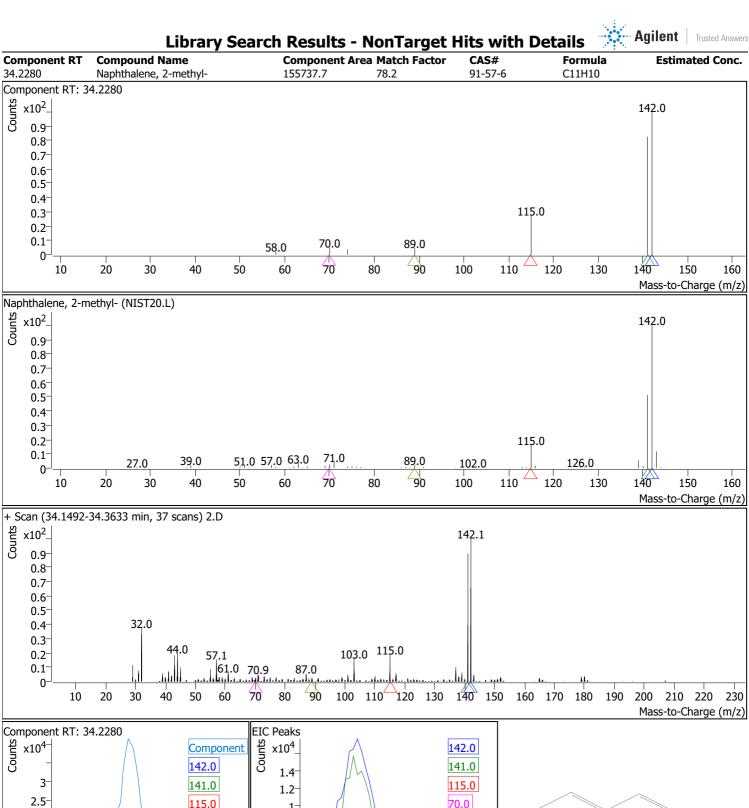
31.6

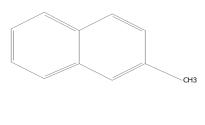


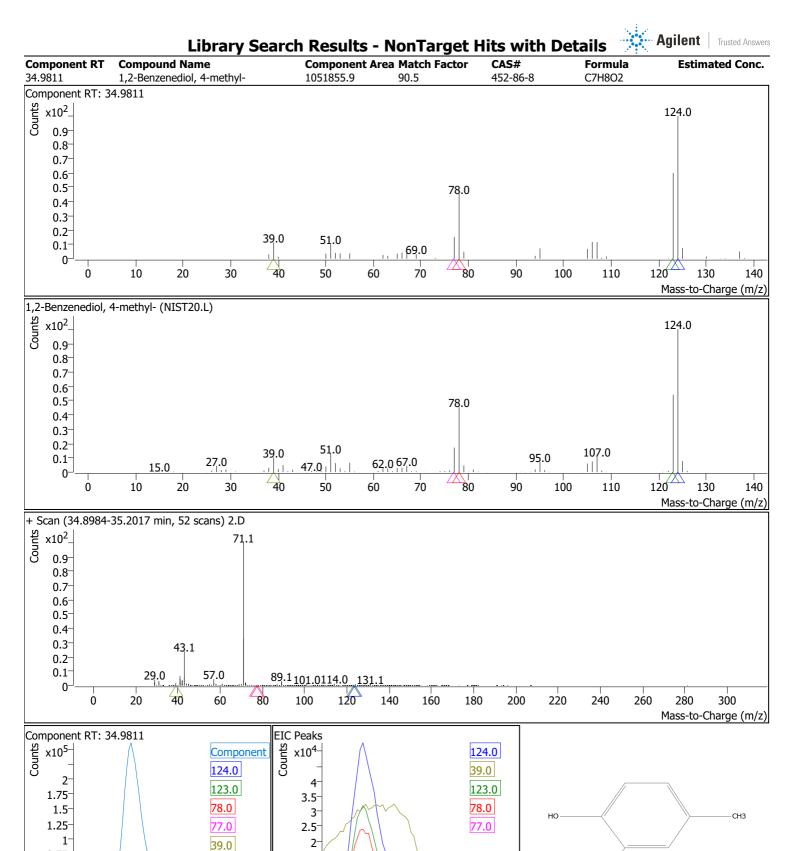














35 35.1 Acquisition Time (min)

1.5

1

0.75

0.5

0.25

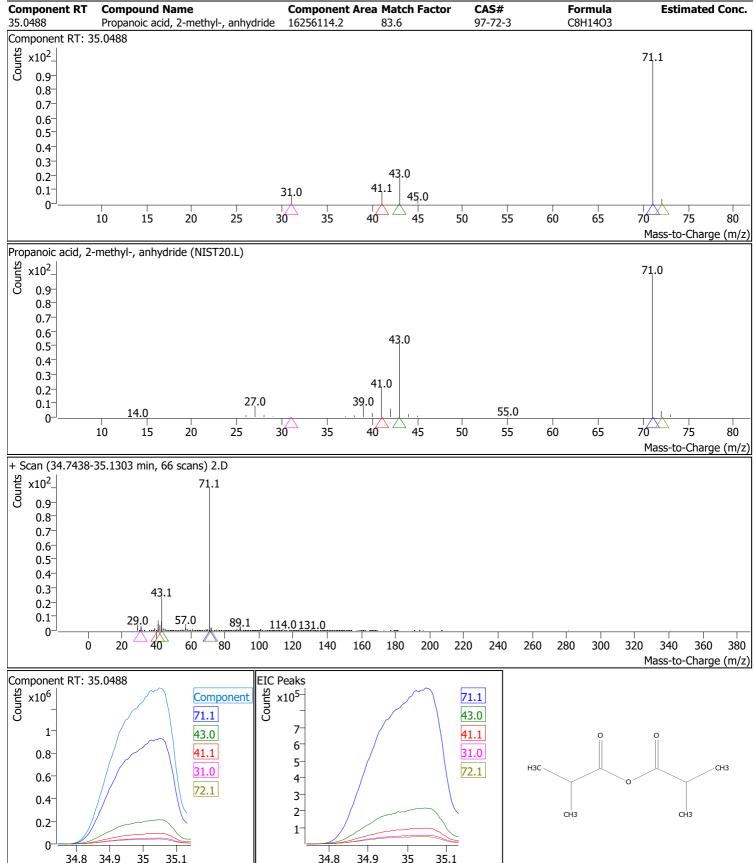
34.9

35

Acquisition Time (min)

35.1





Acquisition Time (min)

### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 145009.1 35.0793 Pentandioic acid, (p-t-butylphenyl) 78.6 212762-88-4 C15H20O4 Component RT: 35.0793 x10<sup>2</sup>\_ 150.0 0.9 135.0 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 0.1 126.0 0-140 100 160 220 240 260 20 40 60 80 120 180 200 280 Mass-to-Charge (m/z) Pentandioic acid, (p-t-butylphenyl) ester (NIST20.L) $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 0.5 150.0 0.4 0.3 0.2 107.0 0.1 41.0 55.065.0 77.087.0 247.0 264.0 177.0 191.0 205.0 219.0 0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 Mass-to-Charge (m/z) + Scan (34.9936-35.4038 min, 70 scans) 2.D x10<sup>2</sup>. 0.9 0.8 0.7 0.6 0.5 0.4 0.3 43.1 0.2 0.1 89.1 101.0114.1 57.0 31.0 0 140 <del>\_\_\_\_</del> 160 Ó 100 120 200 220 240 260 280 20 40 60 80 180 300 Mass-to-Charge (m/z) Component RT: 35.0793 **EIC Peaks** Counts Counts x10<sup>4</sup>x10<sup>4</sup> 150.0 Component 150.0 135.0 1.8 135.0 126.0 1.6 0.8 1.4 136.0 151.0 1.2

35.1 35.2 35.3

Acquisition Time (min)

136.0

0.6

 $0.4^{-}$ 

0.2

151.0

126.0

35.1 35.2 35.3

Acquisition Time (min)

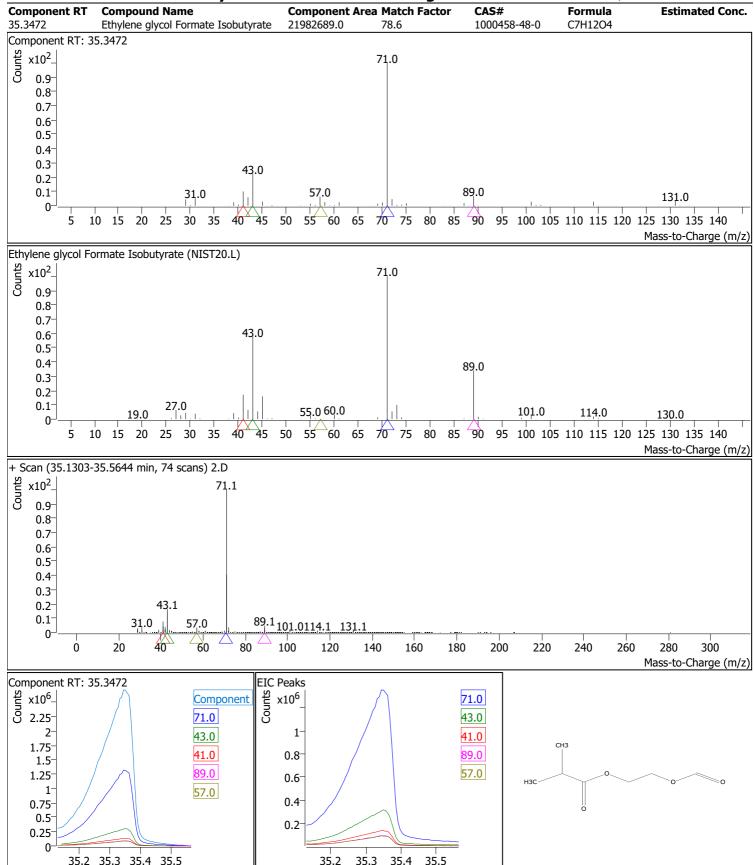
1

0.8

0.6 0.4

0.2

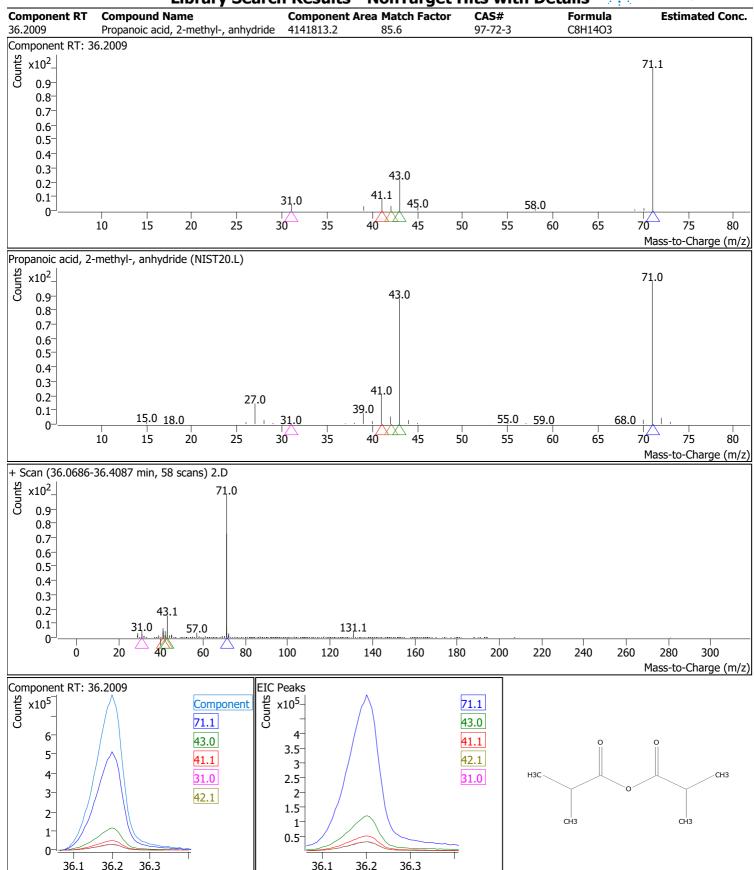




Acquisition Time (min)

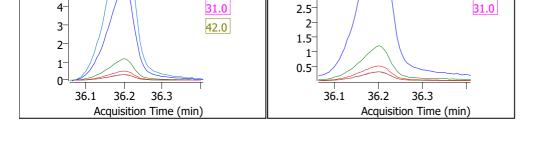




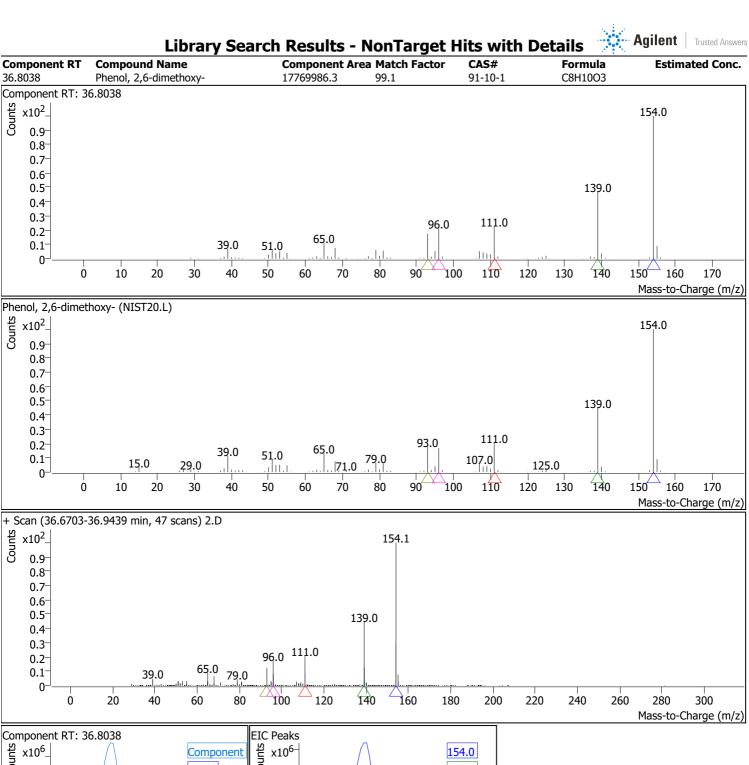


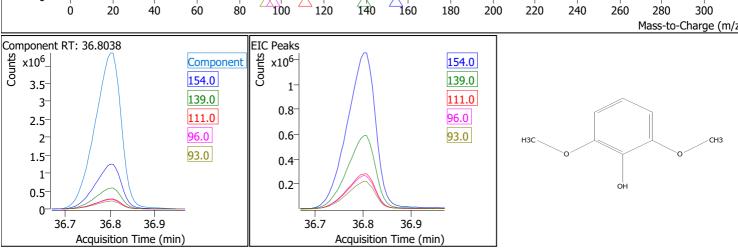
Acquisition Time (min)

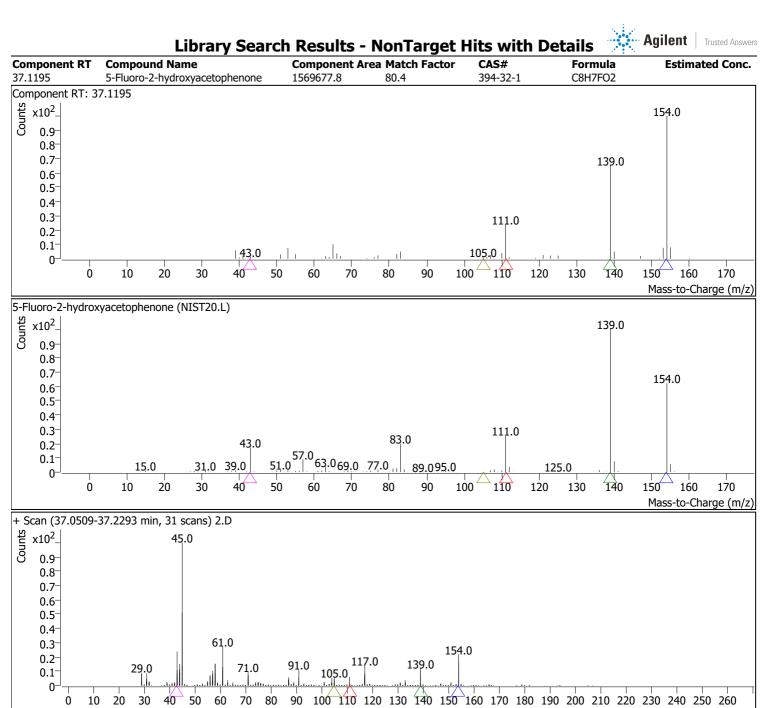
## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.2009 2-Furanmethanol, tetrahydro-4289960.8 84.5 C5H10O2 Component RT: 36.2009 v10<sup>2</sup> 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 0.1 31.0 57.0 100 105 110 10 15 25 30 35 55 60 65 85 90 95 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts 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 (36.0683-36.4087 min, 58 scans) 2.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 43.1 0.1 31.0 57.0 131.1 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 36.2009 Counts Counts x10<sup>5</sup>-71.0 Component 71.0 43.0 6 43.0 41.0 3.5 5 41.0 42.0

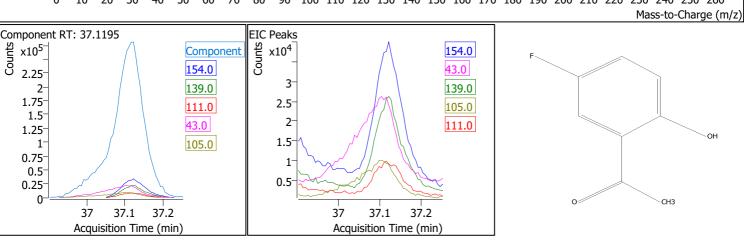


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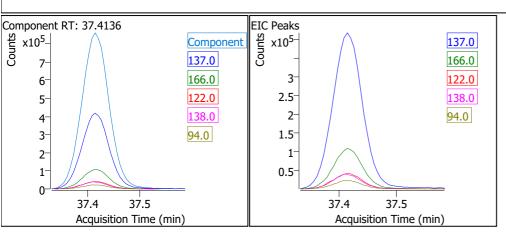


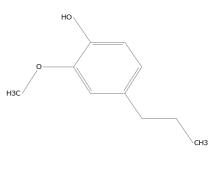






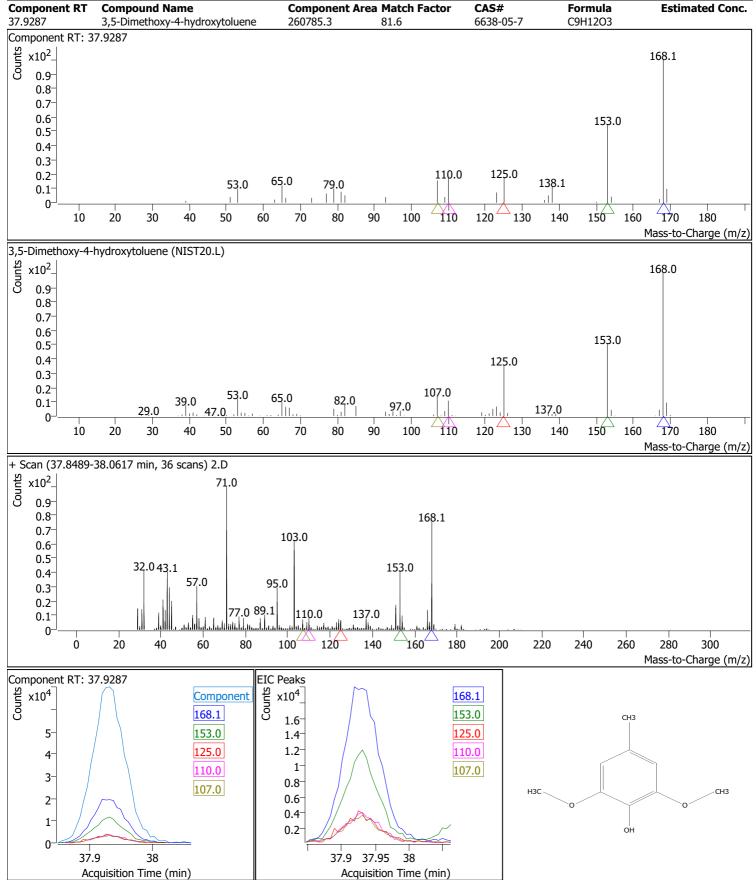
### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4136 Phenol, 2-methoxy-4-propyl-3164872.0 93.8 C10H14O2 Component RT: 37.4136 v10<sup>2</sup> 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 41.0 77.0 160 170 40 120 10 20 30 50 60 80 100 110 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 150 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 180 Mass-to-Charge (m/z) + Scan (37.3303-37.5860 min, 44 scans) 2.D st x10<sup>2</sup> 0.9 137.0 0.8 $0.7^{-}$ 0.6 103.0 0.5 71.0 $0.4^{-}$ 0.3 43.0 0.2 57.0 166.1 0.1 89.1 122.0 10 20 30 40 50 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 60 Mass-to-Charge (m/z) Component RT: 37.4136 **EIC Peaks** x10<sup>5</sup> 137.0 Component





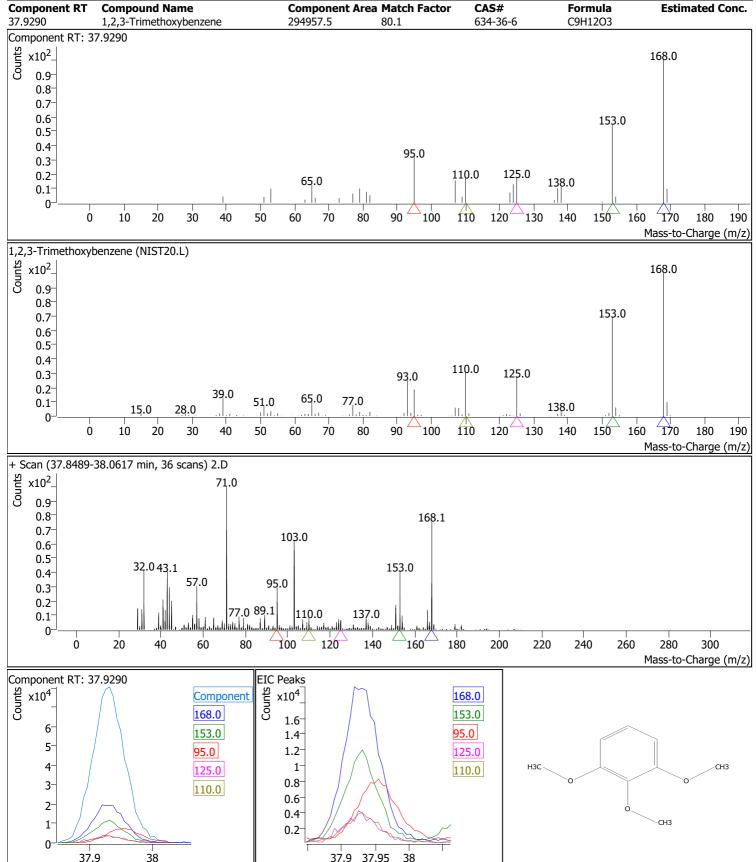












Acquisition Time (min)

## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 38.6225 2-Furanmethanol, tetrahydro-10832043.7 79.1 C5H10O2 Component RT: 38.6225 v10<sup>2</sup> 0.9 71.1 0.8 0.7 0.6 0.5 0.4 43.0 0.3 0.2 41.1 57.0 29.0 0.1 87.0 45.0 55.0 30 85 100 105 110 10 15 25 45 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 61.0 102.0 10 15 20 35 40 50 55 60 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (38.1251-38.8466 min, 122 scans) 2.D st x10<sup>2</sup> 0.9 103.0 0.8 0.7 0.6 0.5 57.0 71.1 $0.4^{-}$ 0.3 0.2 0.1 87.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 38.6225 Counts x10<sup>5</sup>x10<sup>5</sup> Component 71.1 71.1 57.0 6 1.4 43.0 43.0 5 1.2

29.0

41.1

41.1

57.0

29.0

1

0.8

0.6

0.4

0.2

38.2

38.4

38.6

Acquisition Time (min)

4

3

2

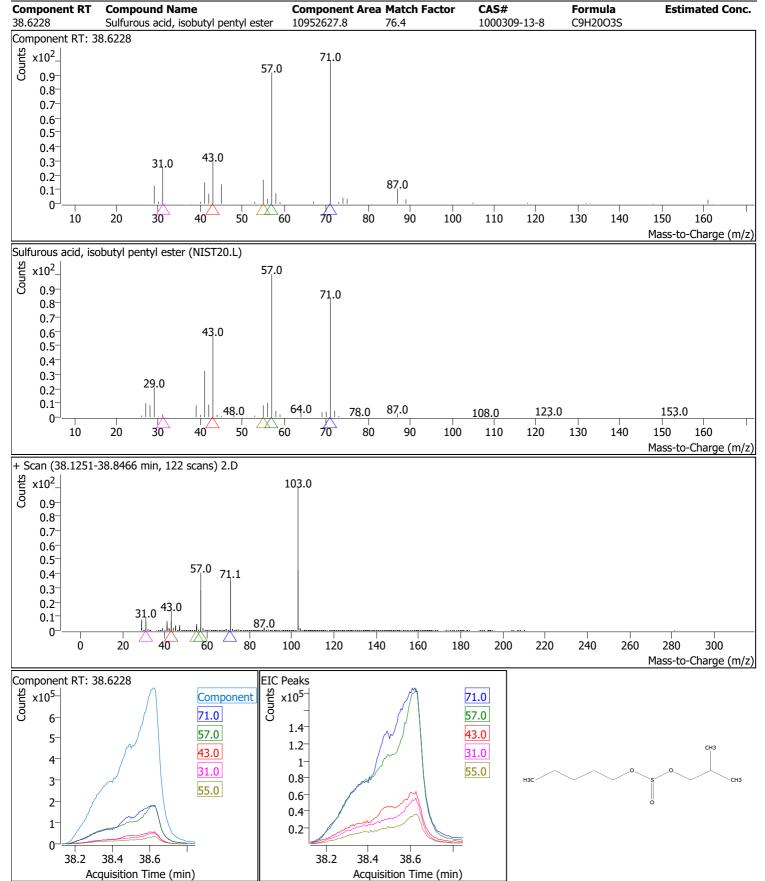
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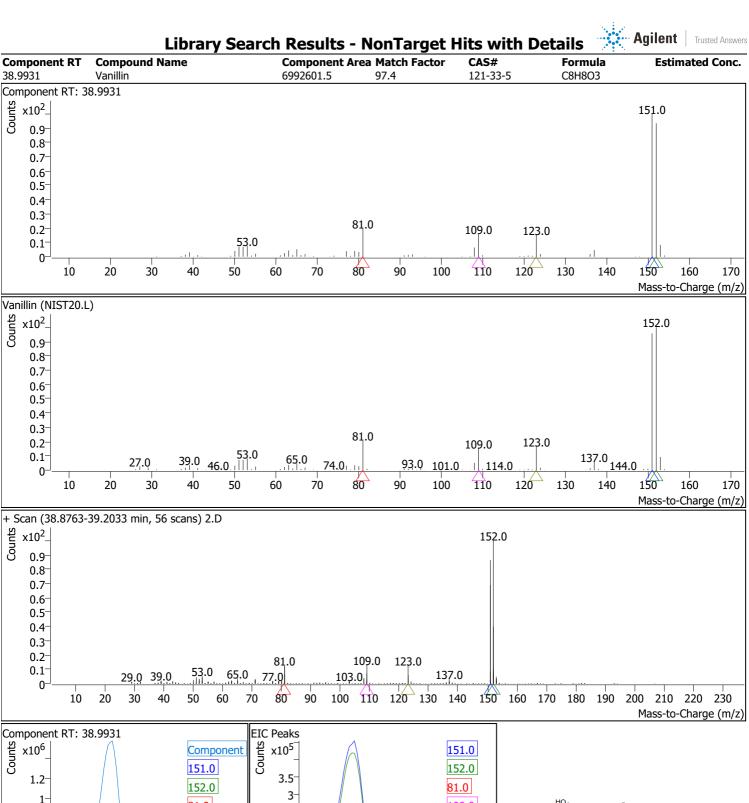
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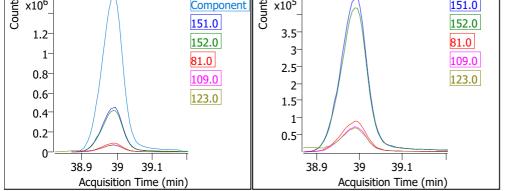
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38.6

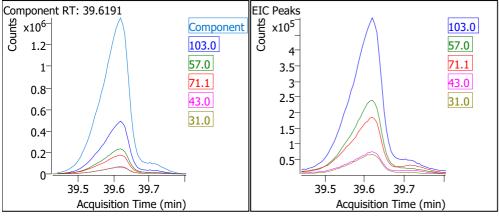






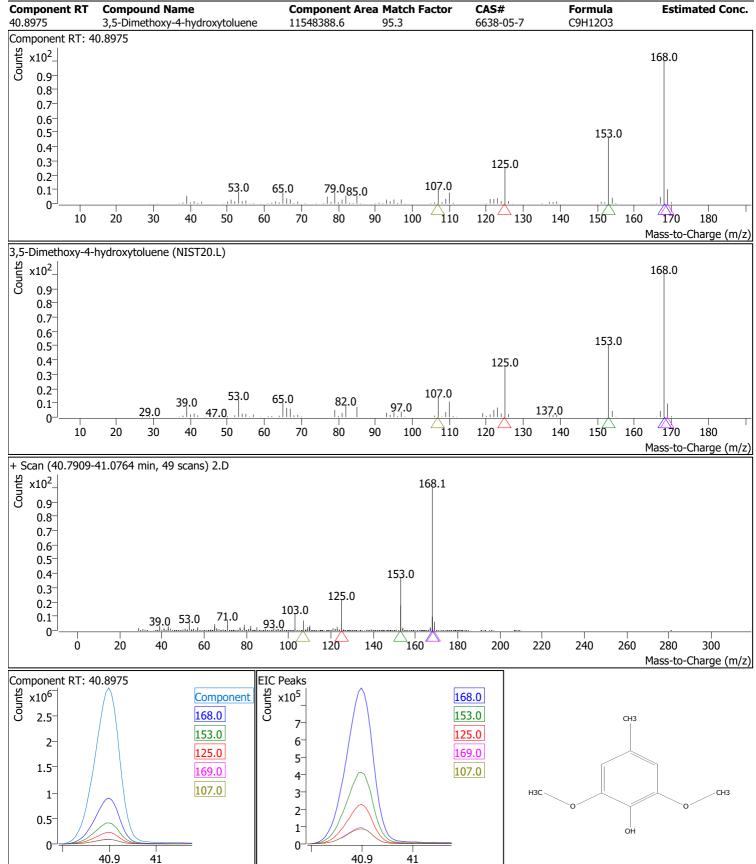


## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 39.6191 1,3-Dioxolane-4-methanol, 2-ethyl-8252841.2 75.0 C6H12O3 Component RT: 39.6191 v10<sup>2</sup> 0.9 103.0 0.8 0.7 0.6 57.0 0.5 0.4 71.1 0.3 0.2 43.0 31.0 0.1 30 40 70 120 130 Ó 10 20 50 80 90 100 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 70 0 10 20 30 40 50 60 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (39.4412-39.8039 min, 62 scans) 2.D st x10<sup>2</sup> 0.9 103.0 0.8 0.7 0.6 57.0 0.5 $0.4^{-}$ 71.0 0.3 0.2 29.1 43.0 0.1 87.0 <del>6</del>0 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 39.6191 Counts Str. x10<sup>6</sup> x10<sup>5</sup> 103.0 Component 103.0 57.0 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.** 93-28-7 Phenol, 2-methoxy-4-(2-propenyl)-, 41.1106 1040935.6 79.8 C12H14O3 acetate Component RT: 41.1106 Counts x10<sup>2</sup>\_ 164.0 0.9 8.0 0.7 0.6 0.5 0.4 149.0 0.3 77.0 91.0 131.0 $0.2^{-}$ 121.0 104.0 0.1 0-150 90 130 30 40 50 60 70 80 100 110 120 140 160 170 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-(2-propenyl)-, acetate (NIST20.L) Counts $x10^{2}$ 164.0 0.9 0.8 0.7 0.6 0.5 149.0 0.4 77.0 0.3 55.0 103.0 91.0 131.0 0.2 51.0 121.0 65.0 137.0 0.1 43.0 82.0 70.0 59.0 0 150 130 30 40 50 60 70 80 90 100 110 120 140 160 170 180 Mass-to-Charge (m/z) + Scan (41.0256-41.2666 min, 41 scans) 2.D st x10<sup>2</sup> 103.0 0.8 0.7 0.6 71.0 0.5 0.4 0.3 43.0 57.0 0.2 89.0 31.0 0.1 0 Ó 80 140 160 180 200 220 240 260 20 40 60 100 280 300 Mass-to-Charge (m/z) Component RT: 41.1106 **EIC Peaks** Counts Counts $x10^{4}$ x10<sup>5</sup> 164.0 Component 149.0 164.0 2.25 4 149.0 77.0 3.5 1.75 131.0 77.0 3 1.5



91.0

91.0

131.0

1.25

0.75

0.5

41.1

41.2

Acquisition Time (min)

0.25

2.5

1.5

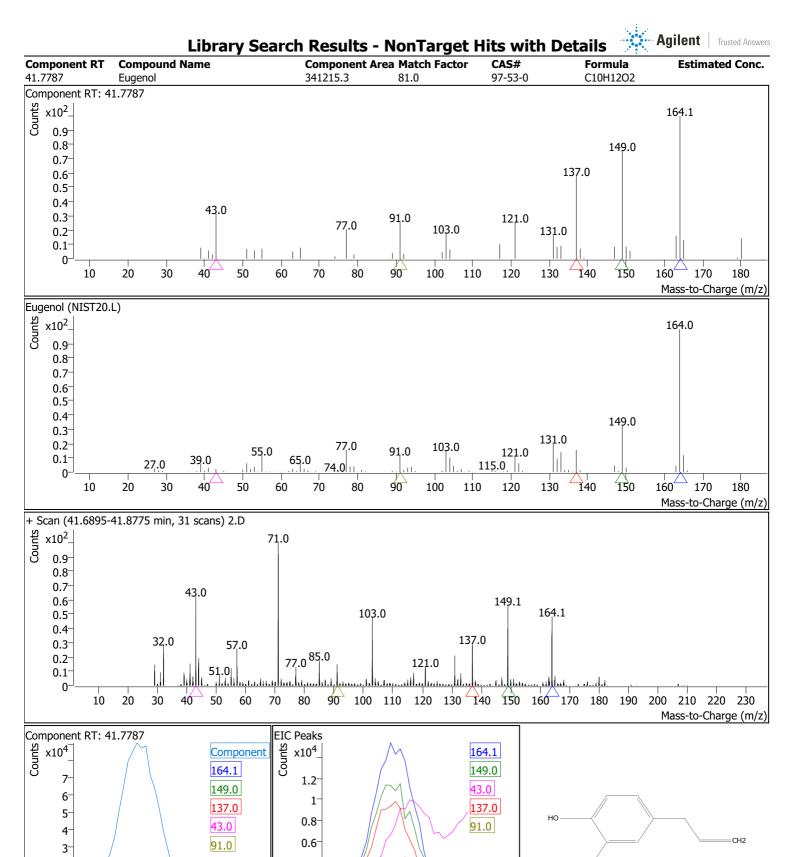
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2

1

41.1

41.2



41.75

41.8

Acquisition Time (min)

41.85

0.4

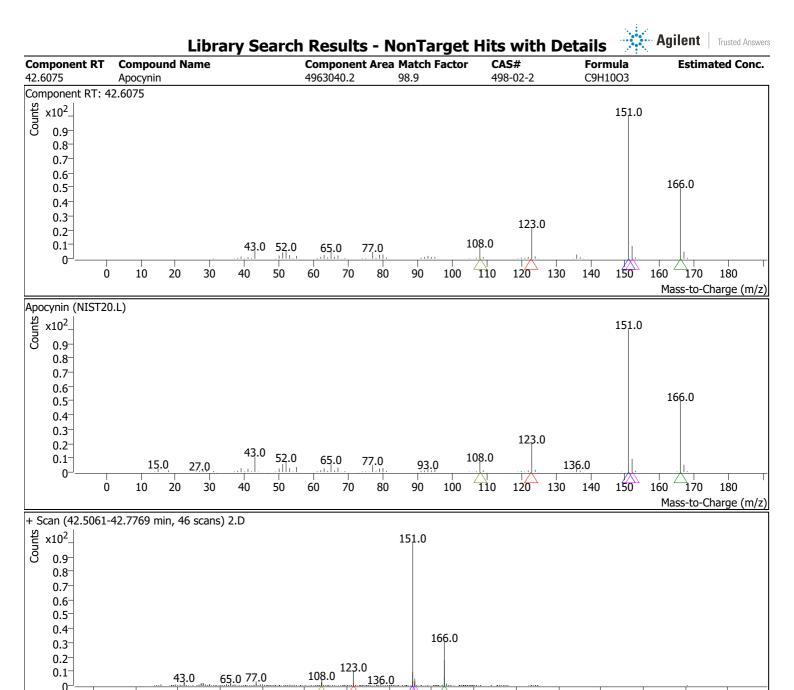
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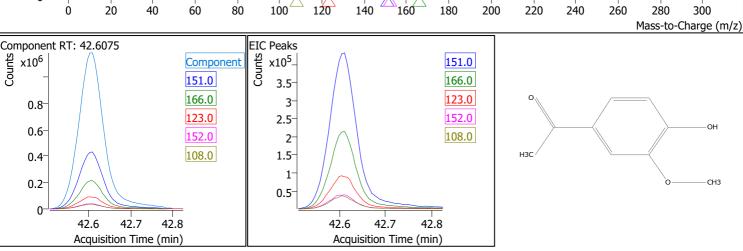
41.75

41.8

Acquisition Time (min)

41.85

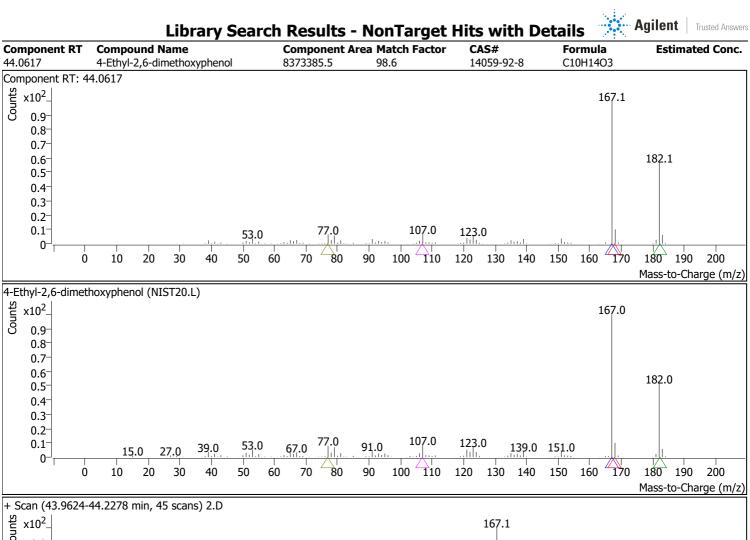


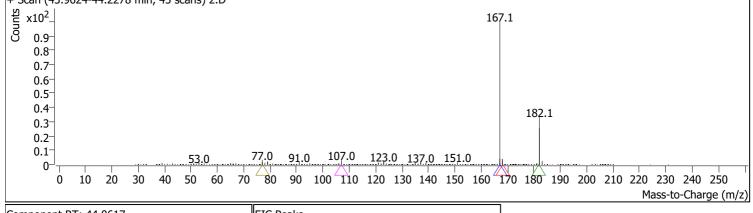


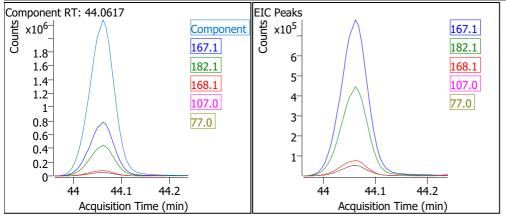
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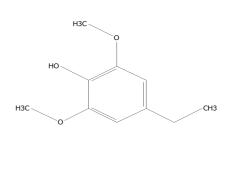
ОН

СНЗ









### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 93.8 44.2931 2-Propanone, 1-(4-hydroxy-3-8338048.4 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.2931 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 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) 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 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 (44.1861-44.4775 min, 50 scans) 2.D x10<sup>2</sup>. 137.0 0.9 0.8 $0.7^{-}$ 0.6 74.0 0.5 0.4 87.0 0.3 180.1 0.2 122.0 43.0 55.0 0.1 94.0 214.2 0 60 100 120 140 180 Ó 20 40 80 160 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 44.2931 Counts Counts x10<sup>6</sup> x10<sup>6</sup>\_ 137.0 Component 180.0 137.0 1.6 0.8 1.4 180.0 122.0 0.7 1.2 138.0 122.0 0.6

44.3

44.4

Acquisition Time (min)

94.0

 $0.5^{-}$ 

 $0.4^{-}$ 

0.3

 $0.2^{-}$ 

0.1

138.0

94.0

1

0.8

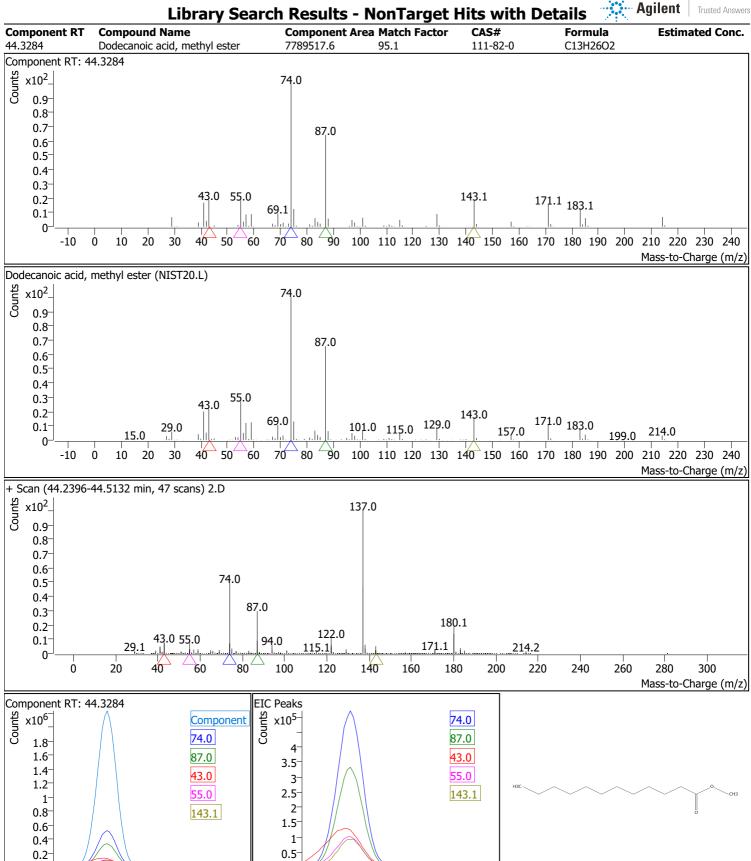
0.6

0.4

0.2

44.3

44.4



44.4 Acquisition Time (min)

44.3

0-

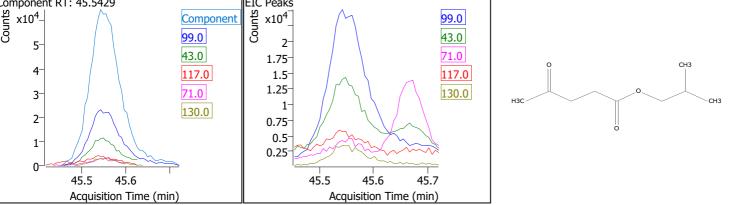
44.3

44.4

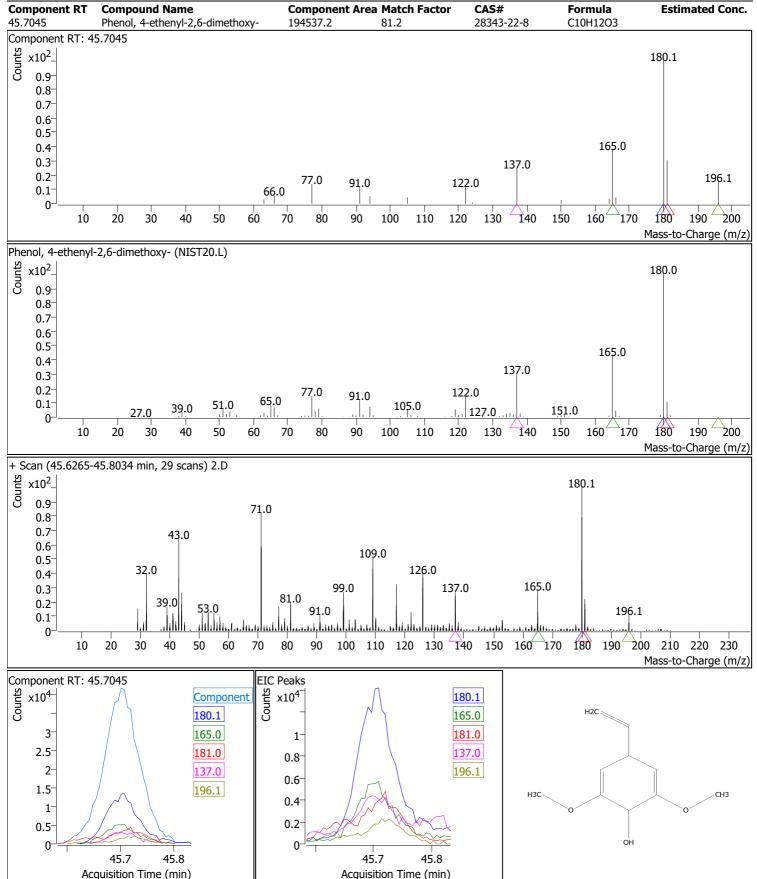
Acquisition Time (min)

44.5

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3757-32-2 45.5429 Pentanoic acid, 4-oxo-, 2-methylpropyl 322435.3 C9H16O3 Component RT: 45.5429 x10<sup>2</sup>\_ 99.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 0.3 117.0 $0.2^{-}$ 71.0 130.0 57.0 0.1 153.0 0-120 70 100 130 0 10 20 30 40 50 60 80 90 110 140 150 160 170 Mass-to-Charge (m/z) Pentanoic acid, 4-oxo-, 2-methylpropyl ester (NIST20.L) St x10<sup>2</sup> 99.0 43.0 0.8 0.7 0.6 0.5 0.4 57.0 0.3 74.0 0.2 27.0 117.0 0.1 15.0 130.0 157.0 0 120 40 100 130 10 20 30 50 60 70 80 90 110 140 150 160 170 Mass-to-Charge (m/z) + Scan (45.5004-45.6072 min, 18 scans) 2.D st x10<sup>2</sup> 0.9 99.0 0.8 43.0 0.7 0.6 0.5 0.4 0.3 117.0 32.0 0.2 57.0 71.0 130.1 0.1 153.0 0 Ó 20 40 100 120 260 280 60 80 140 160 180 200 220 240 300 Mass-to-Charge (m/z) Component RT: 45.5429 **EIC Peaks** Counts Counts x10<sup>4</sup>-99.0 x10<sup>4</sup> Component 99.0 43.0 2-

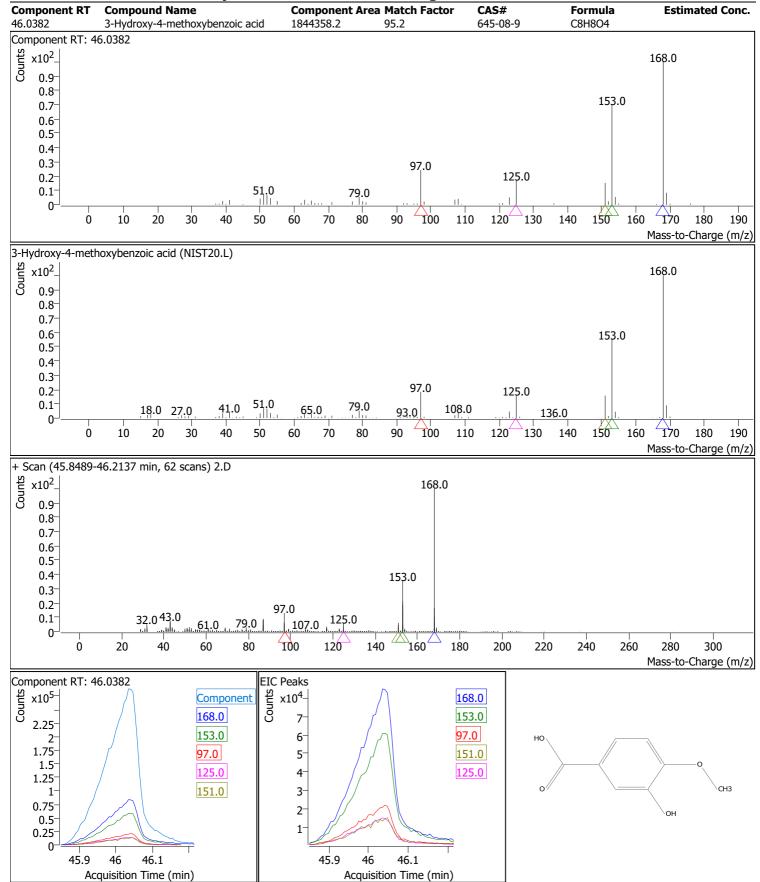












### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 46.4793 1-Propanone, 1-(4-hydroxy-3-1111484.7 91.9 1835-14-9 C10H12O3 methoxyphenyl)-Component RT: 46.4793 Counts x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 $0.2^{-}$ 123.0 108.0 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 29.0 39.0 136.0 164.0 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 (46.3802-46.5408 min, 28 scans) 2.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 180.1 123.0 0.1 108.0 32.0 44.0 65.0 77.0 0 Ó 60 120 180 20 40 80 100 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 46.4793 **EIC Peaks** Counts Counts x10<sup>5</sup>\_ x10<sup>5</sup> 151.0 Component СНЗ 180.0 2.25 151.0 2 1 180.0 123.0 1.75 123.0 0.8 152.0 1.5

46.45

46.5

Acquisition Time (min)

152.0

108.0

0.6

0.4

0.2

1.25

0.75

0.25

46.5

46.6

Acquisition Time (min)

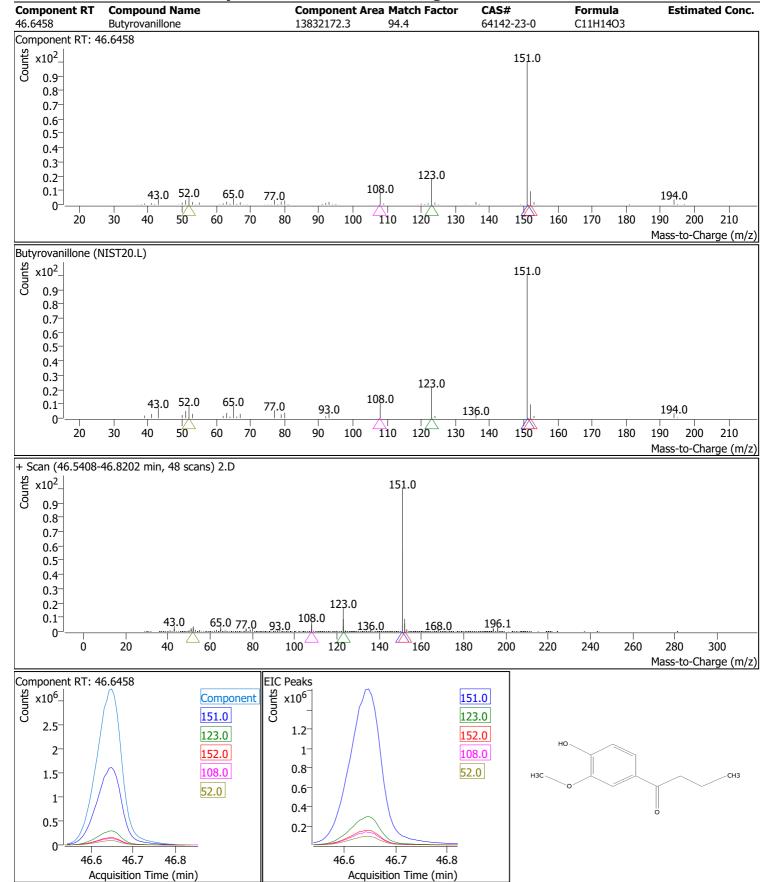
1

108.0

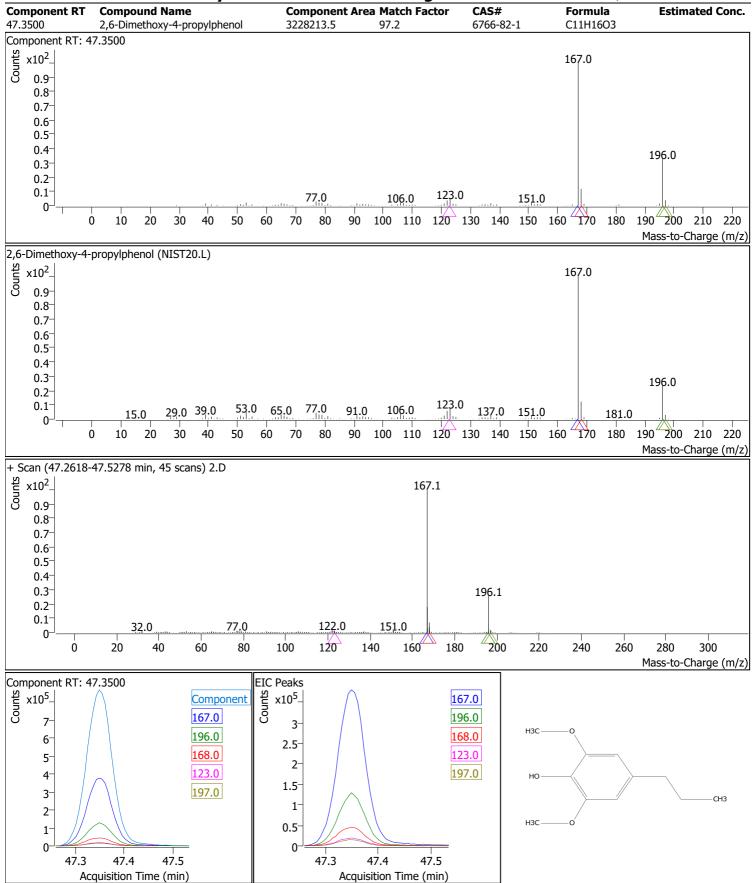
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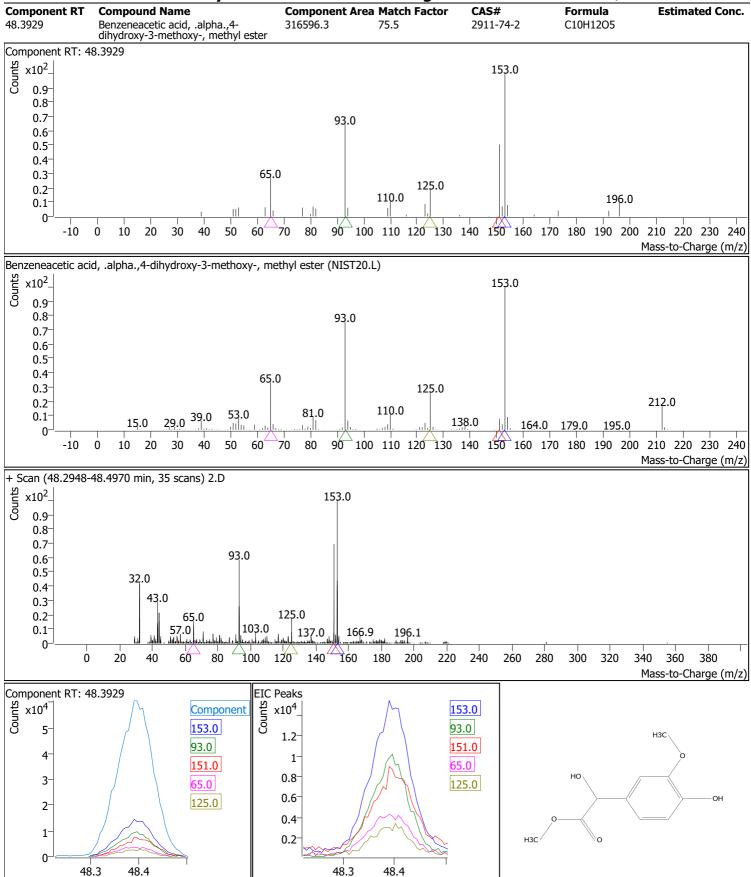






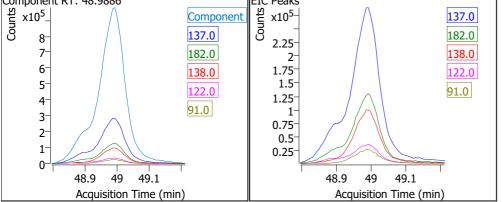






Acquisition Time (min)

### --- 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 48.9886 Benzenepropanol, 4-hydroxy-3-5862365.1 95.6 C10H14O3 methoxy-Component RT: 48.9886 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 91.0 107.0 0.1 0-90 140 180 10 20 30 40 50 60 70 80 100 110 120 130 150 160 170 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 122.0 0.2 77.0 91.0 65.0 106.0 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 (48.8003-49.2063 min, 69 scans) 2.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 182.1 0.3 0.2 65.0 77.0 91.0 107.0 <sup>122.0</sup> 0.1 151.0164.1 32.0 44.0 0 140 40 60 80 100 120 180 260 Ó 20 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 48.9886 **EIC Peaks** Counts Counts x10<sup>5</sup>. x10<sup>5</sup>-137.0 Component 182.0 137.0 8 2.25 7 182.0 138.0 2 6 1.75 122.0 138.0



### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 49.3563 Benzaldehyde, 4-hydroxy-3,5-2524757.3 95.2 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3563 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 79.0 0.1 0-0 10 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) Benzaldehyde, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts $x10^{2}$ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 111.0 0.2 167.0 93.0 139.0 39.0 65.0 51.0 79.0 0.1 15.0 29.0 153.0 123.0 0 160 170 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2701-49.5435 min, 46 scans) 2.D x10<sup>2</sup>\_ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 131.0 194.1 0.1 39.0 51.0 65.0 79.0 96.0 111.0 155.0 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3563 **EIC Peaks** Counts Counts x10<sup>5</sup> 182.0 x10<sup>5</sup>. Component 0 181.0 182.0 4.5 4 1.2 181.0 111.0 3.5 1 111.0 167.0 3 0.8 167.0 183.0 2.5

49.4

Acquisition Time (min)

49.5

2

1

49.3

49.4

Acquisition Time (min)

49.5

1.5

0.5

183.0

0.6

0.4

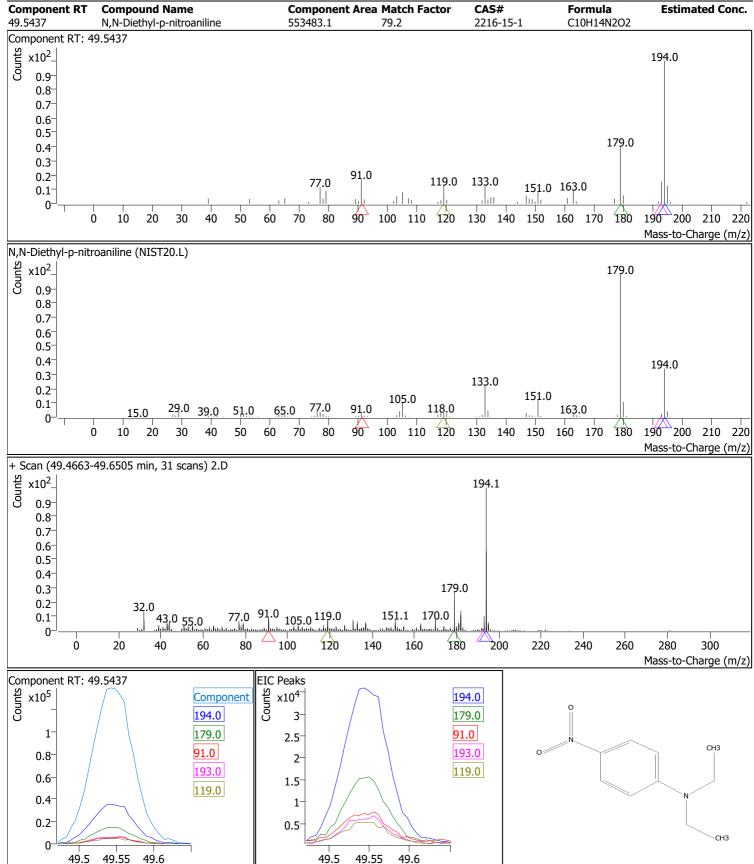
0.2

49.3

ОΉ







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.** 50.4168 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-615087.7 86.3 65996-50-1 C6H5N3O2 dione Component RT: 50.4168 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 123.0 0.1 108.0 77.0 40 55 65 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 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 65 70 80 85 90 60 Mass-to-Charge (m/z) + Scan (50.3106-50.5603 min, 43 scans) 2.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 169.0 0.4 0.3 0.2 81.0 95.0 109.0 197.1 29.0 43.0 57.0 0.1 228.1 139.0 80 20 40 60 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 50.4168 Counts Counts x10<sup>4</sup>⊣ x10<sup>5</sup>. 151.0 Component 123.0 151.0 1 7 123.0 152.0 0.8 6 152.0 108.0 5

50.4

50.5

Acquisition Time (min)

77.0

108.0

77.0

4

3<sup>-</sup> 2<sup>-</sup>

1

0.6

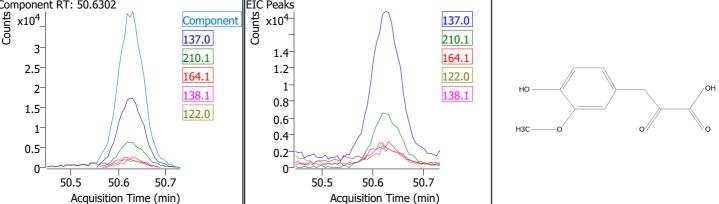
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0.2

50.4

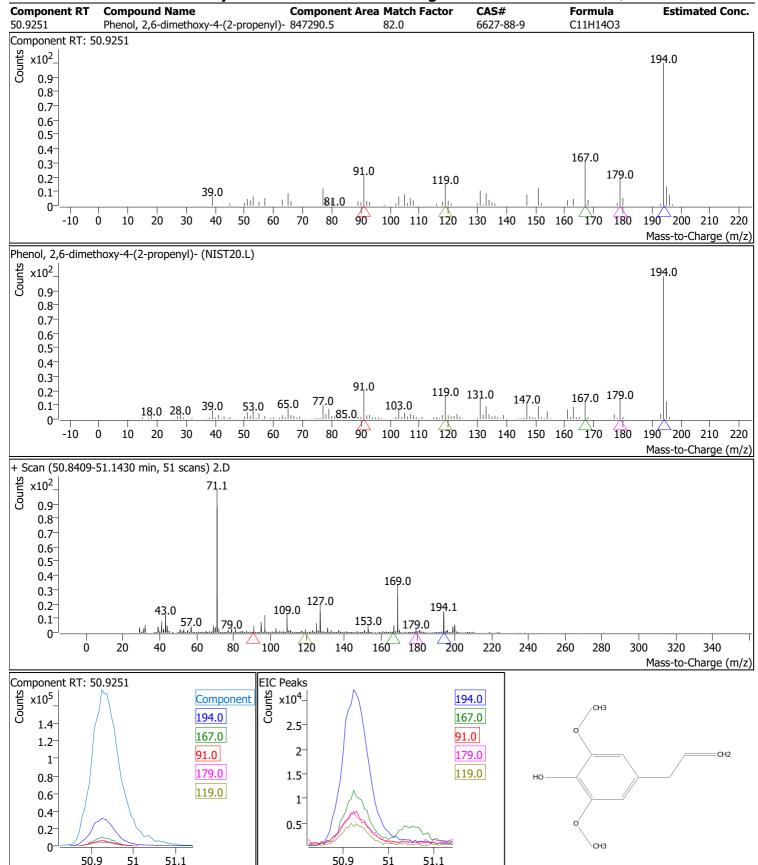
50.5

## ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 50.6302 Phenylacetylformic acid, 4-hydroxy-3- 155122.2 78.6 1081-71-6 C10H10O5 methoxy-Component RT: 50.6302 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 210.1 0.3 $0.2^{-}$ 164.1 122.0 91.0 0.1 150.0 100 110 120 130 140 150 160 170 180 190 200 210 220 230 -10 10 20 50 60 70 80 90 Mass-to-Charge (m/z) Phenylacetylformic acid, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 0.4 210.0 0.3 0.2 164.0 122.0 0.1 65.0 77.0 51.0 28.0 107.0 149.0 0 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 10 20 60 70 80 Mass-to-Charge (m/z) + Scan (50.5543-50.7262 min, 29 scans) 2.D x10<sup>2</sup>. 137.0 0.9 0.8 71.0 0.7 0.6 0.5 32.0 0.4 151.0 43.0 210.1 0.3 0.2 169.0 7.0 103.0 122.0 57.0 193.0 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 50.6302 Counts Counts x10<sup>4</sup>-137.0 x10<sup>4</sup> Component 210.1 137.0









Acquisition Time (min)

### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 210089.8 1000131-52-4 51.0508 2-Cyclohexen-3-ol-1-one, 2-[1-79.8 C8H11NO2 iminoethyl]-Component RT: 51.0508 x10<sup>2</sup>\_ 153.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2 0.1 41.0 103.0 144.0 159.0 0-90 30 40 50 70 80 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) 2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]- (NIST20.L) $x10^{2}$ 153.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 69.0 83.0 97.0 125.0 49.0 55.0 112.0 138.0 0 50 100 30 40 60 70 80 90 110 120 130 140 160 170 Mass-to-Charge (m/z) + Scan (50.9408-51.1133 min, 29 scans) 2.D st x10<sup>2</sup> 0.8 0.7 0.6 0.5 0.4 0.3 169.0 0.2 179.0 194.1 43.0 109.0 127.0 0.1 153.0 57.0 81.0 0 <del>1</del>60 40 60 280 20 80 100 120 140 180 200 220 240 260 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 51.0508 Counts Counts x10<sup>4</sup> 41.0 x10<sup>4</sup> Component 153.0 153.0 0.8 154.0 57.0 3.5 0.7 103.0 3 57.0 0.6 2.5

51.1

Acquisition Time (min)

41.0

103.0

51.1

Acquisition Time (min)

2

1-

0-

1.5

0.5

0.5

0.4

0.3

0.2

0.1

154.0

CH3

#### --- 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- 336745.6 3-methoxyphenyl)-51.7086 4899-74-5 C10H12O4 Component RT: 51.7086 Counts x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 196.0 $0.2^{-}$ 0.1 107.0 0-140 190 200 10 20 30 40 50 60 100 110 120 130 150 160 170 180 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 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 (51.6275-51.8300 min, 34 scans) 2.D x10<sup>2</sup>. 137.1 0.9 0.8 0.7 71.1 0.6 0.5 169.0 0.4 196.1 0.3 103.0 32.0 57.0 0.2 145.1 95.0 122.0 81.0 181.0 0.1 0 20 40 60 100 120 140 160 180 200 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 51.7086 **EIC Peaks** Counts Counts x10<sup>4</sup> x10<sup>4</sup> 137.0 Component 196.0 137.0 H<sub>3</sub>C 6 196.0 122.0 3.5 5 138.0 122.0 3

51.7

Acquisition Time (min)

94.0

51.8

4

3

2

1

51.6

51.7

Acquisition Time (min)

138.0

94.0

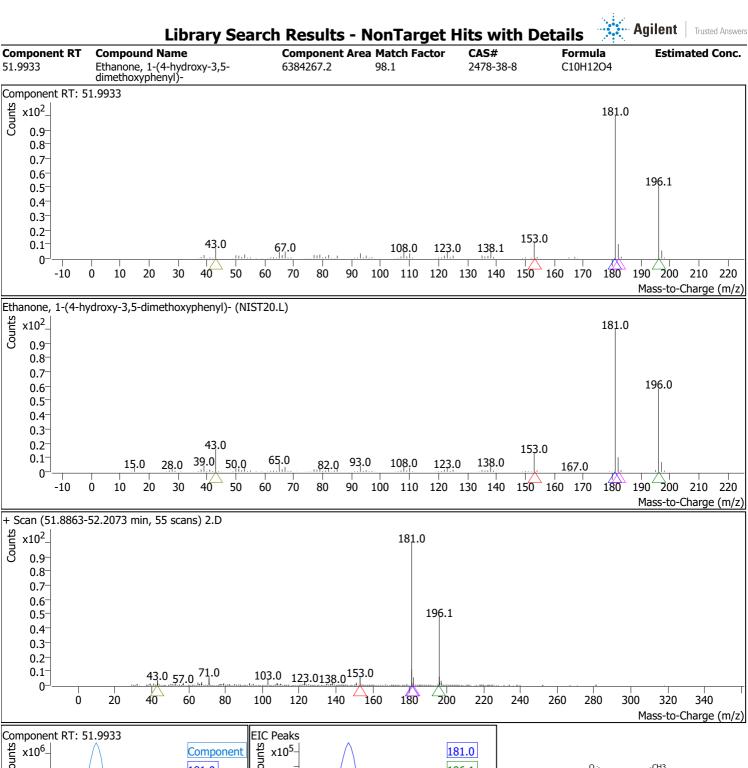
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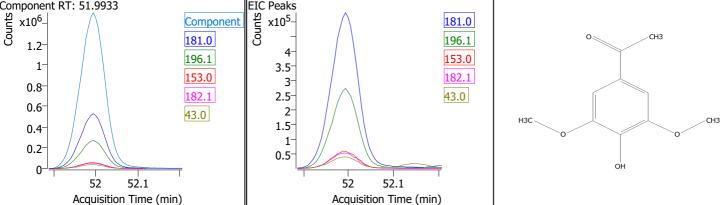
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0.5

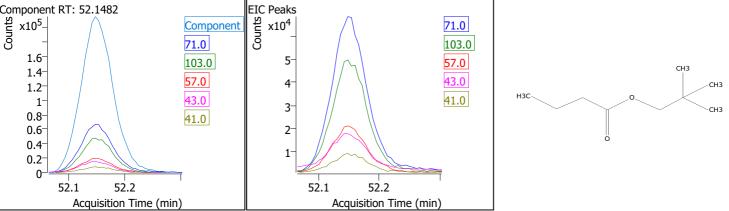
2

1





#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 52.1482 Butanoic acid, 2,2-dimethylpropyl 871583.9 78.5 23361-69-5 C9H18O2 Component RT: 52.1482 x10<sup>2</sup>\_ 71.0 0.9 8.0 103.0 0.7 0.6 0.5 0.4 57.0 0.3 43.0 $0.2^{-}$ 87.0 143.0 0.1 161.0 29.0 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 0 100 10 20 30 40 50 60 70 90 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (52.0706-52.3079 min, 40 scans) 2.D st x10<sup>2</sup> 0.8 0.7 103.0 0.6 0.5 0.4 137.1 0.3 57.0 43.1 0.2 181.0196.0 32.0 151.0 0.1 87.0 40 20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 52.1482 Counts Counts x10<sup>4</sup> x10<sup>5</sup>-71.0 Component 71.0 103.0



#### ··· 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- 292272.3 3-methoxyphenyl)-52.2249 83.7 4899-74-5 C10H12O4 Component RT: 52.2249 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 196.0 0.5 0.4 0.3 $0.2^{-}$ 122,0 0.1 107.0 77.0 168.0 0-140 200 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 180 190 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 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 77.0 55.0 65.0 107.0 0 190 200 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 210 Mass-to-Charge (m/z) + Scan (52.1598-52.2430 min, 15 scans) 2.D x10<sup>2</sup>. 0.9 0.8 103.0 0.7 0.6 0.5 137.1 0.4 57.0 0.3 196.1 43.1 0.2 151.0 181.0 87.0 32.0 0.1 124.0 0 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 52.2249 Counts Counts x10<sup>4-</sup> x10<sup>4</sup> 137.0 Component 196.0 137.0 4.5 H<sub>3</sub>C 2-196.0 124.0 4 1.75 3.5 138.0 138.0 1.5 3

122.0

124.0

2.5

1.5

0.5

52.2

52.3

Acquisition Time (min)

2

1.25

0.75

0.5

0.25

52.2

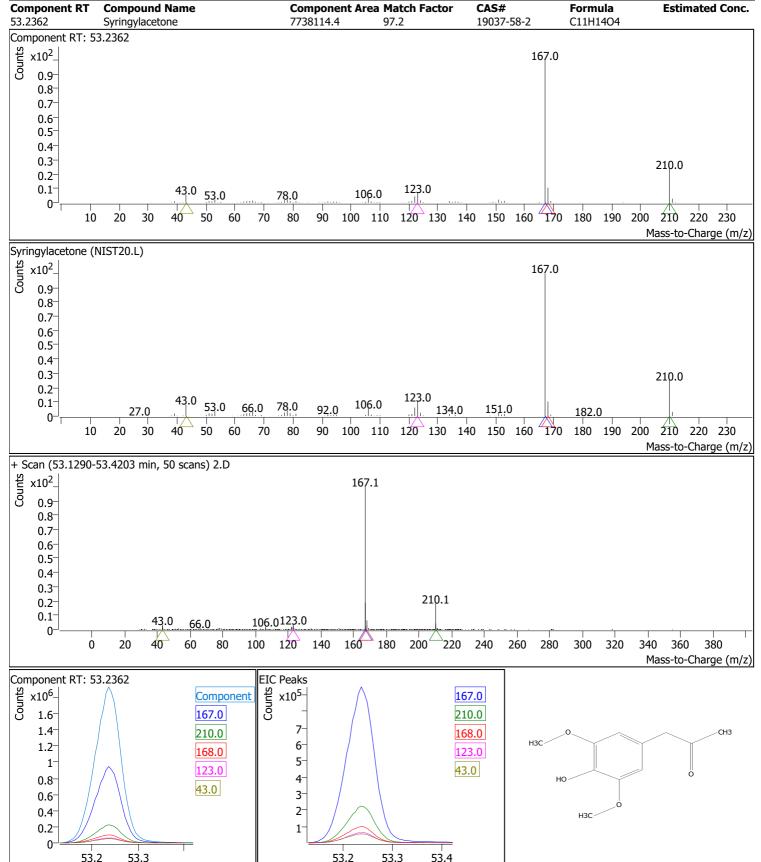
52.3

Acquisition Time (min)

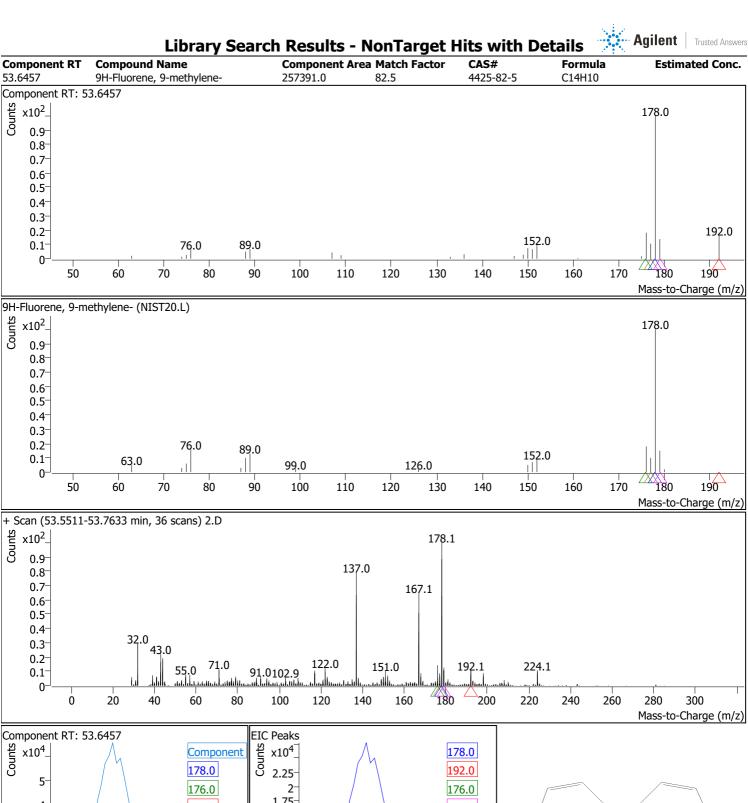
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Acquisition Time (min)



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CH2

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 54.9472 Benzoic acid, 4-hydroxy-3,5-1132096.9 88.5 530-57-4 C9H10O5 dimethoxy-Component RT: 54.9472 x10<sup>2</sup>\_ 198.0 0.9 8.0 0.7 0.6 0.5 0.4 183.0 0.3 127.0 $0.2^{-}$ 109.0 153.0 0.1 137.0 0-110 180 200 10 20 30 40 60 70 80 90 100 120 130 140 150 160 170 190 Mass-to-Charge (m/z) Benzoic acid, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts x10<sup>2</sup>. 198.0 0.9 0.8 0.7 0.6 0.5 0.4 183.0 0.3 127.0 0.2 109.0 81.0 93.0 0.1 155.0 53.0 137.0 29.0 0 180 200 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 210 220 Mass-to-Charge (m/z) + Scan (54.8229-55.1804 min, 61 scans) 2.D x10<sup>2</sup>. 181.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 198.0 0.2 0.1 67.0 93.0 108.0123.0138.0153.0 224.1 0 100 200 20 40 60 80 140 160 180 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 54.9472 **EIC Peaks** Counts Counts x10<sup>5</sup>x10<sup>5</sup> 181.0 Component ОН 198.0 198.0 4.5 1.6 183.0 183.0 1.4 3.5 127.0 127.0 1.2 3

55

Acquisition Time (min)

55.1

109.0

181.0

109.0

2.5

1.5

0.5

2

1

54.9

1

0.8

0.6

0.4

0.2

54.9

55

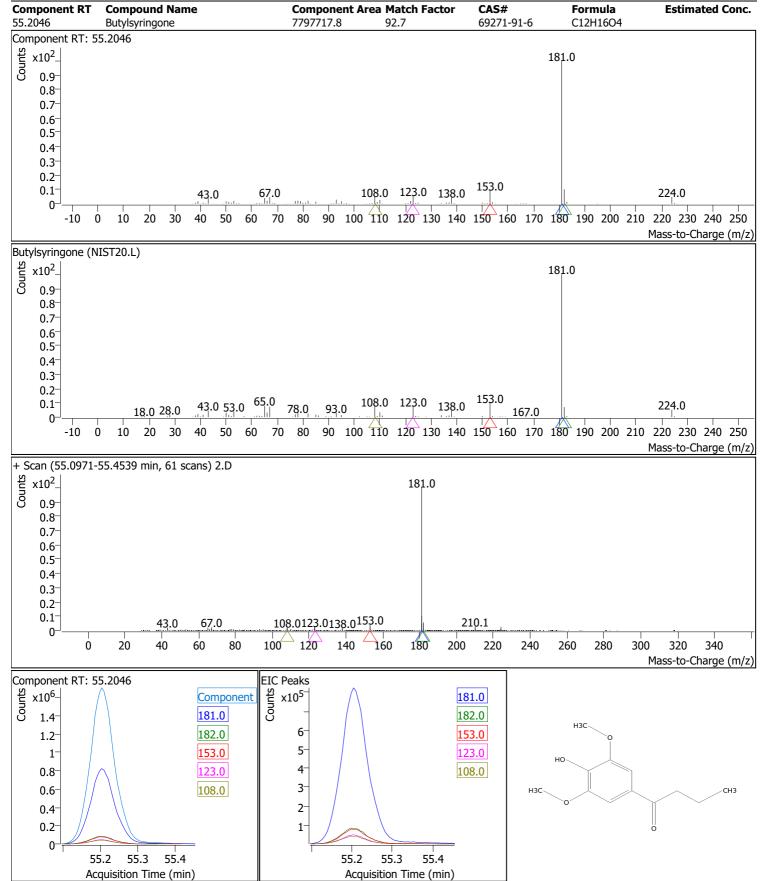
Acquisition Time (min)

55.1

ОН

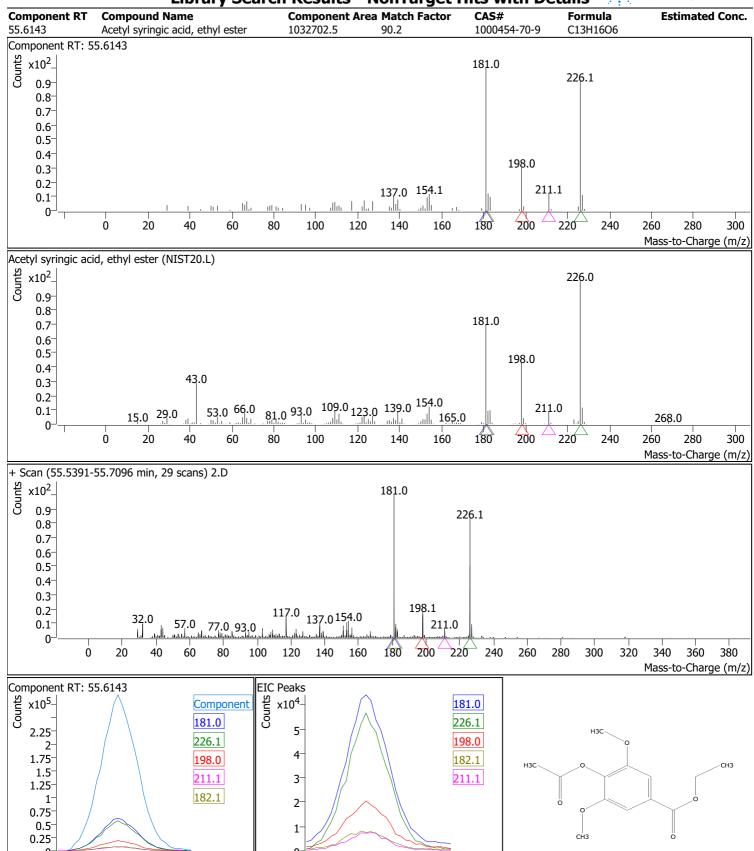






# **Library Search Results - NonTarget Hits with Details**





55.6

55.65

Acquisition Time (min)

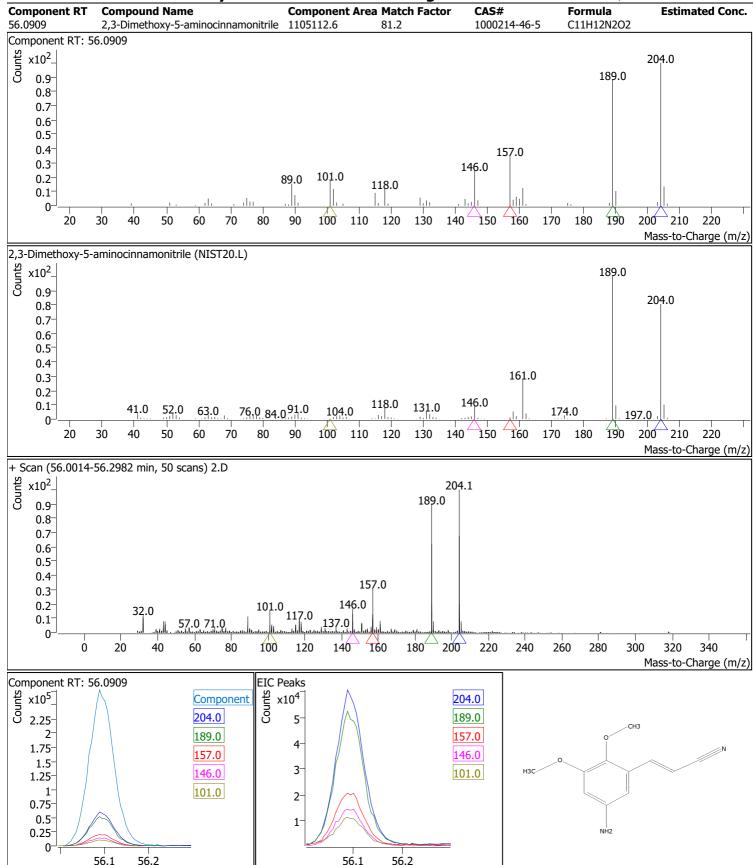
55.7

55.6 55.65

Acquisition Time (min)







Acquisition Time (min)

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol 57.4646 1608727.9 93.6 63543-12-4 C11H16O4 Component RT: 57.4646 x10<sup>2</sup>\_ 168.1 0.9 8.0 212.1 0.7 0.6 0.5 0.4 0.3 153.0 137.0 $0.2^{-}$ 123.0 107.0 77.0 91.0 0.1 aluu مطالتات 0-90 100 110 120 130 140 150 160 170 180 190 200 10 20 30 50 60 80 210 220 230 240 Mass-to-Charge (m/z) 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 212.0 0.6 0.5 0.4 0.3 153.0 0.2 108.0 123.0 137.0 179.0 91.0 77.0 31.039.0 65.0 0.1 85.0 197.0 100 110 120 130 140 150 160 170 180 190 200 10 20 30 60 70 80 90 210 220 230 240 Mass-to-Charge (m/z) + Scan (57.3804-57.6599 min, 48 scans) 2.D x10<sup>2</sup>. 168.1 0.9 212.1 0.8 0.7 0.6 0.5 0.4 0.3 0.2 117.0 77.091.0 0.1 181.1 0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 57.4646 Counts x10<sup>4</sup> 168.1 Component 168.1 167.1 3 5 167.1 212.1 2.5 137.0 212.1 2

57.5

57.6

Acquisition Time (min)

153.0

153.0

137.0

1.5

1<sup>-</sup> 0.5<sup>-</sup>

57.5

57.6

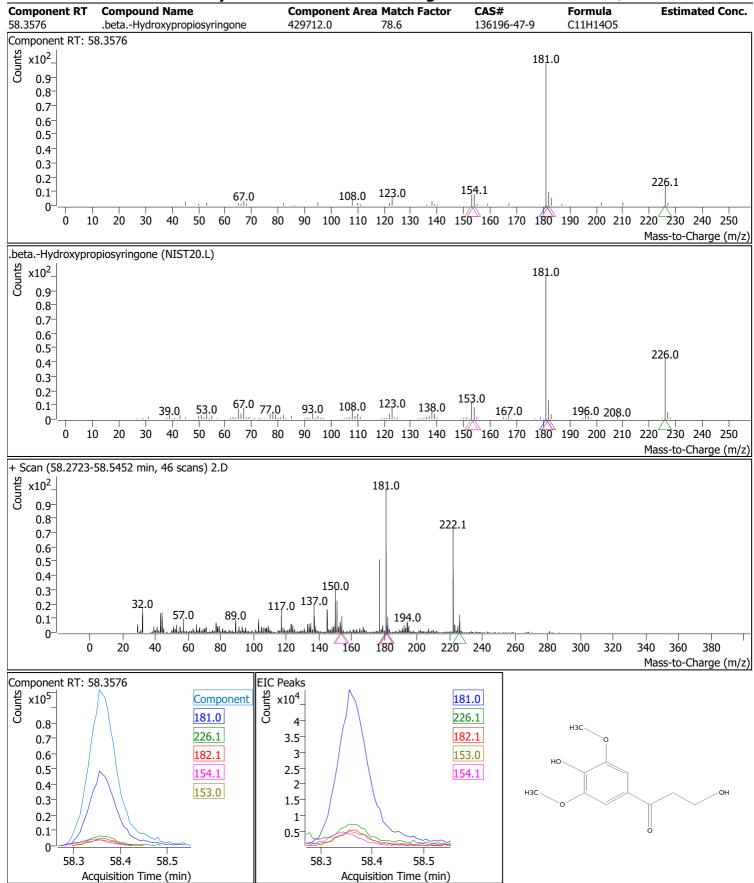
Acquisition Time (min)

3

2

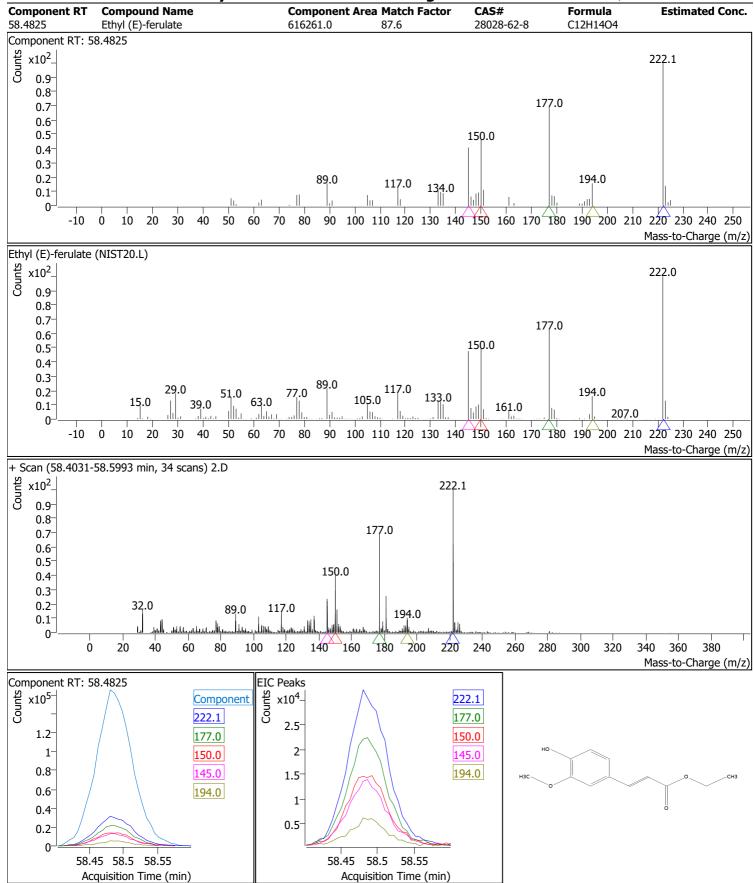




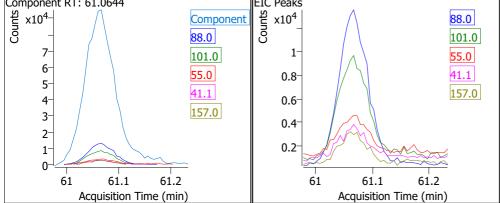






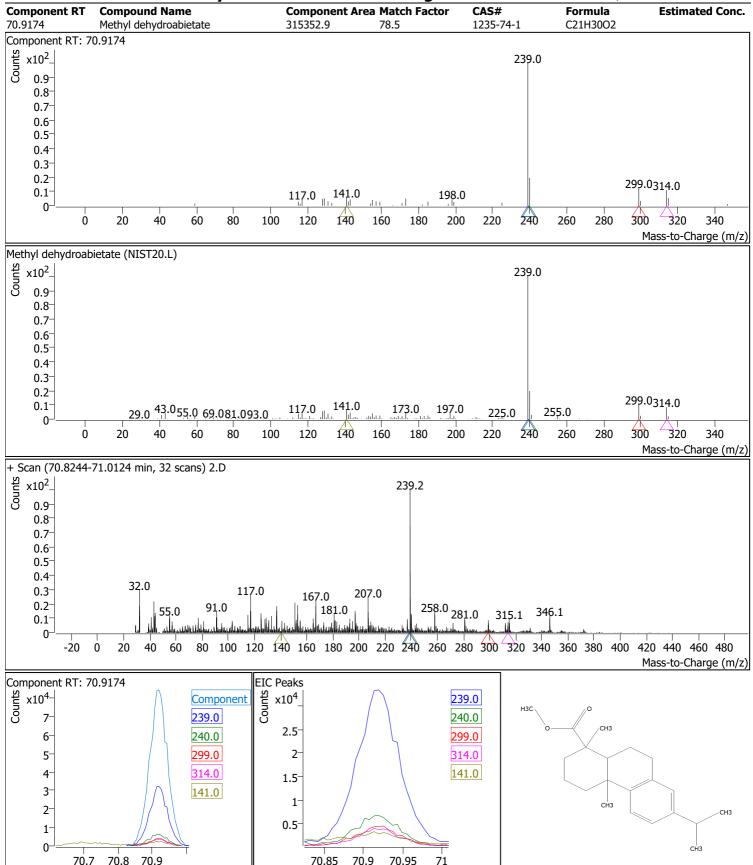


#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 628-97-7 61.0644 Hexadecanoic acid, ethyl ester 385114.9 C18H36O2 Component RT: 61.0644 $x10^{2}$ 88.0 0.9 0.8 $0.7^{-}$ 101.0 0.6 0.5 0.4 0.3 41.1 55.0 157.0 137.0 0.2 29.0 0.1 240.2 160 100 240 20 40 60 80 120 140 180 200 220 260 280 300 320 Mass-to-Charge (m/z) Hexadecanoic acid, ethyl ester (NIST20.L) st x10<sup>2</sup>\_ 0.9-88.0 0.8 0.7 101.0 0.6 0.5 0.4 0.3 157.0 284.0 0.2 43.0 55.0 70.0 241.0 115.0 129.0 143.0 25<u>5</u>.0<sub>269.0</sub> 0.1 $171.0^{185.0199.0213.0}227.0$ 29.0 160 100 20 80 120 140 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) + Scan (60.9956-61.1740 min, 31 scans) 2.D st x10<sup>2</sup> 0.9 103.0 0.8 0.7 149.0 0.6 0.5 57.0 $0.4^{-}$ 137.0 0.3 220.1 32.0 0.2 88.0 117.0 0.1 69.0 240.1 163.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) EIC Peaks Component RT: 61.0644 x10<sup>4</sup> 88.0 Component





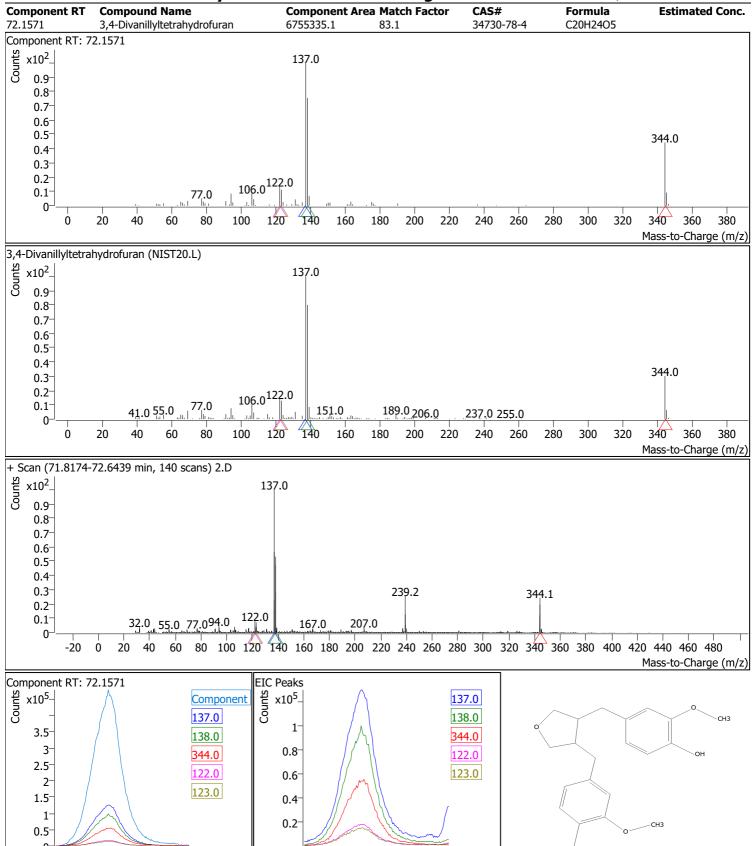




Acquisition Time (min)



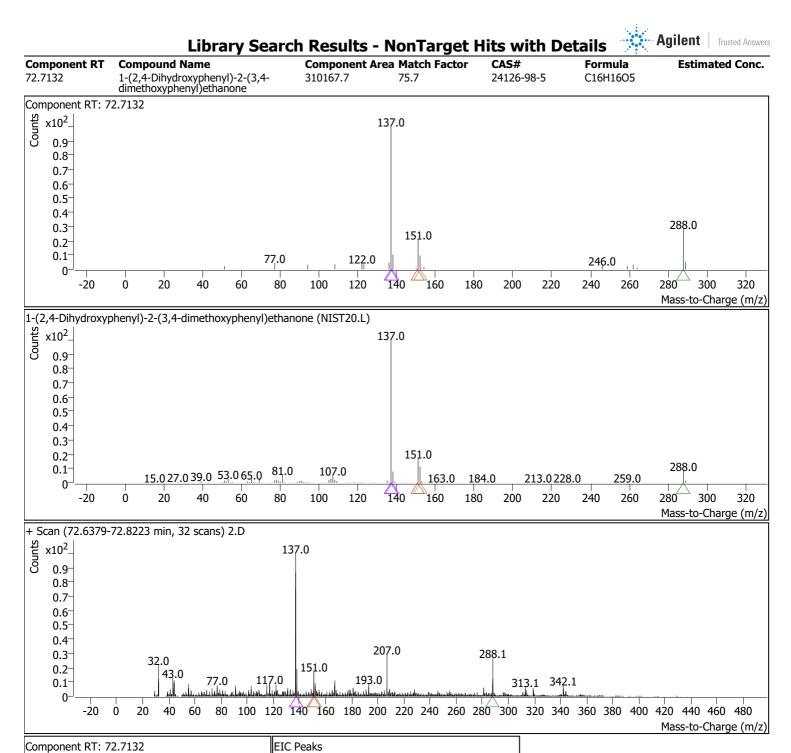


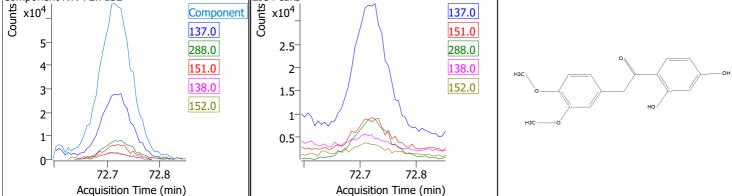


72.2 72.4 72.6

Acquisition Time (min)

72.2 72.4 72.6

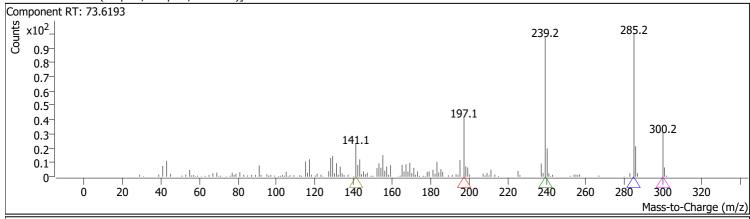


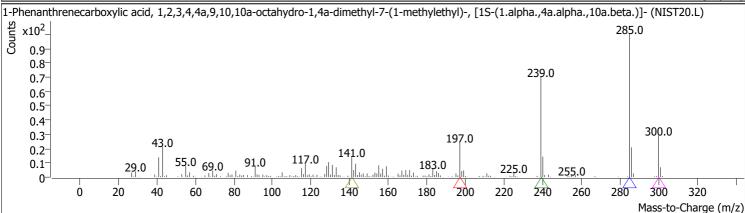


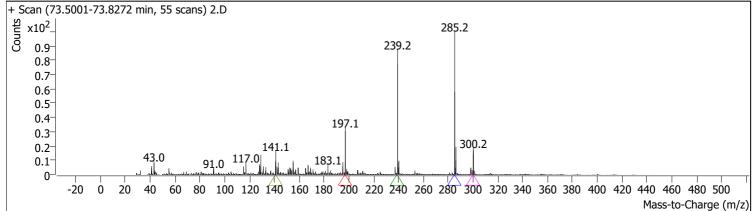
**Compound Name Component RT** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6193

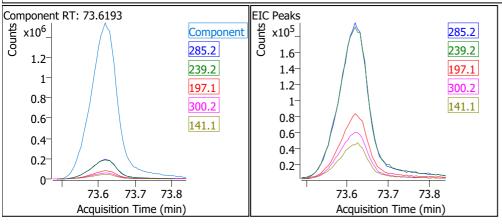
**Component Area Match Factor** 7974946.1 93.1

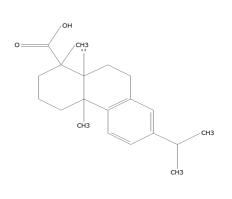
CAS# 5155-70-4 **Formula** C20H28O2 **Estimated Conc.** 

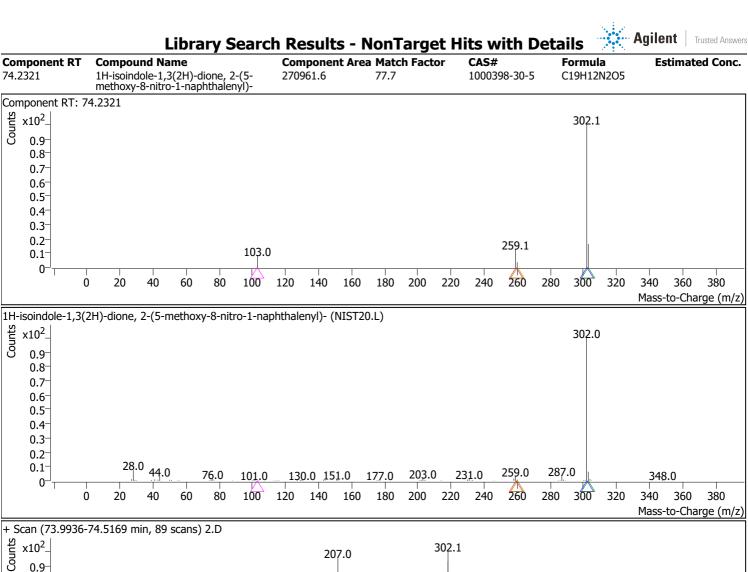


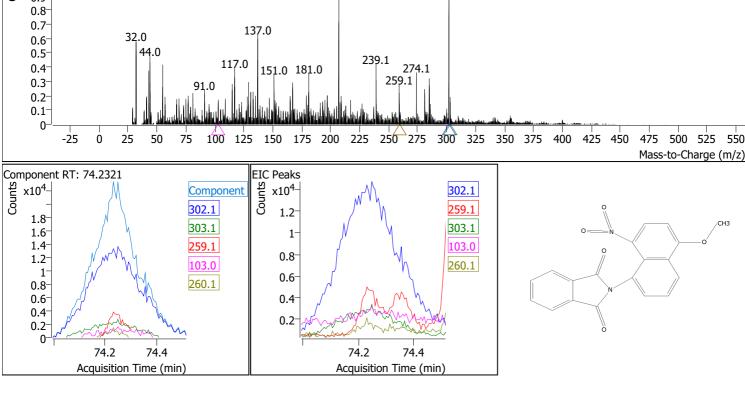












## --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1010363-08-5 74.5711 Silane, diethylnonyloxypropoxy-354036.6 C16H36O2Si Component RT: 74.5711 y x10<sup>2</sup> 0.9 259.0 0.8 $0.7^{-}$ 0.6 0.5 $0.4^{-}$ 0.3 0.2 0.1 212.0 155.0 260 100 160 180 20 40 60 80 120 140 280 Mass-to-Charge (m/z) Silane, diethylnonyloxypropoxy- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 259.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 133.0 145.0 <u>159.0 175.0187.0</u> 0.1 103.0 117.0 260 20 40 60 80 100 120 140 160 180 200 240 280 Mass-to-Charge (m/z) + Scan (74.4753-74.6893 min, 37 scans) 2.D st x10<sup>2</sup> 0.9 259.1 0.8 0.7 0.6 0.5 207.0 $0.4^{-}$ 32.0 55.0 0.3 137.1 167.0 75.0 <sub>95.0</sub> 44.0 0.2 229.1 281.1 0.1 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 Mass-to-Charge (m/z) EIC Peaks Component RT: 74.5711 Counts st x10<sup>4</sup>x10<sup>4</sup> 259.0 Component 2<u>59.0</u> 260.0 3.5 260.0 229.0 6 3-155.0 5 229.0 2.5 212.0 155.0

74.55 74.6 74.65

Acquisition Time (min)

2-

1

1.5

0.5

212.0

3

2

1

74.5

74.6

### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor Component RT Compound Name** CAS# **Formula Estimated Conc.** 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether 75.8864 1091277.6 79.3 22318-87-2 C18H22O4 Component RT: 75.8864 $x10^{2}$ 151.0 0.9 0.8 $0.7^{\circ}$ 0.6 0.5 0.4 0.3 0.2 302.1 65.077.0 91.0 0.1 108.0123.0 60 100 120 300 -20 20 40 140 180 200 220 240 260 280 320 340 Mass-to-Charge (m/z) 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether (NIST20.L) x10<sup>2</sup>\_ 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2-302.0 <u>15.027.039.051.0</u> 65.077.0 91.0 107.0 0.1 165.0 181.0196.0211.0226.0241.0256.0 220 300 20 180 200 240 260 320 340 -20 60 80 100 120 140 160 280 Mass-to-Charge (m/z) + Scan (75.8012-76.0793 min, 47 scans) 2.D Counts x10<sup>2</sup>\_ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 181.0 0.2 207.0 0.1 32.0 55.0 91.0 302.1 167.0 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 20 Mass-to-Charge (m/z) Component RT: 75.8864 EIC Peaks Counts x10<sup>5</sup>\_ x10<sup>5</sup>. 151.0 Component 151.0 152.0 2 1.2 152.0 302.1 1.75 1 1.5 91.0 302.1 0.8 1.25 123.0 91.0 1 0.6

75.9

76

Acquisition Time (min)

123.0

0.4

0.2

0.75

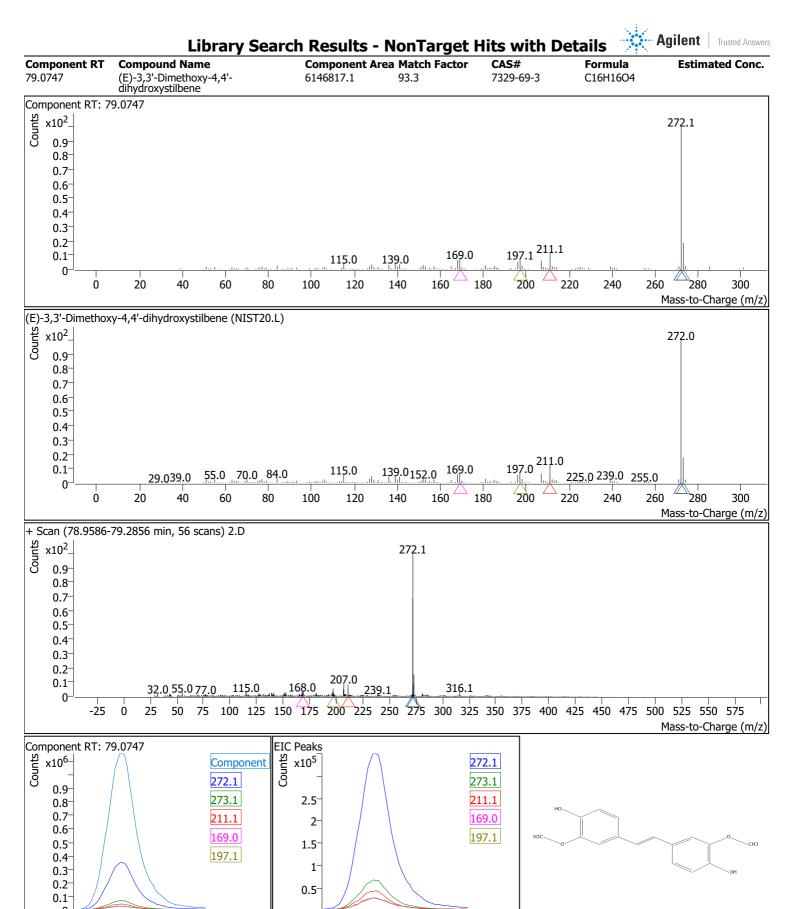
0.5

75.9

76

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.** 75.8864 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-857506.2 88.3 65996-50-1 C6H5N3O2 Component RT: 75.8864 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 0.1 108.0 120.0 90 55 65 85 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 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 55 65 70 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) + Scan (75.8012-76.0807 min, 48 scans) 2.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 181.0 0.2 207.0 91.0 0.1 167.0 302.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 Mass-to-Charge (m/z) Component RT: 75.8864 **EIC Peaks** Counts Counts x10<sup>5</sup> $x10^{5}$ 151.0 Component 152.0 151.0



79.1

79.2

Acquisition Time (min)

79

79.1

79.2

## --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor Component RT Compound Name** CAS# **Formula Estimated Conc.** 80.5379 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-1084953.1 97.3 65996-50-1 C6H5N3O2 dione Component RT: 80.5379 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 0.1 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) 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 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) + Scan (80.4217-80.8018 min, 63 scans) 2.D x10<sup>2</sup>. 181.0 0.9 0.8 0.7 0.6 0.5 151.0 0.4 0.3 0.2 348.1 167.1 207.0 0.1 253.2 281.0 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 Mass-to-Charge (m/z) Component RT: 80.5379 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup> 151.0 Component 152.0 151.0 1 152.0 1.2 52.0 0.8 52.0 1 55.0

80.5 80.6 80.7 80.8

Acquisition Time (min)

80.0

0.8

0.6

0.4

0.2

80.5 80.6 80.7 80.8

Acquisition Time (min)

55.0

80.0

0.6

 $0.4^{\circ}$