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



D:\MassHunter\GCMS\1\methods\RBEL\

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

240501 scan

240502 data.uaf **Analysis File Name** 

Acq. Method File

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

**File Name** 1.D **Path Name** D:\MassHunter\GCMS\1\data\RBEL\240501 scan **Sample Name Sample Type** 1

Acq. Method Path Acq. Operator Acq. Date-Time 5/1/2024 1:36:47 PM

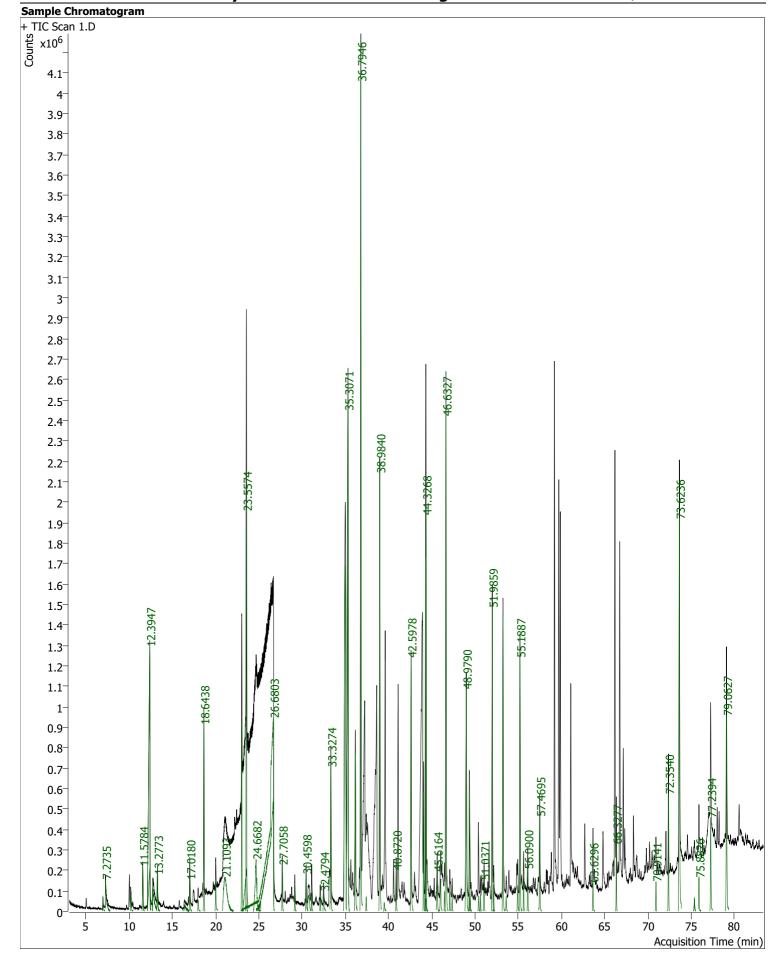
**Instrument Name** GCMSD Dil. 1

Component RT Compound Name		CAS#	Formula	Component	Match Factor	Estimated
6.9745	3-Furaldehyde	498-60-2	C5H4O2	<b>Area</b> 234391.9	95.7	Conc.
7.2735	1,3-Propanediol	504-63-2	C3H8O2	1263556.9	96.0	
10.1875	Ethanedioic acid, diethyl ester	95-92-1	C6H10O4	478276.3	75.0	
11.5784	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	1041610.3	78.5	
12.3947	Butyrolactone	96-48-0	C4H6O2	12958594.4	97.7	
12.3974	2-Propenal	107-02-8	C3H4O	2114377.4	78.1	
12.7378	(S)-(+)-1,2-Propanediol	4254-15-3	C3H8O2	1369287.5	79.3	
12.7378	Acetoin	513-86-0	C4H8O2	1449576.9	79.2	
13.2773	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	922641.6	76.5	
13.2773	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	817371.6	76.0	
16.4438	Ethane, 1,1,1-triethoxy-	78-39-7	C8H18O3	399182.1	75.5	
16.4440	Ethyl 2,2-diethoxypropionate	7476-20-2	C9H18O4	399225.1	75.8 75.8	
17.0180	Acetoin	513-86-0	C4H8O2	690174.9	79.6	
17.9778	Phenol	108-95-2	C6H6O	254152.5	93.3	
18.6438	Diisoamyl ether	544-01-4	C10H22O	3396460.2	98.2	
20.0201	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	703403.8	95.0	
21.1093	1,3,5-Trioxane	110-88-3	C3H6O3	4648194.3	77.4	
23.0255	1-Octanol	111-87-5	C8H18O	3779230.8	98.4	
23.5574	Phenol, 2-methoxy-	90-05-1	C7H8O2	8383926.4	98.5	
23.6130	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	3230331.3	82.1	
24.6682	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	3228314.2	87.8	
25.1522	1,3,5,7-Tetroxane	293-30-1	C4H8O4	648304.1	78.0	
26.6801	2-Propanone, 1-hydroxy-	116-09-6	C3H6O2	22515463.1	80.1	
26.6803	Glycerin	56-81-5	C3H8O3	37962614.8	80.5	
27.7058	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	1010279.2	81.3	
29.1581	Creosol	93-51-6	C8H10O2	525521.9	97.3	
30.4598	1,3-Dioxolane, 2-butyl-4-methyl-	74094-60-3	C8H16O2	834040.1	79.0	
30.7535	Catechol	120-80-9	C6H6O2	925875.3	86.6	
31.1051	1-Propanone, 1-(5-methyl-2-thienyl)-	59303-13-8	C8H10OS	343736.1	76.1	
32.0956	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	234475.9	90.1	
32.4794	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	538517.7	94.6	
33.3274	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	2832530.1	97.6	
35.0048	Ethylene glycol Formate Isobutyrate	1000458-48-0	C7H12O4	17452974.0	83.5	
35.3071	2,3-dihydroxypropyl isobutyrate	1010458-45-6	C7H14O4	17670321.0	79.5	
35.3074	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	17616193.8	78.2	
36.1579	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	4021958.6	82.2	
36.7946	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	16652182.6	97.9	
37.4113	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	240330.3	80.4	
38.9840	Vanillin	121-33-5	C8H8O3	9553029.9	99.0	
39.4888	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	227800.9	89.7	
40.8720	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	776796.4	92.5	
42.5978	Apocynin	498-02-2	C9H10O3	5395989.4	99.2	
44.0450	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	2188782.0	97.5	
44.2850	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	7255885.9	93.9	
44.2924	4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-1H-pyrazole	98816-47-8	C9H12N2O2	329057.9	75.7	
44.3268	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6825508.8	94.9	
45.6164	Pentanoic acid, 4-oxo-, 2-methylpropyl ester	3757-32-2	C9H16O3	991790.5	85.1	
46.0282	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	913799.3	90.7	
46.4726	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	384241.8	83.3	
46.6327	Butyrovanillone	64142-23-0	C11H14O3	10320359.6	95.3	
47.0806	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	352815.4	82.6	
47.3445	Homosyringaldehyde	87345-52-6	C10H12O4	249662.5	83.0	
48.9790	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	6788098.5	96.4	
49.3444	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2605242.4	96.7	
49.4061	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	366053.3	84.2	
49.4209	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	383468.5	78.5	
50.4127	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	326279.1	80.6	
50.6291	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	1081-71-6	C10H10O5	303107.7	79.6	
51.0371	Butanoic acid, (tetrahydro-2-furanyl)methyl ester	2217-33-6	C9H16O3	665275.7	77.4	
51.9859	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	6385500.3	97.5	
52.1417	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	553692.7	76.7	
53.2264	Syringylacetone	19037-58-2	C11H14O4	5978717.1	97.7	
53.5885	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	308310.5	79.4	
54.9294	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	621745.1	85.0	

# Library Search Results - NonTarget Hits with Details



Component R	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
55.1887	Butylsyringone	69271-91-6	C12H16O4	5238788.3	92.8	
55.6079	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	586028.4	87.9	
56.0900	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	821559.2	79.6	
57.4695	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	2046714.7	92.7	
63.6296	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	592568.4	76.5	
66.3277	(E)-9-Octadecenoic acid ethyl ester	6114-18-7	C20H38O2	1204905.9	89.6	
70.9141	Methyl dehydroabietate	1235-74-1	C21H30O2	544068.0	83.3	
72.3540	Methyl dehydroabietate	1235-74-1	C21H30O2	2231742.9	76.5	
73.6236	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	10413462.8	93.3	
75.3528	Cyclotetradecane	295-17-0	C14H28	268574.4	84.5	
75.3538	Undecane, 4-cyclohexyl-	13151-79-6	C17H34	316799.7	84.8	
75.8826	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	771065.1	92.0	
77.2394	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	2195585.6	76.2	
79.0627	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	4958162.3	92.6	



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3-Furaldehyde 498-60-2 6.9745 234391.9 95.7 C5H4O2 Component RT: 6.9745 y x10<sup>2</sup> 0.9 96.0 0.8 $0.7^{-}$ 0.6 39.0 0.5 0.4 0.3 0.2 67.0 0.1 53.0 0 65 10 15 20 25 30 35 45 50 55 60 75 80 85 90 100 105 Mass-to-Charge (m/z) 3-Furaldehyde (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 95.0 0.8 0.7 0.6 0.5 39.0 0.4 0.3 0.2 67.0 29.0 0.1 50.0 26.0 55.0 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 (6.9236-7.1780 min, 43 scans) 1.D st x10<sup>2</sup> 0.9 95.0 0.8 0.7 0.6 0.5 39.0 $0.4^{-}$ 0.3 44.0 0.2 0.1 0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 6.9745 **EIC Peaks** Counts x10<sup>4</sup> Counts x10<sup>4</sup>– 96.0 Component 96.0 95.0 1.4 3.5 95.0 39.0 1.2 3 38.0 39.0 1 2.5 67.0 38.0 0.8 2 67.0 0.6

7 7.05 7.1 7.15 Acquisition Time (min)

0.4

0.2

6.95

1.5

0.5

1

7.1

#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 7.2735 1,3-Propanediol 1263556.9 96.0 504-63-2 C3H8O2 Component RT: 7.2735 y x10<sup>2</sup> 0.9 57.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 43.0 0.2 0.1 39.0 5 15 25 55 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 49.0 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 (7.2376-7.7786 min, 91 scans) 1.D st x10<sup>2</sup> 0.9 58.0 0.8 31.0 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: 7.2735 EIC Peaks Counts x10<sup>5</sup> x10<sup>4</sup>\_ 57.0 Component 57.0 58.0 3 1.2 58.0 31.0 1 2.5 43.0 31.0 0.8 2-43.0 45.0

7.4 7.5 7.6 7.7

Acquisition Time (min)

1.5

1

0.5

45.0

0.6

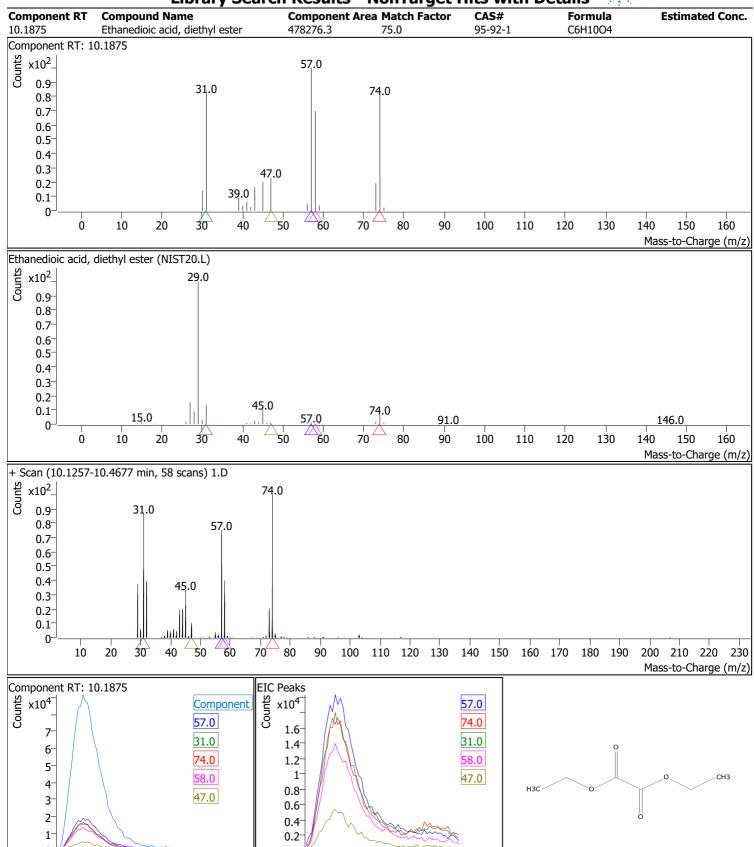
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7.3 7.4 7.5 7.6 7.7







10.2

10.3

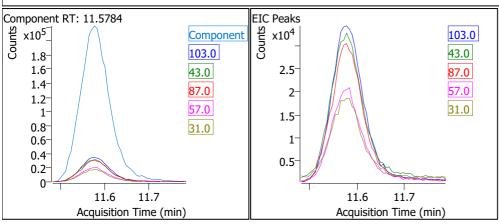
Acquisition Time (min)

10.4

10.3

Acquisition Time (min)

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 11.5784 Propane, 1,1-diethoxy-1041610.3 78.5 C7H16O2 Component RT: 11.5784 v10<sup>2</sup> 0.9 103.0 43.0 87.0 0.8 0.7 57.0 0.6 31.0 0.5 0.4 0.3 0.2 117.0 0.1 0 40<sup>2</sup> 30 70 130 10 20 50 60 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 70.0 131.0 130 0 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.4925-11.7327 min, 41 scans) 1.D St x10<sup>2</sup> 0.9 87.0 103.0 0.8 0.7 29.0 0.6 57.0 0.5 $0.4^{-}$ 0.3 0.2 117.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.5784 **EIC Peaks** x10<sup>4</sup> 103.0 Component



Н3С <

# --- 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 12.3947 Butyrolactone 12958594.4 97.7 C4H6O2 Component RT: 12.3947 v10<sup>2</sup> 0.9 42.1 0.8 0.7 0.6 86.0 0.5 0.4 29.0 56.0 0.3 39.0 0.2 0.1 0 25 55 75 20 30 35 40 50 65 70 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 (12.1015-12.5414 min, 74 scans) 1.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 86.0 56.0 29.0 0.3 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: 12.3947 Counts Counts 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



29.0

56.0

12.2 12.3 12.4 12.5

Acquisition Time (min)

0.6

0.4

0.2

2

1

1.5

0.5

12.2

12.3

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12.4

Acquisition Time (min)

12.5

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 12.3974 2-Propenal 2114377.4 78.1 107-02-8 C3H4O Component RT: 12.3974 y x10<sup>2</sup> 0.9 39.0 56.0 55.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 0.3 0.2 54.0 0.1 54 56 20 22 24 26 28 30 32 36 38 42 46 50 52 58 60 Mass-to-Charge (m/z) 2-Propenal (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 56.0 0.8 0.7 55.0 0.6 0.5 26.0 29.0 0.4 0.3 0.2 38.0 25.0 27.0 0.1 57.0 36.0 52.0 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 58 60 Mass-to-Charge (m/z) + Scan (12.1023-12.5057 min, 68 scans) 1.D St x10<sup>2</sup> 0.9 0.8 0.7 $0.6^{-}$ 0.5 $0.4^{-}$ 86.0 56.0 29.0 0.3 0.2 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 12.3974 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup> Component 56.0 39.0 39.0 0.9 1.6 56.0 55.0 0.8 1.4 0.7 55.0 54.0 1.2 H2C 0.6

54.0

101.0

0.8

0.6

0.4

0.2

12.2 12.3

12.4

Acquisition Time (min)

0.5

0.4

0.3

0.2

12.2

12.3

12.4

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.** 4254-15-3 12.7378 (S)-(+)-1,2-Propanediol 1369287.5 C3H8O2 Component RT: 12.7378 v10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 0.1 30.0 55.0 0 30 25 55 65 70 75 10 15 20 35 50 60 80 Mass-to-Charge (m/z) (S)-(+)-1,2-Propanediol (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 31.0 0.1 27.0 61.0 57.0 19.0 39.0 30 45 10 15 20 25 35 40 50 55 60 65 70 75 80 Mass-to-Charge (m/z) + Scan (12.7050-13.1895 min, 82 scans) 1.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 29.0 0.1 102.0 87.0 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: 12.7378 **EIC Peaks** Counts Counts x10<sup>4</sup>\_ 45.0 Component 45.0 43.0 7 0.9 43.0 42.0 H3C 0.8 6 $0.7^{-}$ 46.0 46.0 5

12.8 12.9

30.0

13.1

13

Acquisition Time (min)

0.6

0.5

 $0.4^{-}$ 

0.3

0.2<sup>-</sup> 0.1<sup>-</sup> 0<sup>-</sup>

12.8

13

13.2

Acquisition Time (min)

42.0

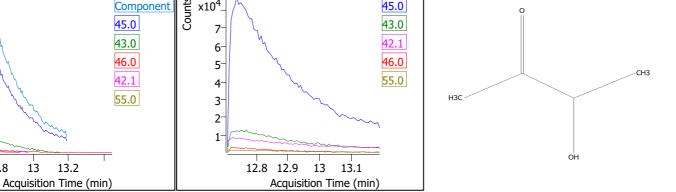
30.0

4

3

2

# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1449576.9 513-86-0 12.7378 Acetoin C4H8O2 Component RT: 12.7378 y x10<sup>2</sup> 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 0.1 30.0 55.0 55 25 30 65 70 75 80 85 95 20 60 90 Mass-to-Charge (m/z) Acetoin (NIST20.L) St x10<sup>2</sup>\_0.9 45.0 0.8 0.7 0.6 43.0 0.5 0.4 0.3 0.2 88.0 0.1 73.0 55 20 25 30 35 40 50 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.7029-13.1895 min, 82 scans) 1.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 0.2 29.0 0.1 102.0 87.0 40 10 20 30 50 <sup>2</sup>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: 12.7378 **EIC Peaks** Counts Counts x10<sup>4</sup>\_ 45.0 Component 45.0 43.0 7 0.9 43.0 42.1 0.8 6 $0.7^{-}$



0.6

0.5

 $0.4^{-}$ 

0.3

0.2 0.1 0-

12.8

13

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-(2-methoxyethoxy)propanoic acid, O-acetyl-13.2773 922641.6 76.5 1000506-61-7 C8H14O5 Component RT: 13.2773 x10<sup>2</sup> 103.0 0.9 8.0 43.0 87.0 0.7 0.6 57.0 0.5 31.0 0.4 0.3 $0.2^{-}$ 0.1 0-130 140 0 10 20 30 40 50 70 80 90 100 110 120 150 160 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 40 90 130 0 10 20 30 50 70 80 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (13.1957-13.4333 min, 40 scans) 1.D st x10<sup>2</sup> 103.0 45.0 0.8 0.7 0.6 87.0 0.5 57.0 29.0 0.4 0.3 0.2 0.1 117.1 0 40 90 190 200 210 220 230 10 20 30 50 60 70 80 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 13.2773 **EIC Peaks** Counts Counts x10<sup>5</sup> $x10^{4}$ 103.0 Component 103.0 43.0 1.4 2.5 43.0 87.0 1.2 87.0 45.0 2

13.3

13.4

Acquisition Time (min)

13.5

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13.3 13.4 13.5

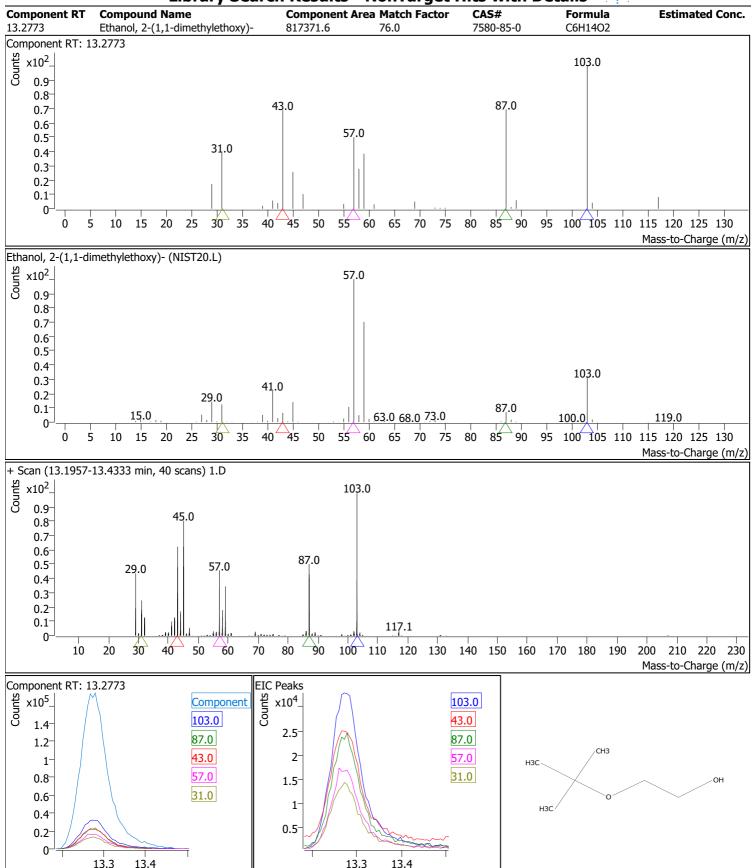
Acquisition Time (min)

1.5

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.** 78-39-7 16.4438 Ethane, 1,1,1-triethoxy-399182.1 75.5 C8H18O3 Component RT: 16.4438 $x10^{2}$ 61.0 89.0 117.0 0.9 0.8 $0.7^{-}$ 43.0 0.6 31.0 0.5 75.0 0.4 0.3 0.2 0.1 90 70 140 150 10 20 30 40 50 60 80 100 110 120 130 160 Mass-to-Charge (m/z) Ethane, 1,1,1-triethoxy- (NIST20.L) st x10<sup>2</sup> 0.9 61.0 0.8 43.0 0.7 117.0 0.6 89.0 0.5 0.4 31.0 0.3 27.0 0.2 0.1 147.0 70.0 82.0 <sup>∠</sup>90 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (16.3310-16.5787 min, 42 scans) 1.D Counts $x10^{2}$ 117.0 0.9 32.0 0.8 0.7 0.6 0.5 59.0 89.0 43.0 $0.4^{-}$ 0.3 103.0 75.0 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: 16.4438 Counts Counts x10<sup>3</sup> Component 117.0 61.0 СНЗ 89.0 2 117.0



16.6

Acquisition Time (min)

16.8

1.5

1

0.5

16.4

16.6

Acquisition Time (min)

16.8

59.<u>0</u>

43.0

3

2

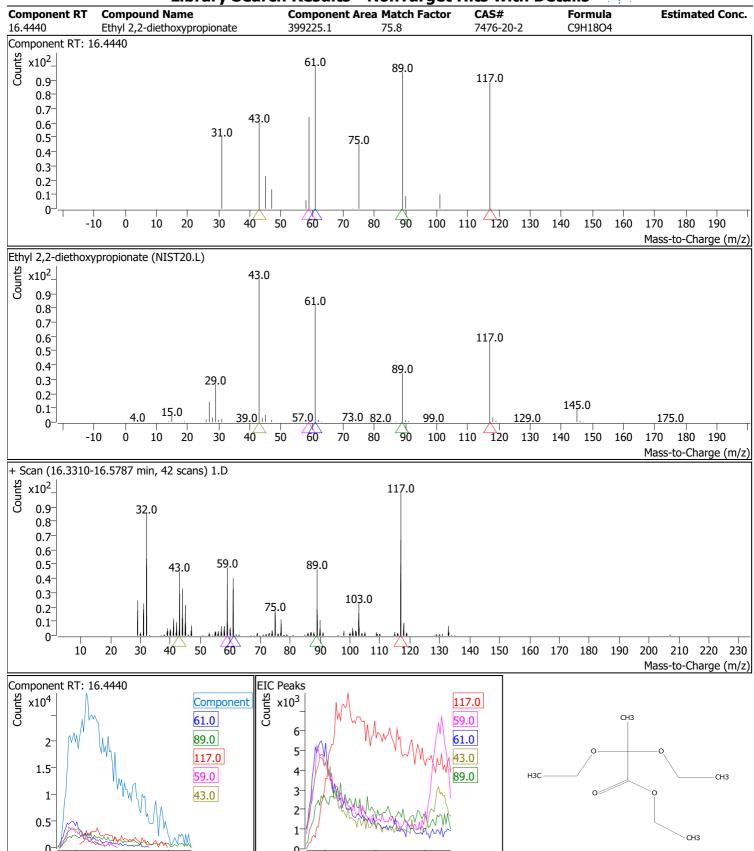
16.4

СНЗ

-CH3

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





16.6

Acquisition Time (min)

16.8

16.4

16.4

16.6

Acquisition Time (min)

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 513-86-0 17.0180 Acetoin 690174.9 79.6 C4H8O2 Component RT: 17.0180 y x10<sup>2</sup> 0.9 45.0 0.8 0.7 43.0 0.6 0.5 0.4 0.3 57.0 88.0 0.2 0.1 73.0 39.0 25 40 65 70 75 80 85 90 95 20 30 35 50 Mass-to-Charge (m/z) Acetoin (NIST20.L) St x10<sup>2</sup>\_0.9 45.0 0.8 0.7 0.6 43.0 0.5 0.4 0.3 0.2 88.0 0.1 73.0 45 20 25 30 35 40 50 55 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (16.9297-17.2298 min, 50 scans) 1.D St x10<sup>2</sup> 0.9 0.8 0.7 0.6 0.5 103.0 $0.4^{-}$ 0.3 117.0 88.0 0.2 29.0 57.0 0.1 75.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 17.0180 EIC Peaks Counts Counts x10<sup>4</sup> 45.0 Component 45.0 43.0 4 1.2 43.0 103.0 3.5 1 57.0 88.0 3-



17.1

Acquisition Time (min)

17.2

57.0

нзс

2.5

1.5

0.5

2

1

88.0

103.0

0.8

0.6

0.4

0.2

17

17.1

Acquisition Time (min)

17.2

ОН

-CH3

#### --- 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 17.9778 Phenol 254152.5 93.3 Component RT: 17.9778 v10<sup>2</sup> 0.9 94.0 0.8 $0.7^{-}$ 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 55.0 63.0 50.0 95 25 55 65 75 85 90 20 30 35 40 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 95 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) + Scan (17.9089-18.2496 min, 58 scans) 1.D St x10<sup>2</sup> 0.9 0.8 43.0 0.7 94.0 0.6 0.5 0.4 32.0 0.3 103.0 117.0 0.2 75.0 133.0 0.1 0-60 Ó 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 17.9778 Counts Counts x10<sup>4</sup> 94.0 Component 94.0 66.0 2-66.0 1.75 65.0 3.5 39.0 65.0 1.5 3

95.0

1.25

0.75 0.5 0.25

1

0-

18

18.1

Acquisition Time (min)

18.2

39.0

95.0

2.5

1.5

0.5

18

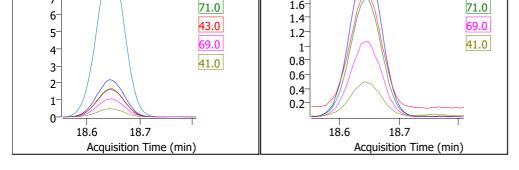
18.1

Acquisition Time (min)

18.2

2

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3396460.2 544-01-4 18.6438 Diisoamyl ether 98.2 C10H22O Component RT: 18.6438 v10<sup>2</sup> 0.9 70.0 0.8 43.0 $0.7^{-}$ 0.6 0.5 0.4 0.3 55.0 101.0 0.2 29.0 0.1 70 20 100 130 10 30 40 50 60 80 90 110 120 140 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) S x10<sup>2</sup> 0.9 43.0 70.0 0.8 0.7 0.6 0.5 0.4 0.3 101.0 55.0 0.2 29.0 0.1 79.0 85.0 91.0 97.0 70 10 20 30 40 50 60 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (18.5528-18.7490 min, 34 scans) 1.D St x10<sup>2</sup> 0.9 0.8 43.1 0.7 0.6 0.5 0.4 0.3 61.0 0.2 101.1 29.1 0.1 117.0



20

Component RT: 18.6438

Counts

7

60

Component 70.0

80

100

EIC Peaks

x10<sup>5</sup>\_

1.8

1.6

120

140

160

180

70.0

43.0

200

220

240

260

280

300 Mass-to-Charge (m/z)

#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 80-71-7 20.0201 2-Cyclopenten-1-one, 2-hydroxy-3-703403.8 95.0 C6H8O2 methyl-Component RT: 20.0201 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 $0.2^{-}$ 43.0 0.1 0-<del>7</del>0 30 35 45 50 55 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 (19.9156-20.2415 min, 55 scans) 1.D $x10^{2}$ 0.9 0.8 0.7 43.0 0.6 0.5 0.4 112.0 0.3 31.0 0.2 55.0 69.0 0.1 84.0 103.0 0 Ó 20 40 60 80 100 200 220 260 120 140 160 180 240 280 300 Mass-to-Charge (m/z) Component RT: 20.0201 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>4</sup> 112.0 Component 112.0 69.0 3-69.0 55.0 1 2.5 55.0 83.0 0.8 2-83.0 41.0 нзс 0.6 1.5 41.0 0.4 1

0.5

20

20.1

Acquisition Time (min)

20.2

0.2

20

20.1

Acquisition Time (min)

20.2

ОН

#### -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4648194.3 110-88-3 21.1093 1,3,5-Trioxane 77.4 C3H6O3 Component RT: 21.1093 v10<sup>2</sup> 0.9 89.0 43.0 61.0 0.8 0.7 0.6 31.0 0.5 0.4 0.3 0.2 45.0 0.1 56.0 0 <sup>1</sup>45 <del>-9</del>0 25 55 75 10 15 20 30 35 40 50 60 65 70 80 85 95 100 Mass-to-Charge (m/z) 1,3,5-Trioxane (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 31.0 0.8 61.0 89.0 0.7 0.6 0.5 0.4 29.0 0.3 0.2 0.1 44.0 14.0 56.0 0-45 <del>2</del>0 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.7715-22.0548 min, 215 scans) 1.D st x10<sup>2</sup> 0.9 0.8 0.7 0.6 43.0 0.5 0.4 0.3 0.2 31.0 89.0 0.1 117.0 Ó 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.1093 **EIC Peaks** Counts Counts x10<sup>5</sup> 61.0 Component 89.0 43.0 1.2 43.0 89.0 31.0 1 61.0 0.8 0.8 60.0 31.0

21.5

Acquisition Time (min)

0.6

0.4

0.2

21

60.0

0.6

0.4

0.2

21

21.5

## --- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0255 1-Octanol 3779230.8 98.4 111-87-5 C8H18O Component RT: 23.0255 v10<sup>2</sup> 0.9 56.0 0.8 41.1 69.1 $0.7^{-}$ 84.1 29.0 0.6 0.5 0.4 0.3 0.2 0.1 55 100 105 110 115 120 125 130 135 140 45 50 65 70 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 55 20 25 35 40 45 50 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9361-23.2323 min, 50 scans) 1.D st x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 31.0 55.1 0.2 69.1 84.1 0.1 103.0 117.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 23.0255 EIC Peaks Counts Counts x10<sup>5</sup> 56.0 Component 56.0 55.0 7 55.0 41.1 0.8 6 41.1 69.1 5 0.6

23.1

Acquisition Time (min)

23.2

69.1

70.1

0.4

0.2

4

3

2

1

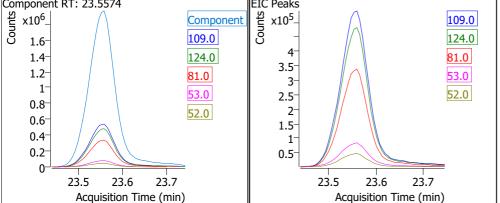
23.1

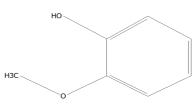
Acquisition Time (min)

23

23.2

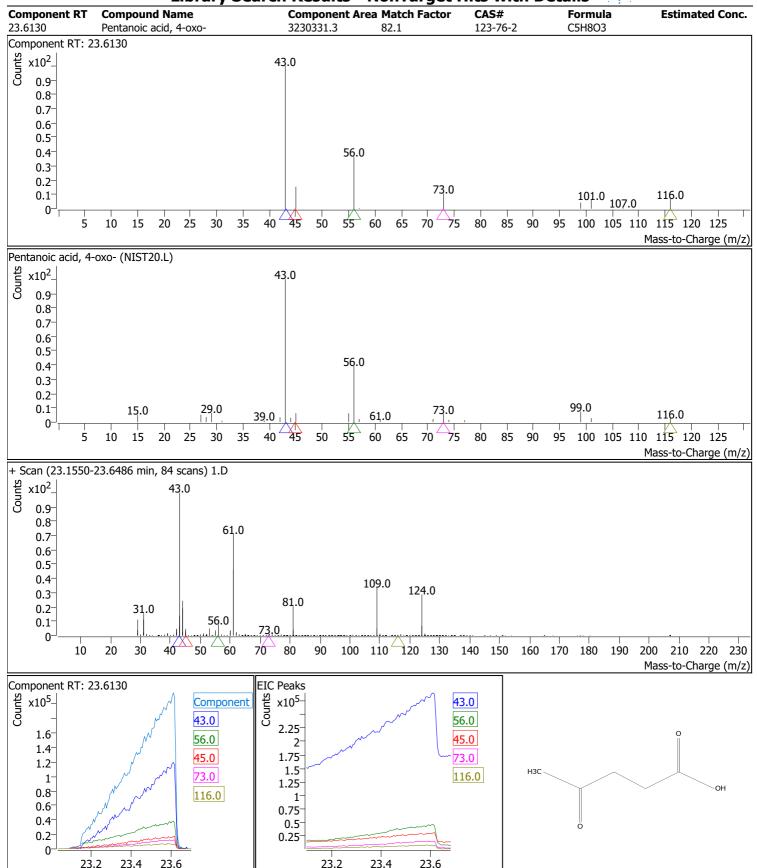
#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.5574 Phenol, 2-methoxy-8383926.4 98.5 C7H8O2 Component RT: 23.5574 v10<sup>2</sup> 0.9 109.0 124.0 0.8 $0.7^{-}$ 81.0 0.6 0.5 0.4 0.3 0.2 53.0 39.0 0.1 63.0 50 80 110 10 20 30 40 60 70 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 109.0 124.0 0.8 0.7 0.6 0.5 81.0 0.4 0.3 0.2 53.0 27.0 39.0 0.1 65.0 18.0 77.0 95.0 50 110 10 20 30 40 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4464-23.7437 min, 51 scans) 1.D st x10<sup>2</sup> 0.9 0.8 0.7 61.0 0.6 109.0 0.5 124.0 $0.4^{-}$ 81.0 0.3 31.0 0.2 56.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.5574 Counts x10<sup>6</sup> x10<sup>5</sup> 109.0 Component 109.0 124.0 1.6 1.4 124.0 81.0 3.5



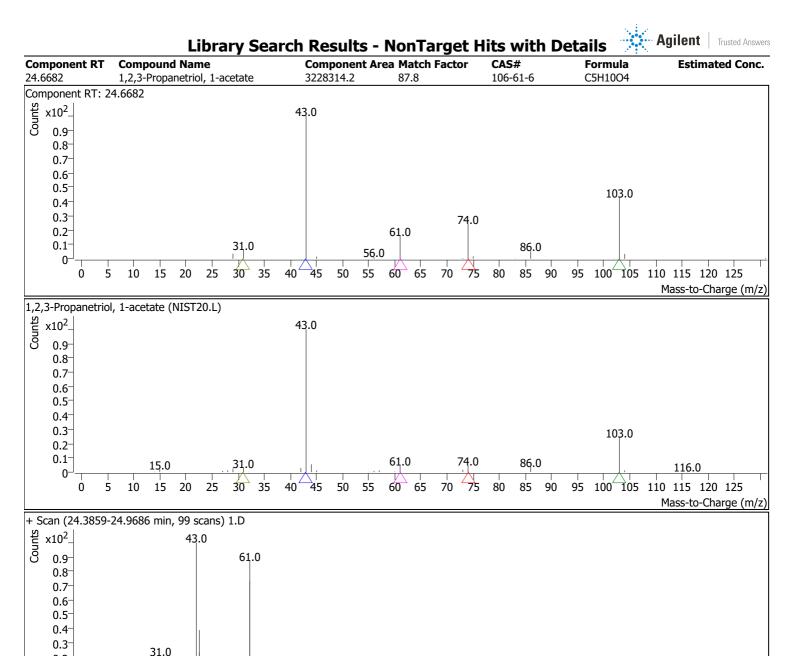


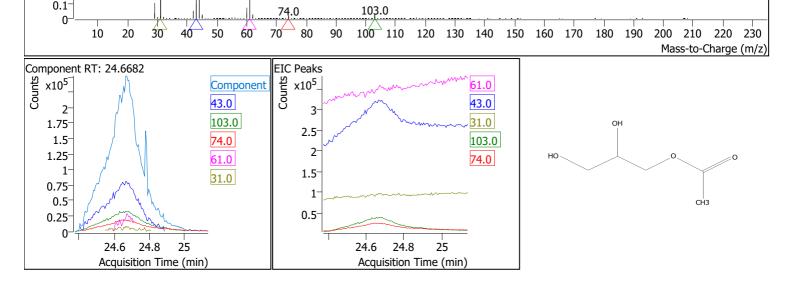
# **Library Search Results - NonTarget Hits with Details**





Acquisition Time (min)





# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 293-30-1 25.1522 1,3,5,7-Tetroxane 648304.1 78.0 C4H8O4 Component RT: 25.1522 y x10<sup>2</sup> 0.9 61.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 91.0 120 30 35 40 50 55 65 70 75 100 105 110 115 125 Mass-to-Charge (m/z) 1,3,5,7-Tetroxane (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 61.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 91.0 0.1 44.0 89.0 121.0 120 125 30 35 40 45 50 55 60 65 70 75 80 85 100 105 110 115 Mass-to-Charge (m/z) + Scan (25.1470-25.1708 min, 5 scans) 1.D St x10<sup>2</sup>\_ 0.9 43.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 31.0 0.2 0.1 55.0 117.0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 25.1522 Counts Counts x10<sup>5</sup> Component 61.0 61.0 91.0 3 3.5 91.0 92.0 3 2.5 92.0 122.0 2.5 2

25

Acquisition Time (min)

99.0

25.2

99.0

122.0

25.2

1.5

0.5

1

0-

24.8

2

1

24.8

25

Acquisition Time (min)

1.5

# --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 2-Propanone, 1-hydroxy-22515463.1 116-09-6 C3H6O2 26.6801 80.1 Component RT: 26.6801 y x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 31.0 0.1 29.0 40.0 0 30 40 75 25 35 55 65 10 15 20 50 60 80 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy- (NIST20.L) S x10<sup>2</sup> 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 15.0 29.0 0.1 27.0 45.0 30 45 65 70 10 15 20 25 35 40 50 55 60 80 Mass-to-Charge (m/z) + Scan (24.9745-26.7893 min, 306 scans) 1.D st x10<sup>2</sup> 0.9 61.0 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 80 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 26.6801 EIC Peaks Counts Counts x10<sup>5</sup> x10<sup>5</sup> 43.0 Component 31.0 43.0 3 СНЗ 31.0 29.0 2.5 42.1 3 42.1 2 73.0 29.0

25.5

26

Acquisition Time (min)

26.5

1.5

73.0

2

1

25.5

26

Acquisition Time (min)

26.5

OH

## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 37962614.8 56-81-5 26.6803 Glycerin 80.5 C3H8O3 Component RT: 26.6803 v10<sup>2</sup> 0.9 43.0 61.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 74.0 5 15 25 30 75 10 20 35 40 45 55 70 80 Mass-to-Charge (m/z) Glycerin (NIST20.L) x10<sup>2</sup>\_ 0.9 61.0 43.0 0.8 0.7 0.6 0.5 31.0 0.4 0.3 15.0 0.2 27.0 0.1 19.0 55.0 58.0 74.0 39.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 Mass-to-Charge (m/z) + Scan (24.9745-26.7893 min, 306 scans) 1.D st x10<sup>2</sup> 0.9 61.0 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 0.1 60 Ó 20 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 26.6803 EIC Peaks Counts Counts x10<sup>5</sup> Component 61.0 43.0 43.0 4.5 4 61.0 31.0 6 3.5 31.0 60.0 3 5



24

25

Acquisition Time (min)

26

60.0

62.0

3

2

1

25

Acquisition Time (min)

26

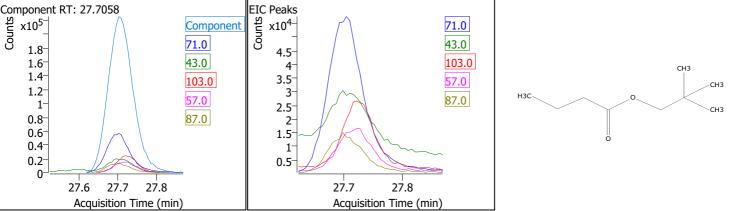
2.5

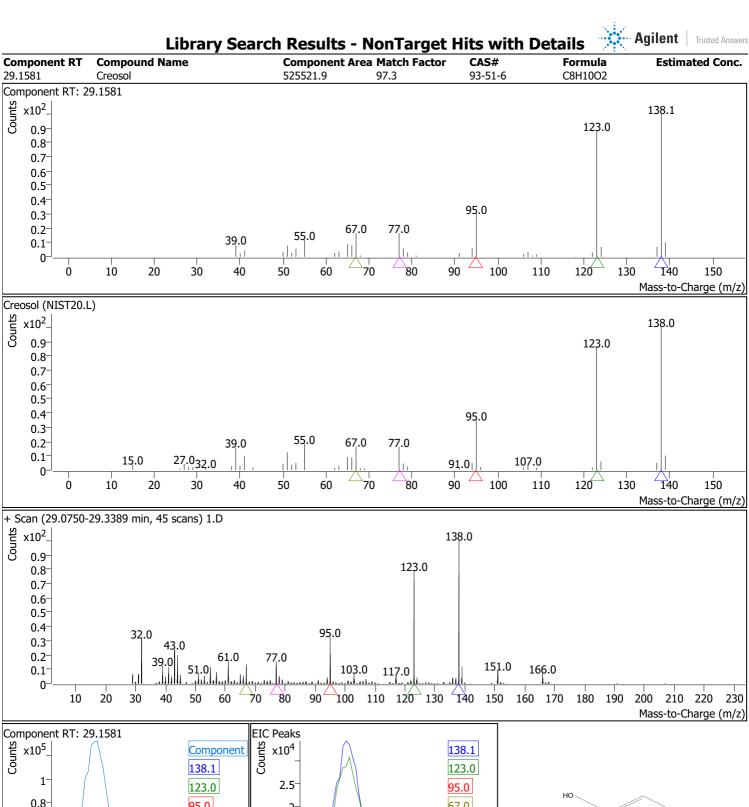
1.5

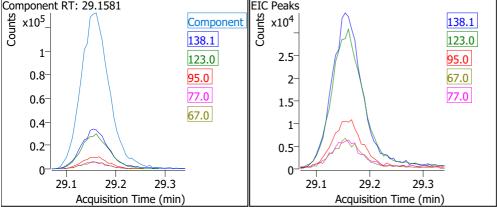
62.0

ОН

#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 81.3 27.7058 Butanoic acid, 2,2-dimethylpropyl 1010279.2 23361-69-5 C9H18O2 Component RT: 27.7058 x10<sup>2</sup>\_ 71.0 0.9 8.0 0.7 0.6 0.5 43.0 103.0 0.4 0.3 57.0 87.0 31.0 $0.2^{-}$ 0.1 0-70 10 20 30 40 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 40 50 60 70 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6293-27.8393 min, 35 scans) 1.D x10<sup>2</sup>. 71.0 0.9 0.8 0.7 43.0 0.6 0.5 0.4 103.0 0.3 31.0 57.0 0.2 87.0 0.1 0 70 90 190 200 210 220 230 10 20 30 40 50 60 80 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) **EIC Peaks**

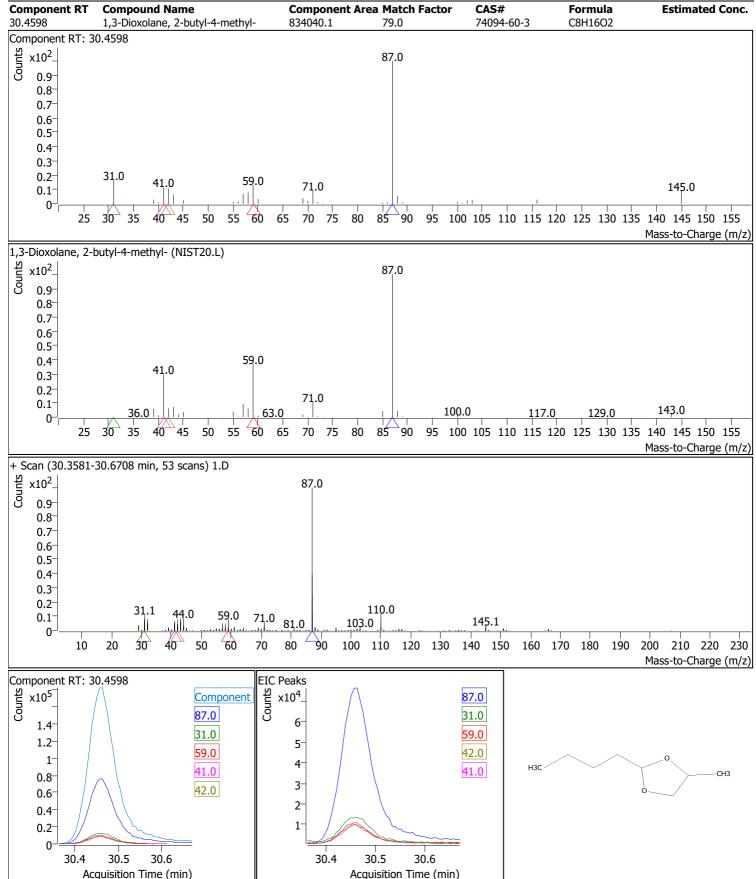






# **Library Search Results - NonTarget Hits with Details**





# --- 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 30.7535 Catechol 925875.3 86.6 C6H6O2 Component RT: 30.7535 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 92.0 53.0 81.0 0.1 100 105 110 115 120 125 50 55 60 85 95 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 (30.6115-30.9919 min, 64 scans) 1.D St x10<sup>2</sup>\_ 0.9 110.0 0.8 0.7 0.6 0.5 $0.4^{-}$ 0.3 64.0 0.2 92.0 103.0 0.1 81.0 10 20 50 60 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 30.7535 **EIC Peaks** Counts st x10<sup>4</sup>-110.0 Component 110.0 64.0 6 64.0 3 63.0 5 63.0 2.5 81.0 4

92.0

92.0

81.0

3

2

1

30.8

31

Acquisition Time (min)

31.2

2-

1.5

0.5

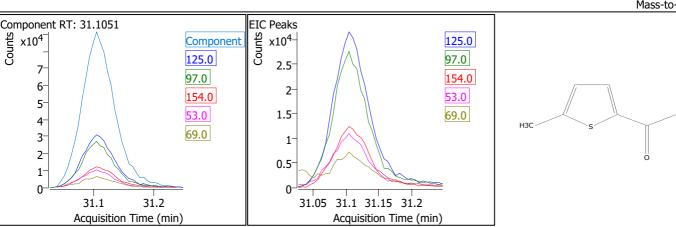
1

30.7

30.8

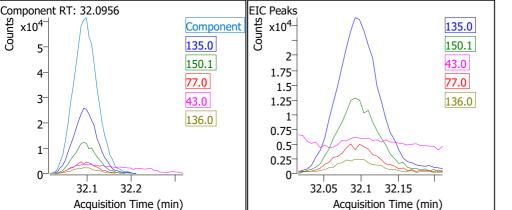
30.9

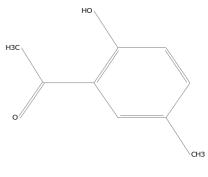
# - Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 59303-13-8 31.1051 1-Propanone, 1-(5-methyl-2-thienyl)-343736.1 **C8H10OS** Component RT: 31.1051 v10<sup>2</sup> 0.9 125.0 97.0 0.8 0.7 0.6 0.5 154.0 0.4 53.0 0.3 69.0 0.2 0.1 50.0 $\frac{4}{70}$ 100 160 10 20 30 40 50 80 110 120 130 140 150<sup>4</sup> 170 Mass-to-Charge (m/z) 1-Propanone, 1-(5-methyl-2-thienyl)- (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 125.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 154.0 0.1 27.0 57.0 63.0 69.0 75.0 90 10 20 30 40 50 60 80 100 110 130 140 150<sup>4</sup> 160 170 Mass-to-Charge (m/z) + Scan (31.0326-31.2298 min, 34 scans) 1.D st x10<sup>2</sup> 0.9 125.0 0.8 0.7 0.6 97,.0109.0 0.5 0.4 81.0 0.3 154.0 53.0 0.2 29.0 87.0 0.1 100 20 40 60 80 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 31.1051 **EIC Peaks** St x10<sup>4</sup>-Counts 125.0 Component 125.0 97.0 2.5 7

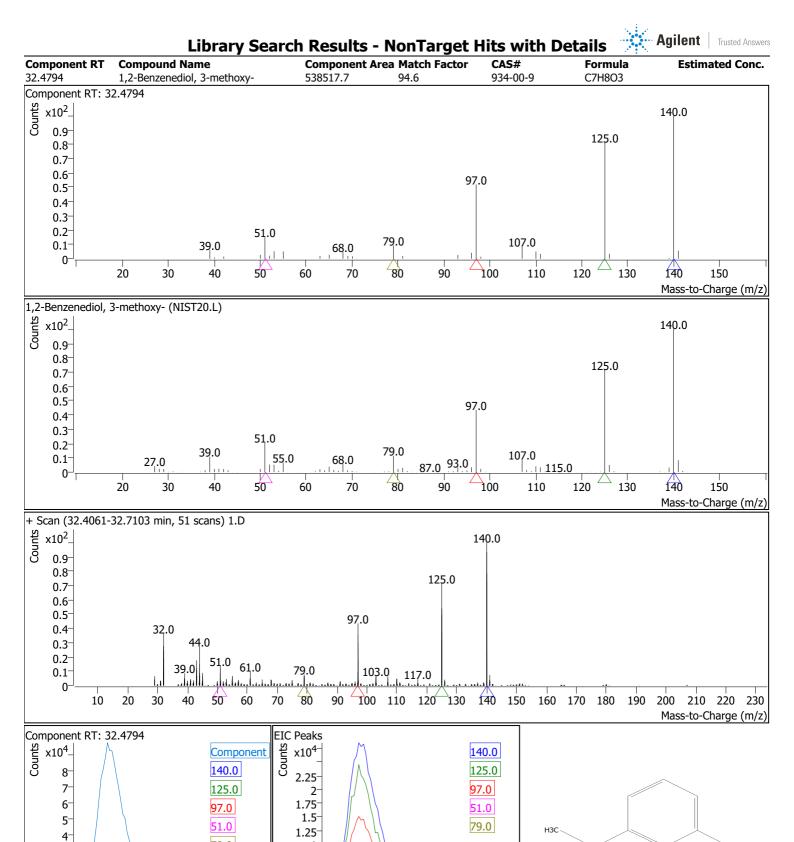


-СН3

#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1450-72-2 32.0956 Ethanone, 1-(2-hydroxy-5-234475.9 90.1 C9H10O2 methylphenyl)-Component RT: 32.0956 x10<sup>2</sup>\_ 135.0 0.9 8.0 0.7 0.6 150.1 0.5 0.4 0.3 43.0 77.0 $0.2^{-}$ 0.1 53.0 39.0 0-150 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 150.0 0.5 0.4 0.3 107.0 0.2 77.0 51.0 0.1 27.0 63.0 85.091.0 131.0 121.0 0 130 150 10 20 30 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0159-32.2109 min, 33 scans) 1.D st x10<sup>2</sup> 0.9 135.0 0.8 0.7 0.6 103.0 150.1 0.5 0.4 0.3 75.0 57.0 32.0 0.2 96.1 61.0 0.1 <u>. . بدنده استطاد</u> 100 110 120 130 140 150 160 170 180 190 200 210 220 230 10 20 30 40 50 60 70 80 90 Mass-to-Charge (m/z) Component RT: 32.0956 **EIC Peaks** Counts Counts x10<sup>4</sup>x10<sup>4</sup> 135.0 Component НО 150.1 135.0 5 2 150.1 43.0 **Н3С** 1.75 4 77.0 77.0 1.5









32.5

32.6

Acquisition Time (min)

32.7

79.0

0.75

0.5

0.25

3

2

1

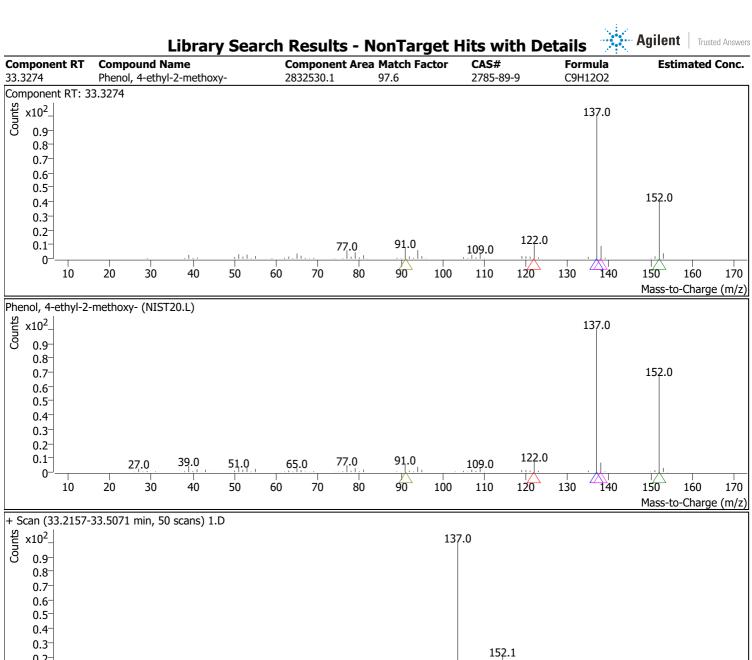
32.5

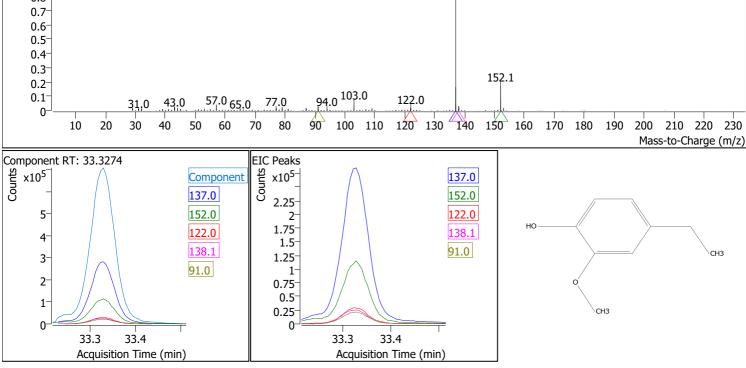
32.6

Acquisition Time (min)

32.7

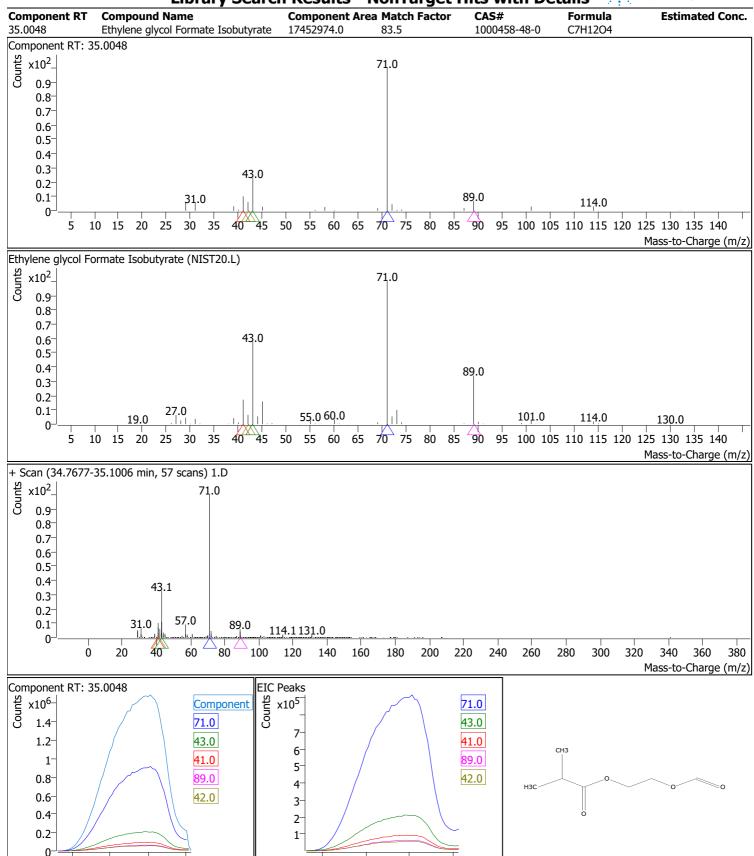
ОН





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





34.9

35

Acquisition Time (min)

34.8

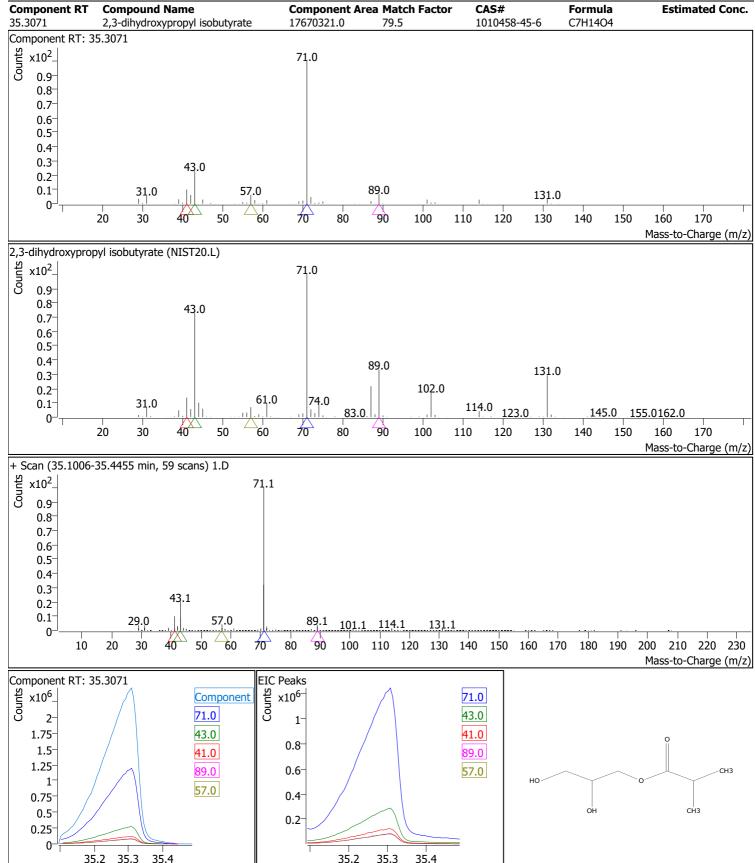
34.8

34.9

35

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

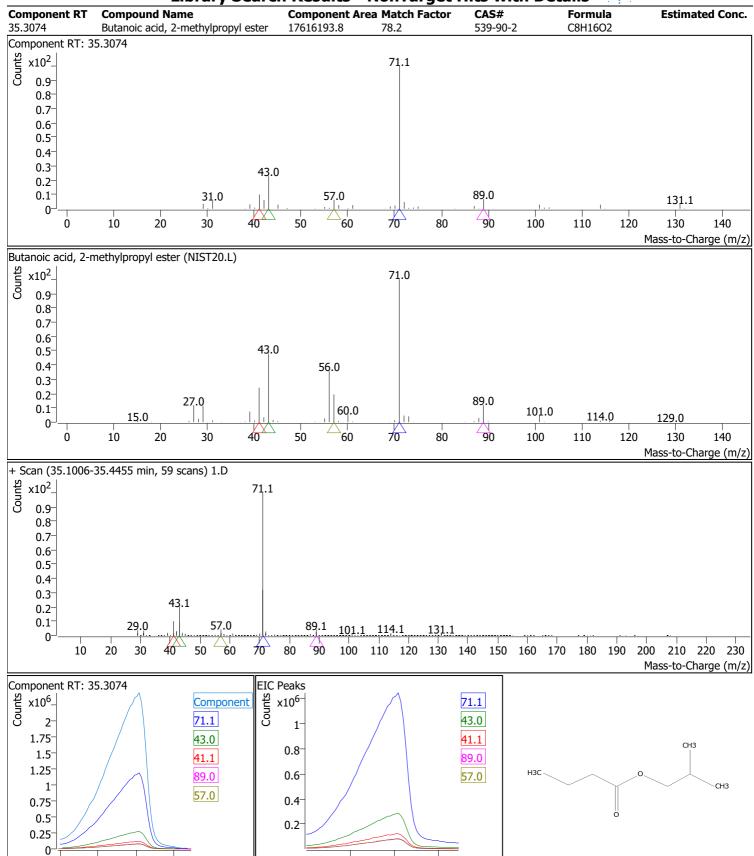




Acquisition Time (min)

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





35.2

35.3

Acquisition Time (min)

35.4

35.2

35.3

Acquisition Time (min)

35.4

## -- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.1579 2-Furanmethanol, tetrahydro-4021958.6 82.2 C5H10O2 Component RT: 36.1579 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 25 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 35 40 45 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.0342-36.3672 min, 57 scans) 1.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: 36.1579 Counts Counts x10<sup>5</sup>\_ 71.0 Component 71.0 43.0 3.5 6 43.0 41.0 3 5 131.0 41.0 2.5

31.0



131.0

31.0

2

1

36.1

36.2

Page 39 of 81

Acquisition Time (min)

36.3

1.5

0.5

4

3

2

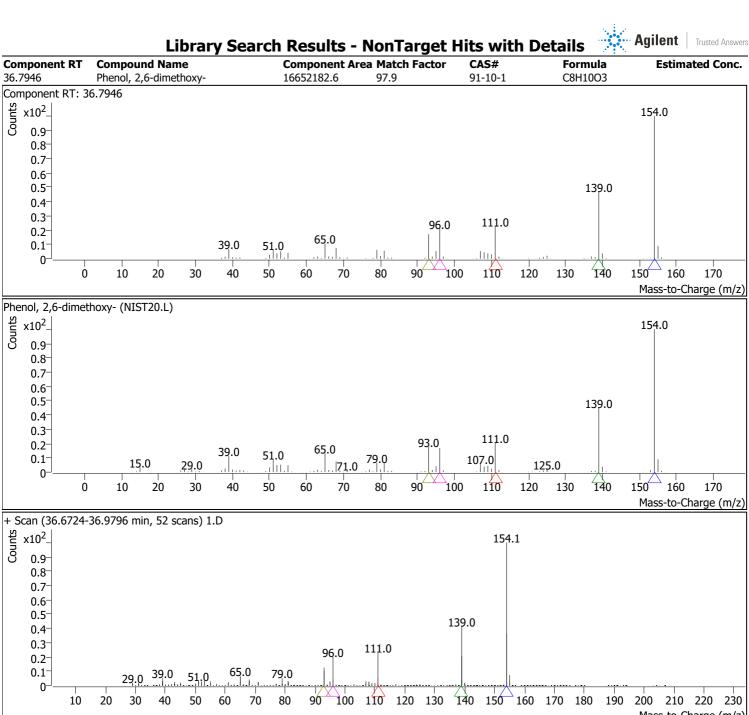
1

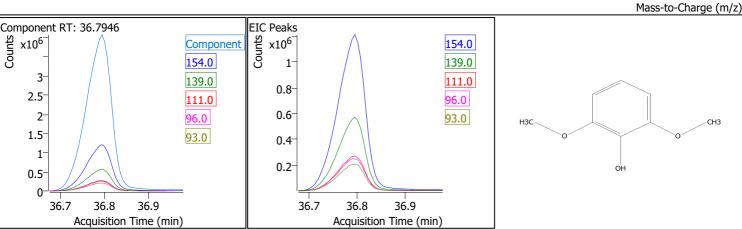
36.1

36.2

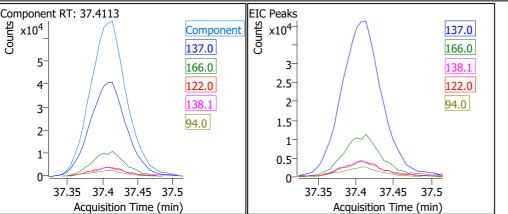
Acquisition Time (min)

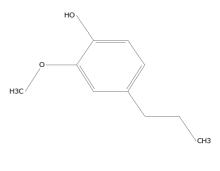
36.3

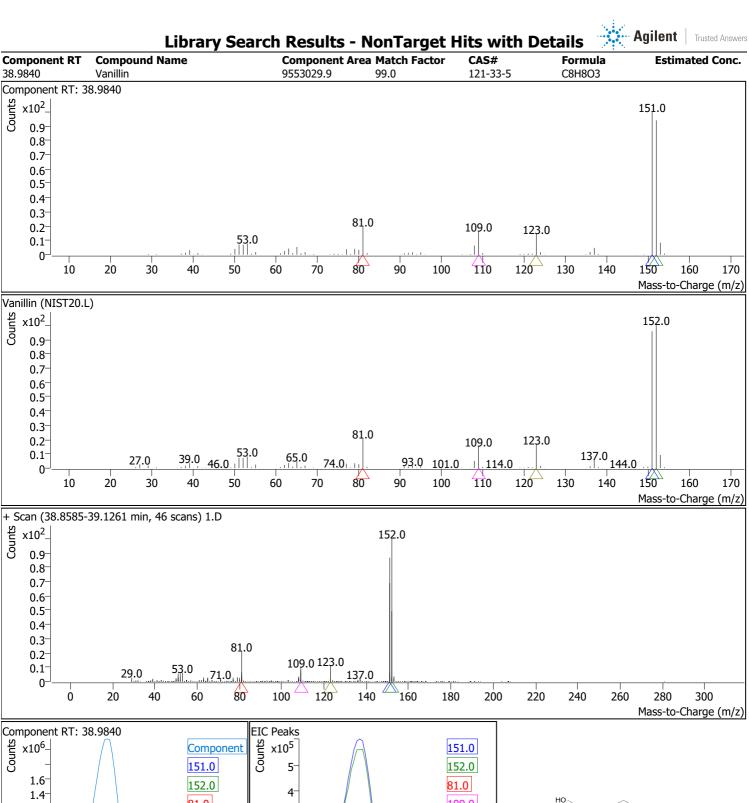


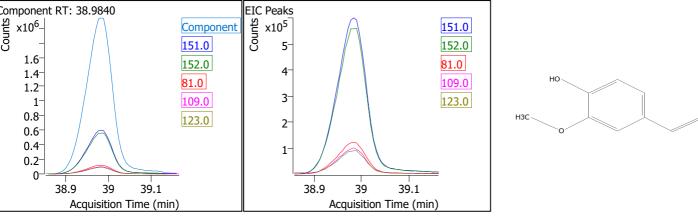


#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4113 Phenol, 2-methoxy-4-propyl-240330.3 80.4 C10H14O2 Component RT: 37.4113 v10<sup>2</sup> 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 77.0 85.0 94.0 160 - 170 120 10 20 30 40 50 110 130 180 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 0.4 166.0 0.3 15.0 29.0 0.2 39.0 122.0 0.1 51.0 66.0 149.0 140 160 170 0 10 20 30 40 50 60 70 80 90 100 110 120 130 150 180 Mass-to-Charge (m/z) + Scan (37.3380-37.4850 min, 25 scans) 1.D st x10<sup>2</sup> 0.9 103.0 71.1 0.8 0.7 43.0 0.6 0.5 57.0 $0.4^{-}$ 137.1 0.3 29.0 0.2 89.0 166.1 0.1 117.0 131.1 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: 37.4113 Counts Counts x10<sup>4</sup> 137.0 Component 137.0 166.0 5 3 166.0 138.1



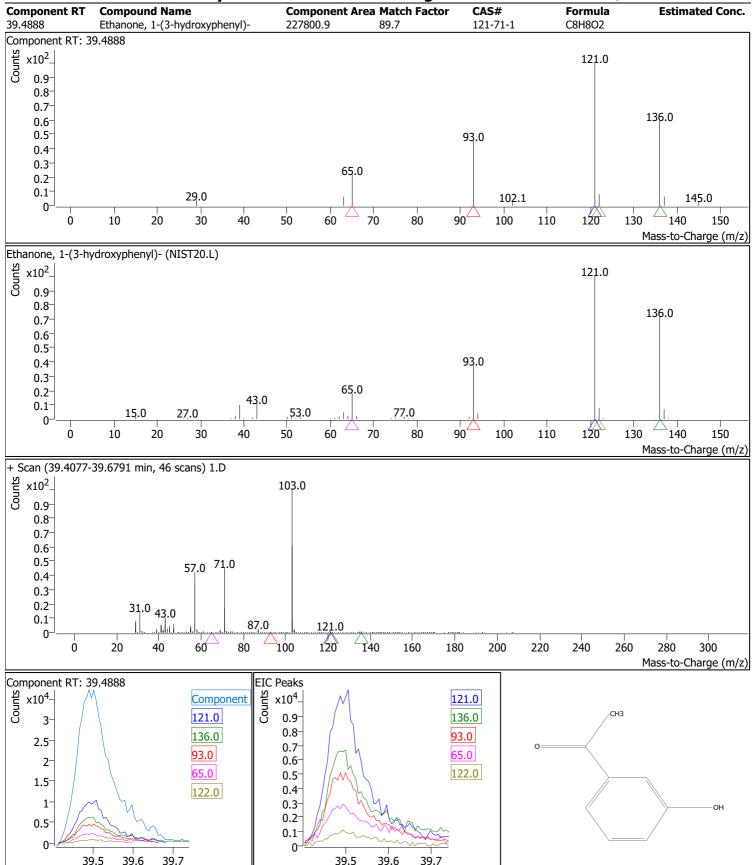






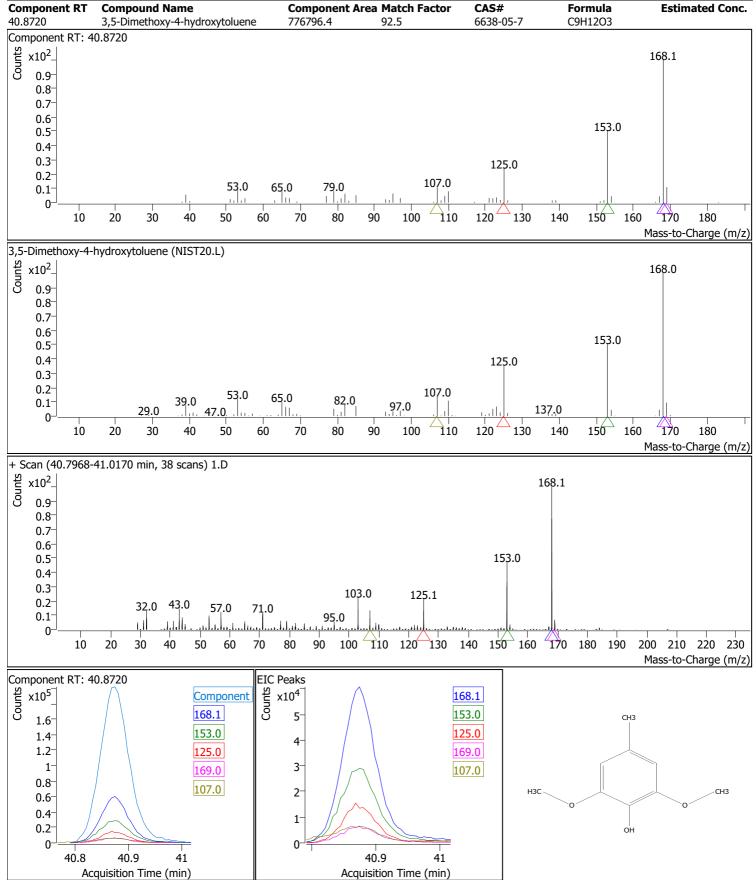




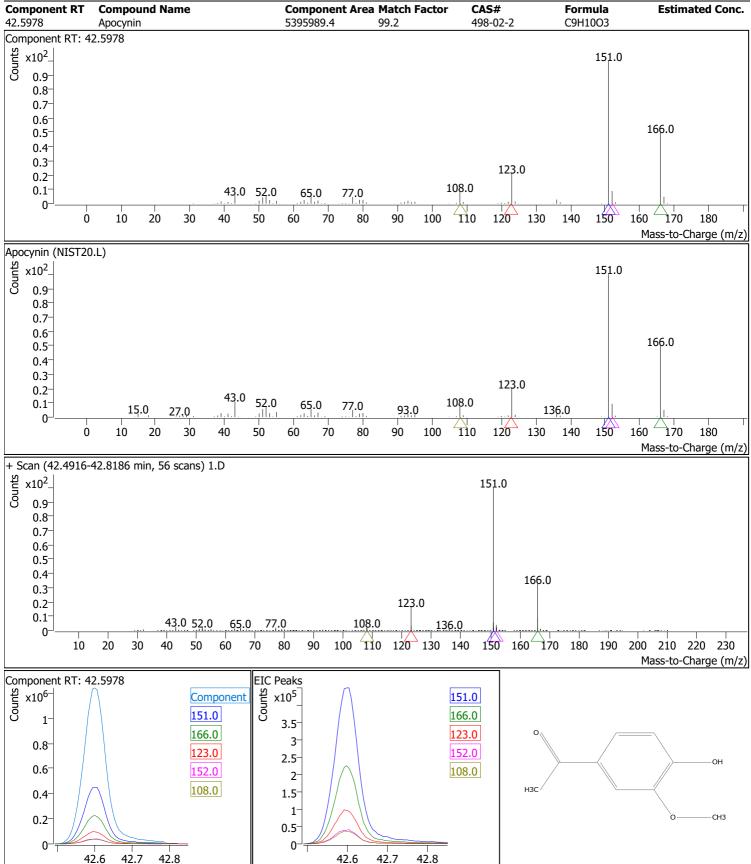






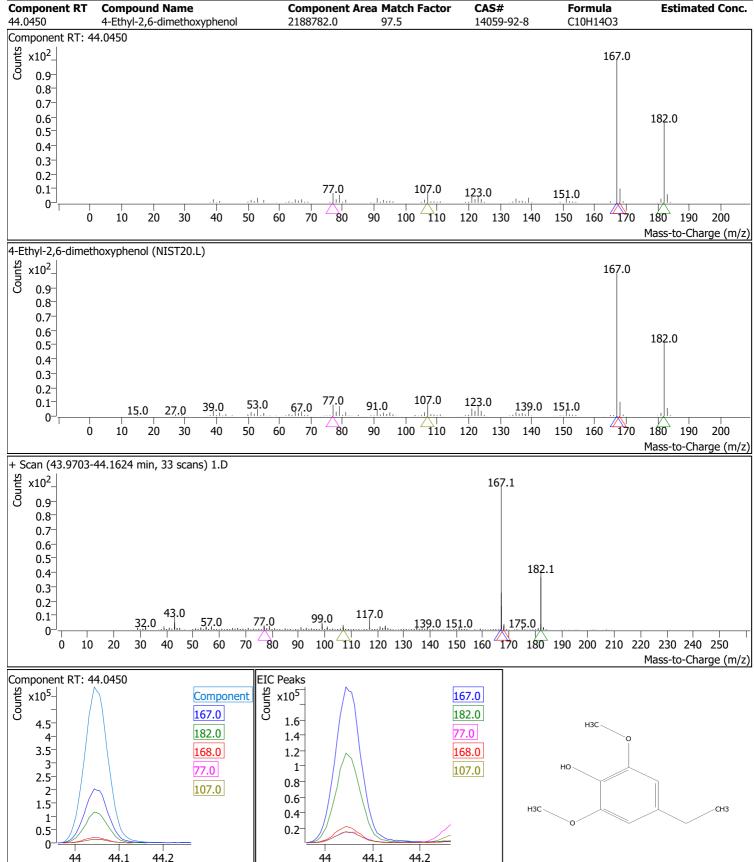






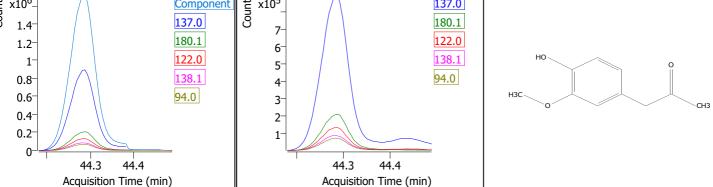
# Library Search Results - NonTarget Hits with Details



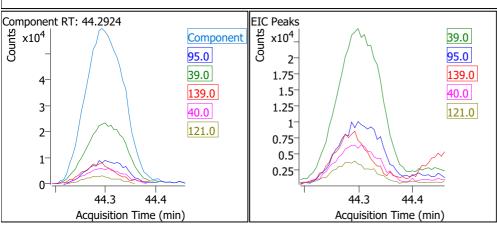


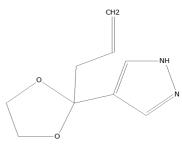
Acquisition Time (min)

#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 44.2850 2-Propanone, 1-(4-hydroxy-3-7255885.9 93.9 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.2850 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 $0.2^{-}$ 122.0 0.1 77.0 66.0 39.0 51.0 120 180 20 30 40 50 60 70 80 100 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 66.0 85.0<sup>9</sup>1.0 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.1803-44.4597 min, 48 scans) 1.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 74.0 0.4 0.3 87.0 180.1 0.2 43.0 122.0 94 N 0.1 171.1 214.2 0 140 180 220 0 20 40 60 80 100 120 160 200 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 44.2850 Counts Counts x10<sup>5</sup> 137.0 x10<sup>6</sup>\_ Component 180.1 137.0 1.4 7 180.1 122.0 1.2 6



#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.2924 4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-329057.9 75.7 98816-47-8 C9H12N2O2 1H-pyrazole Component RT: 44.2924 x10<sup>2</sup>\_ 95.0 0.9 39.0 8.0 139.0 0.7 0.6 0.5 0.4 0.3 121.0 $0.2^{-}$ 0.1 0-30 35 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 Mass-to-Charge (m/z) 4-[2-(2-Propenyl)-1,3-dioxolan-2-yl]-1H-pyrazole (NIST20.L) $x10^{2}$ 95.0 139.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 39.0 0.1 68.0 53.0 80.0 92.0 0 95 100 105 110 115 120 125 130 135 140 145 150 35 50 55 60 65 70 75 80 85 90 Mass-to-Charge (m/z) + Scan (44.2040-44.4062 min, 35 scans) 1.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 74.0 0.5 0.4 180.1 0.3 87.0 0.2 122.0 55.0 94.0 0.1 157.1 <sup>17</sup>1.1 115.1 129.1 214.2 0 40 120 140 Ó 20 60 80 100 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.2924 **EIC Peaks** Counts Counts x10<sup>4</sup> $x10^{4}$ 39.0 Component CH2 95.0 95.0 2



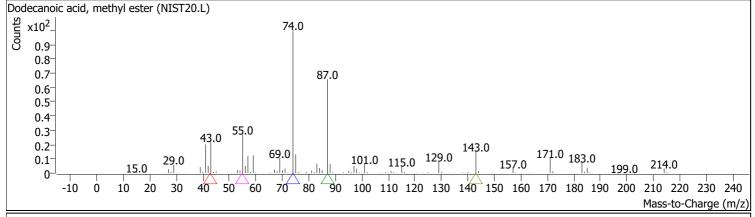


# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3268 Dodecanoic acid, methyl ester 6825508.8 111-82-0 C13H26O2 Component RT: 44.3268 Counts $x10^{2}$ 74.0 0.9 0.8 $0.7^{-}$ 87.0 0.6 0.5 0.4 0.3 43.0 55.0 143.0 0.2 69.0 0.1

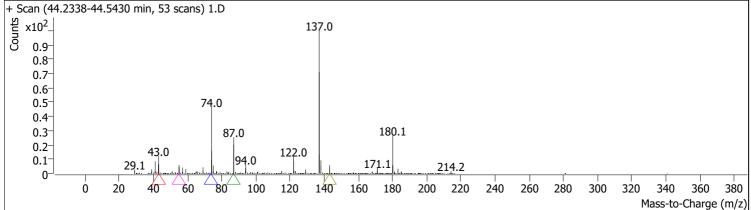
100 110 120

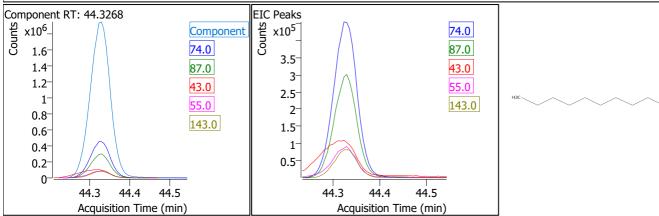
130 140 150 160 170 180 190 200 210 220 230 240

Mass-to-Charge (m/z)



70





#### --- 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 45.6164 Pentanoic acid, 4-oxo-, 2-methylpropyl 991790.5 85.1 C9H16O3 Component RT: 45.6164 x10<sup>2</sup>\_ 99.0 0.9 8.0 0.7 0.6 0.5 43.0 0.4 0.3 $0.2^{-}$ 117.0 130.0 0.1 120 30 100 130 10 20 40 50 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 40 100 120 130 10 20 30 50 60 70 80 90 110 140 150 160 170 Mass-to-Charge (m/z) + Scan (45.4884-45.8273 min, 58 scans) 1.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 0.2 71.0 32.0 55.0 180.0 0.1 130.0 159.0 0 Ó 40 60 100 120 200 260 280 20 80 140 160 180 220 240 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 45.6164 st x10<sup>5</sup>-Counts x10<sup>4</sup>– 99.0 Component 99.0 43.0 7-1.4 43.0 117.0 6 1.2 117.0 71.1 5

45.7

Acquisition Time (min)

45.8

130.0

1

0.8

0.6

0.4

45.6

45.7

Acquisition Time (min)

45.8

71.1

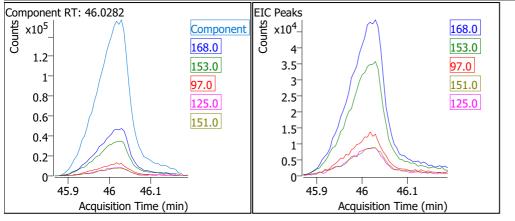
130.0

4

3-

2-

#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 645-08-9 46.0282 3-Hydroxy-4-methoxybenzoic acid 913799.3 90.7 C8H8O4 Component RT: 46.0282 v10<sup>2</sup> 0.9 168.0 0.8 153.0 0.7 0.6 0.5 0.4 0.3 97.0 125.0 0.2 51.0 79.0 0.1 0 100 50 150 10 20 30 40 60 70 80 90 110 120 130 140 180 190 Mass-to-Charge (m/z) 3-Hydroxy-4-methoxybenzoic acid (NIST20.L) st x10<sup>2</sup> 0.9 168.0 0.8 0.7 0.6 153.0 0.5 0.4 0.3 97.0 0.2 125.0 51,0 0.1 79.0 65.0 108.0 18.0 27.0 93.0 136.0 170 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 180 190 Mass-to-Charge (m/z) + Scan (45.8817-46.1603 min, 47 scans) 1.D st x10<sup>2</sup> 0.9 168.0 0.8 0.7 153.0 0.6 0.5 87.0 43.0 $0.4^{-}$ 0.3 97.0 117.0 0.2 32.0 61.0 ....77.0 ..<u>.ا.ا.ا</u>... 107.0 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 46.0282



#### --- 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 46.4726 384241.8 83.3 C10H12O3 methoxyphenyl)-Component RT: 46.4726 x10<sup>2</sup> 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 $0.2^{-}$ 123.0 0.1 108.0 52.0 77.0 137.0 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 (46.3803-46.5289 min, 26 scans) 1.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 117.0 0.4 0.3 180.0 0.2 32.0 43.1 75.0 87.1 99.0 0.1 55.0 137.0 161.0 0 40 60 100 120 180 260 Ó 20 80 140 160 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 46.4726 **EIC Peaks** Counts Counts x10<sup>4</sup>\_ x10<sup>6</sup> 151.0 Component /СН3 151.0 123.0 1 7 180.0 152.0 0.8 6 108.0 123.0

46.5

Acquisition Time (min)

180.0

46.6

5

4

3

2

1

46.4

46.5

Acquisition Time (min)

152.0

108.0

46.6

0.6

0.4

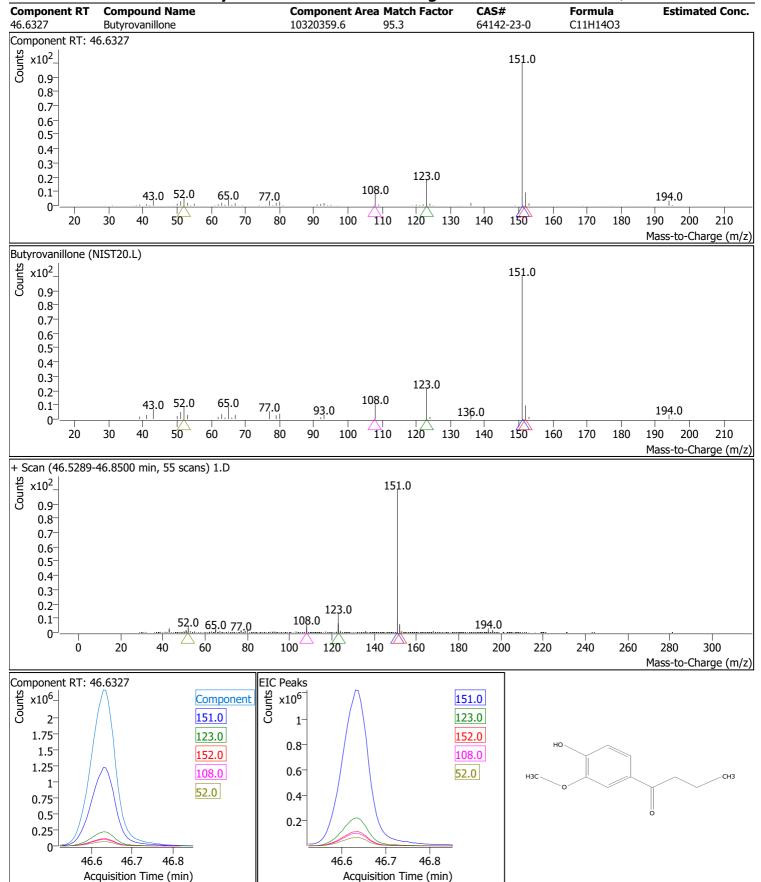
0.2

46.4

нзс







#### ... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 47.0806 (E)-2,6-Dimethoxy-4-(prop-1-en-1-352815.4 82.6 C11H14O3 yl)phenol Component RT: 47.0806 x10<sup>2</sup>\_ 194.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 91.0 119.0 131.1 $0.2^{-}$ 147.0 167.1 179.0 77.0 103.0 0.1 0-10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 97.0 27.0 .85.0 0 130 140 150 160 170 90 20 50 60 70 80 100 110 120 180 190 200 210 220 Mass-to-Charge (m/z) + Scan (47.0058-47.1830 min, 30 scans) 1.D x10<sup>2</sup>. 194.1 0.9 99.0 0.8 0.7 0.6 43.0 0.5 0.4 117.0 151.0 0.3 32.0 87.0 57.0 131.0 0.2 71.0 167.0 0.1 0 200 Ó 20 40 60 80 100 120 140 160 180 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 47.0806 **EIC Peaks** Counts Counts x10<sup>4</sup>x10<sup>4</sup>-194.0 Component 194.0 91.0 7 1.6 **Н3С** 91.0 131.1 1.4 6 131.1 119.0 1.2 5 119.0 147.0 1 НО 4

0.8

0.6

0.4

0.2

47.05

47.1

Acquisition Time (min)

47.15

147.0

47.05 47.1 47.15

Acquisition Time (min)

3

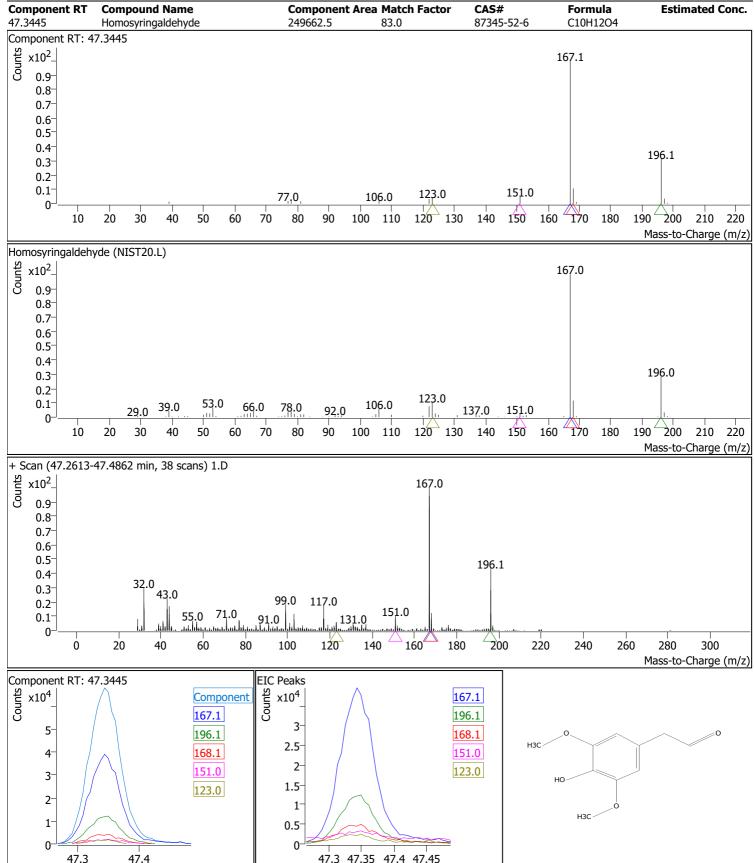
2

1

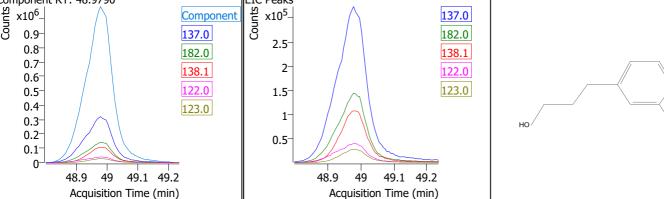
НЗС



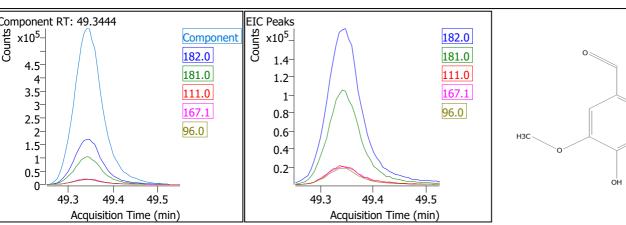


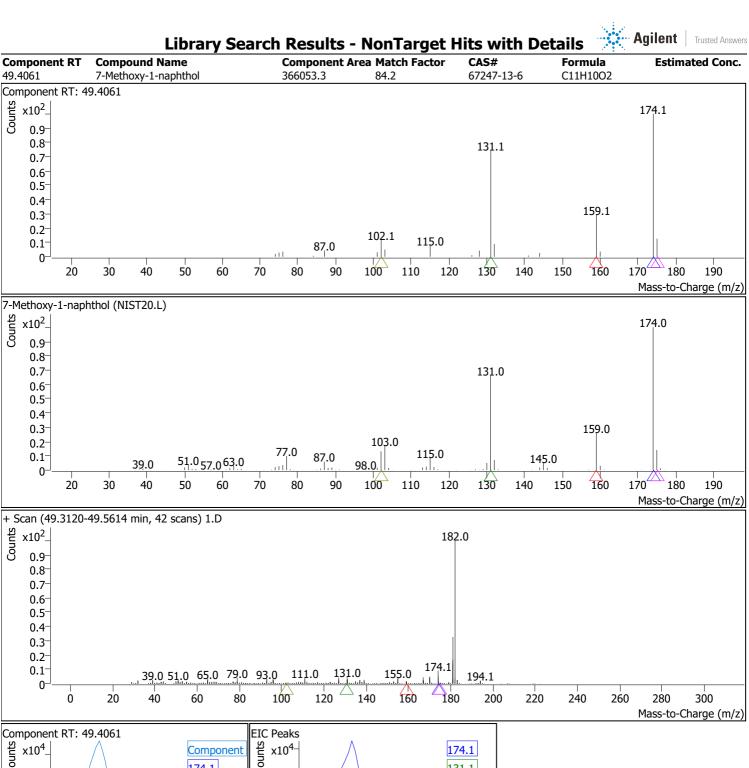


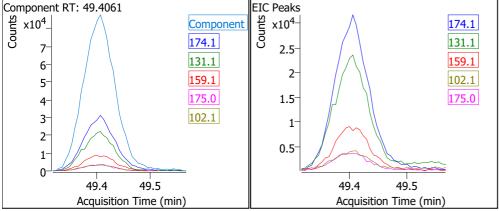
#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 48.9790 Benzenepropanol, 4-hydroxy-3-6788098.5 96.4 C10H14O3 methoxy-Component RT: 48.9790 x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 182.0 0.4 0.3 $0.2^{-}$ 122.0 77.0 91.0 0.1 107.0 0-140 180 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 0.2 122.0 77.0 91.0 65.0 106.0 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 (48.8136-49.1806 min, 61 scans) 1.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 182.1 0.2 0.1 107.0 122.0 32.0 51.0 65.0 77.0 91.0 149.0 0 40 60 100 140 180 Ó 20 80 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 48.9790 **EIC Peaks** Counts x10<sup>6</sup>\_ x10<sup>5</sup>– 137.0 Component 182.0 0.9 137.0 2.5 0.8 182.0 138.1 0.7 2-138.1 122.0 0.6



#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.3444 Benzaldehyde, 4-hydroxy-3,5-2605242.4 96.7 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3444 x10<sup>2</sup>\_ 182.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 167.1 111.0 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 0 110 160 170 10 20 30 40 50 60 70 80 90 100 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2586-49.5257 min, 45 scans) 1.D x10<sup>2</sup>\_ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 174.1 0.1 39.0 51.0 65.0 79.0 93.0 111.0 131.0 155.0 0 Ó 40 80 100 120 180 20 60 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 49.3444 Counts Counts x10<sup>5</sup>x10<sup>5</sup>-182.0 Component 0 181.0 182.0 1.4 4.5 181.0 111.0 1.2 3.5 111.0 167.1 1-

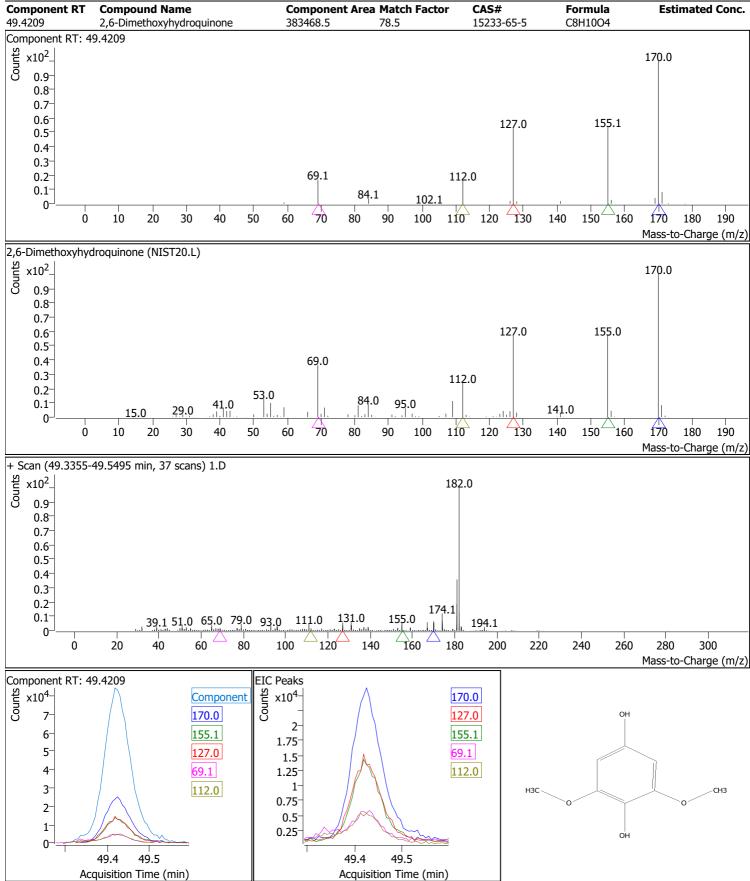












## ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 50.4127 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-326279.1 80.6 65996-50-1 C6H5N3O2 dione Component RT: 50.4127 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 0.1 108.0 52.0 80.0 100 105 110 115 120 125 130 135 140 145 65 70 75 80 85 90 95 150 155 160 165 Mass-to-Charge (m/z) Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L) st x10<sup>2</sup> 0.9 151.0 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 65 70 75 80 85 90 Mass-to-Charge (m/z) + Scan (50.3047-50.5350 min, 39 scans) 1.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 81.0 169.0 0.3 197.0 0.2 43.0 57.0 71.0 95.0 228.1 139.0 183.0 0.1 0 40 60 80 100 Ó 20 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 50.4127 EIC Peaks Counts Counts x10<sup>4</sup> x10<sup>4-</sup> 151.0 Component 151.0 52.0 6 5 108.0 108.0 5 52.0 80.0 4

50.4

Acquisition Time (min)

136.0

50.5

80.0

136.0

50.5

3

2

1

50.4

Acquisition Time (min)

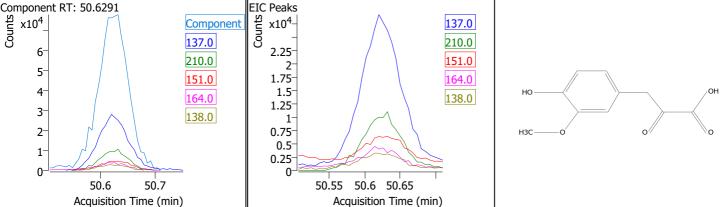
3-

2

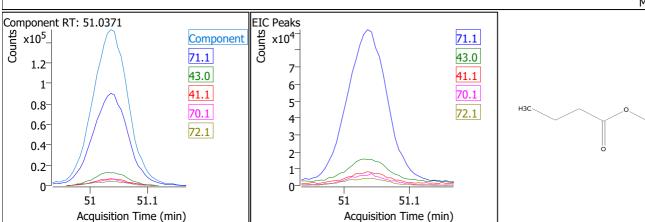
1

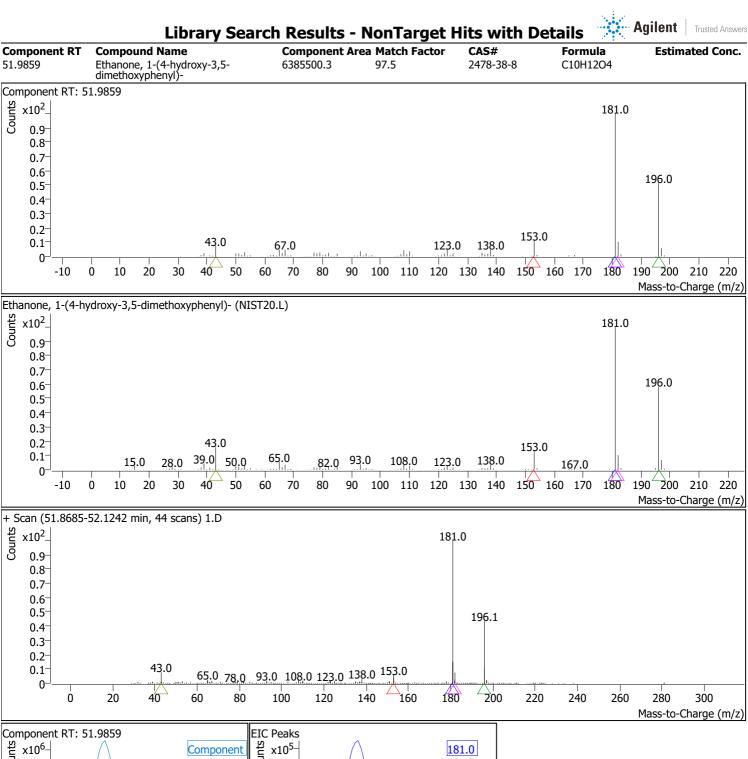
0-

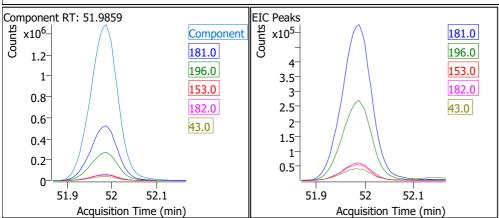
# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 50.6291 Phenylacetylformic acid, 4-hydroxy-3- 303107.7 1081-71-6 C10H10O5 methoxy-Component RT: 50.6291 Counts x10<sup>2</sup>\_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 210.0 0.3 151.0 164.0 $0.2^{-}$ 122.0 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 -10 20 50 60 70 90 Mass-to-Charge (m/z) Phenylacetylformic acid, 4-hydroxy-3-methoxy- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 0.4 210.0 0.3 0.2 164.0 0.1 65.0 77.0 51.0 107.0 149.0 0 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 20 70 80 Mass-to-Charge (m/z) + Scan (50.5524-50.7059 min, 26 scans) 1.D x10<sup>2</sup>. 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 210.1 0.2 151.0 0.1 91.0103.0 164.0 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z)

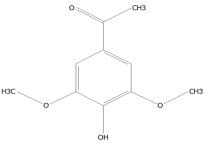


#### --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Butanoic acid, (tetrahydro-2-furanyl)methyl ester 2217-33-6 51.0371 665275.7 77.4 C9H16O3 Component RT: 51.0371 x10<sup>2</sup>\_ 71.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 43.0 0.1 39.0 57.0 87.0 0-10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) Butanoic acid, (tetrahydro-2-furanyl)methyl ester (NIST20.L) St x10<sup>2</sup> 71.0 0.8 0.7 0.6 0.5 0.4 43.0 0.3 0.2 84.0 27.0 0.1 55.0 <u>60.0</u> 15.0 67.0 101.0 114.0 10 15 20 25 30 35 40 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (50.9350-51.1669 min, 40 scans) 1.D st x10<sup>2</sup> 0.8 0.7 0.6 0.5 0.4 0.3 32.0 43.1 0.2 153.0 167.0 0.1 95.0 117.0 131.0 194.1 0 40 60 100 260 280 300 Ó 20 80 120 140 160 180 200 220 240 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 51.0371 Counts Counts x10<sup>4</sup> x10<sup>5</sup>. 71.1 Component 71.1 43.0 1.2 43.0 41.1

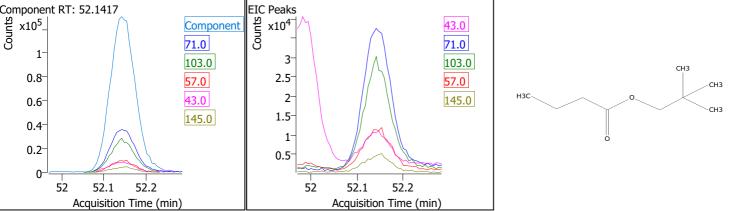






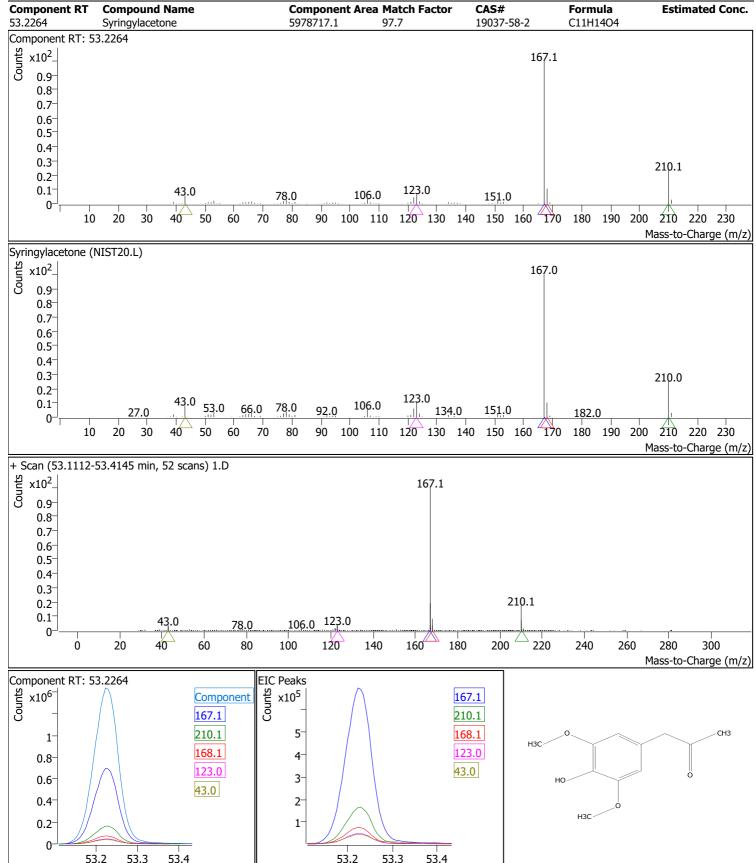


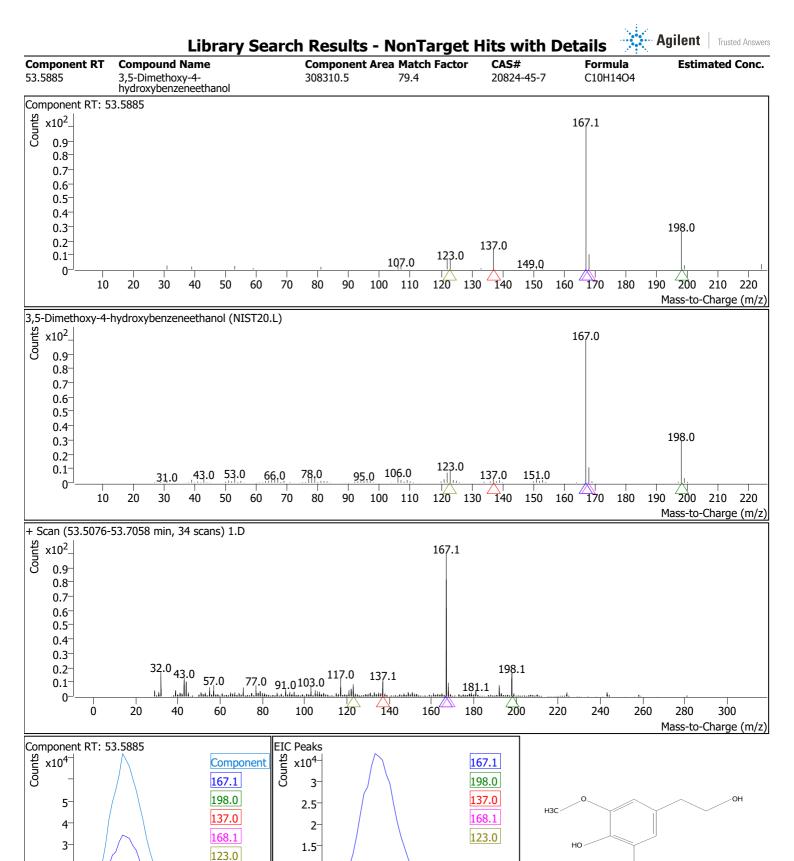
#### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 52.1417 Butanoic acid, 2,2-dimethylpropyl 553692.7 76.7 23361-69-5 C9H18O2 Component RT: 52.1417 x10<sup>2</sup>\_ 71.0 0.9 8.0 103.0 0.7 0.6 0.5 0.4 57.0 0.3 43.0 $0.2^{-}$ 145.0 87.0 0.1 70 10 20 30 50 60 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L) St x10<sup>2</sup> 71.0 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. 0 100 140 150 10 20 30 40 50 60 70 90 110 120 130 160 170 Mass-to-Charge (m/z) + Scan (52.0575-52.2431 min, 32 scans) 1.D st x10<sup>2</sup> 103.0 0.8 0.7 0.6 0.5 0.4 57.0 181.0 196.0 43.0 0.3 137.0 0.2 32.0 77.0 151.0 0.1 122.0 0 Ó 60 80 100 20 40 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 52.1417 x10<sup>4</sup> x10<sup>5</sup>. 43.0 Component











53.6

Acquisition Time (min)

1

0.5

2

1

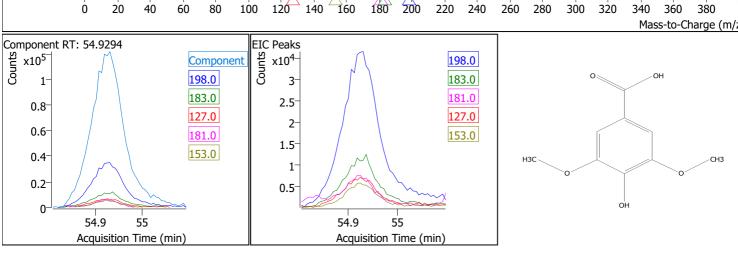
53.6

Acquisition Time (min)

53.7

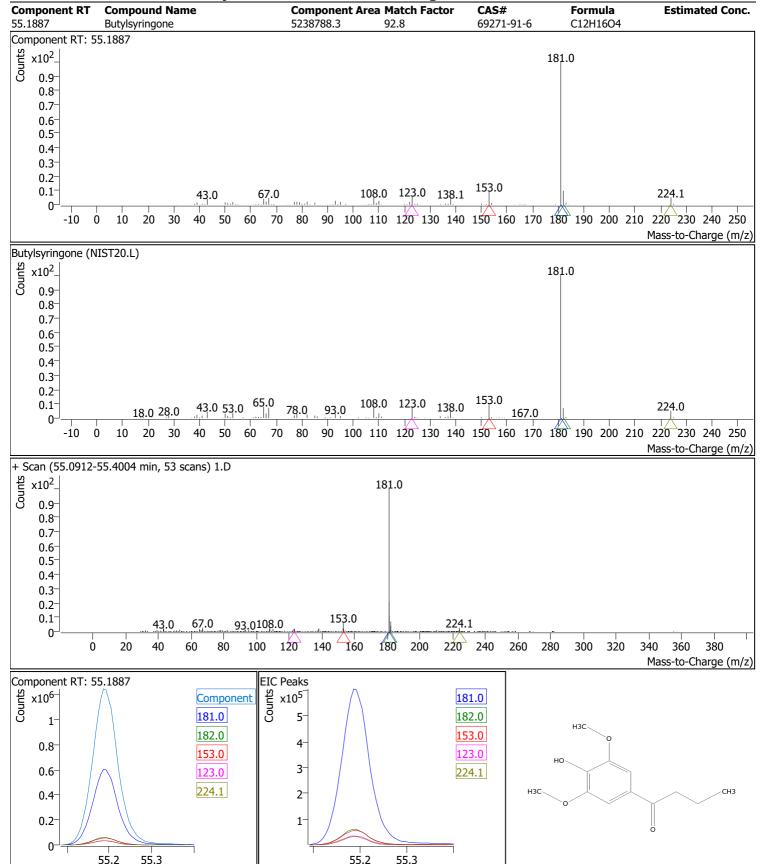
H3C

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 54.9294 Benzoic acid, 4-hydroxy-3,5-621745.1 85.0 530-57-4 C9H10O5 dimethoxy-Component RT: 54.9294 x10<sup>2</sup>\_ 198.0 0.9 8.0 0.7 0.6 0.5 0.4 183.0 0.3 127.0  $0.2^{-}$ 153.0 109.0 0.1 0-180 200 10 20 30 40 60 70 80 90 100 110 120 130 140 150 160 170 190 210 220 Mass-to-Charge (m/z) Benzoic acid, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts  $x10^{2}$ 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 50 60 70 80 90 100 110 120 130 140 150 160 170 190 210 220 Mass-to-Charge (m/z) + Scan (54.8217-55.0972 min, 47 scans) 1.D x10<sup>2</sup>. 198.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 178.1 0.2 57.0 77.0 0.1 0 180 200 20 40 60 80 100 140 160 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 54.9294 Counts Counts x10<sup>4</sup> 198.0 x10<sup>5</sup> Component ОН 198.0 183.0 3-1 183.0 181.0 2.5 0.8 127.0 127.0



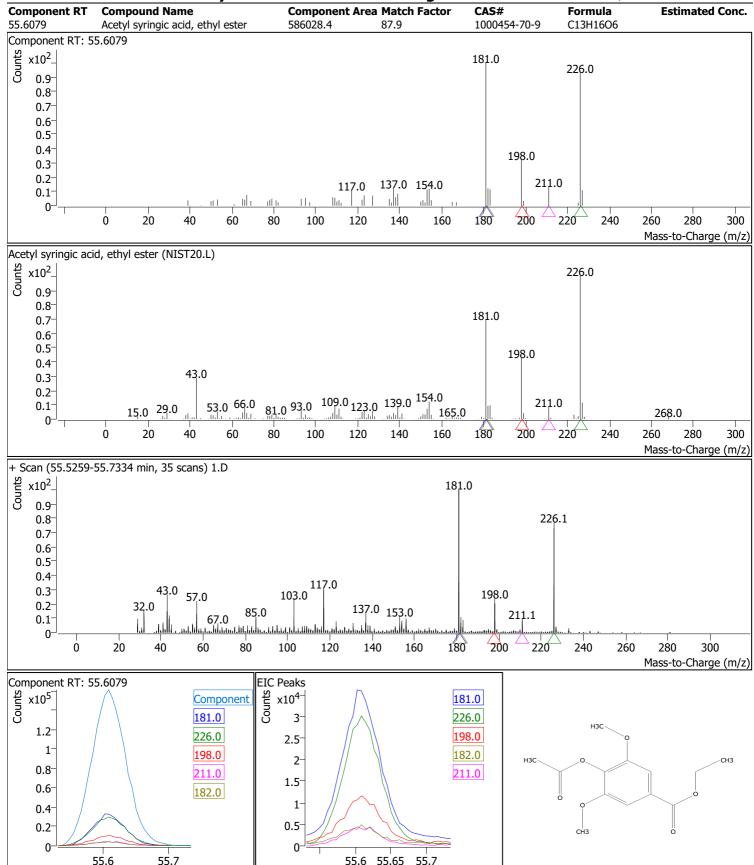






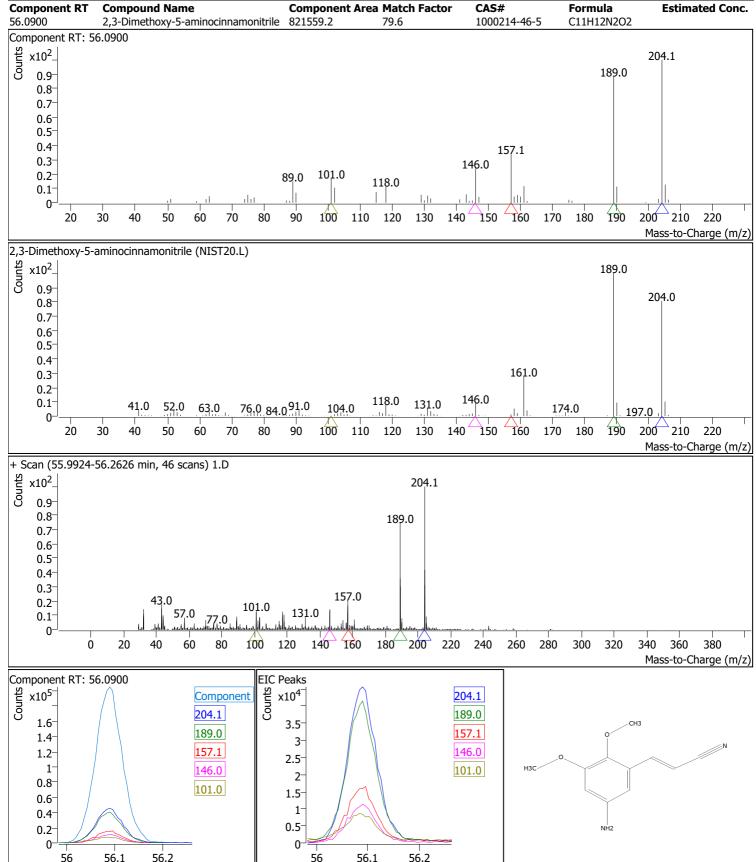












#### ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol 57.4695 2046714.7 92.7 63543-12-4 C11H16O4 Component RT: 57.4695 x10<sup>2</sup>\_ 168.1 0.9 8.0 212.1 0.7 0.6 0.5 0.4 0.3 153.0 $0.2^{-}$ 137.0 123.0 107.0 91.0 0.1 متنايات 0-100 110 120 130 140 150 160 170 180 190 200 10 20 30 50 60 80 90 210 220 230 240 Mass-to-Charge (m/z) 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 212.0 0.6 0.5 0.4 0.3 153.0 0.2 108.0 123.0 137.0 179.0 91.0 77.0 65.0 0.1 31.039.0 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 (57.3507-57.6540 min, 52 scans) 1.D x10<sup>2</sup>. 167.1 0.9 0.8 0.7 0.6 212.1 0.5 0.4 0.3 0.2 43.0<sub>57.0</sub> 137.0 0.1 77.091.0 0 140 180 200 0 20 40 60 80 100 120 160 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 57.4695 Counts Counts x10<sup>4</sup> x10<sup>5</sup> 168.1 Component 167.1 168.1 6 3.5 167.1 212.1 3 5 137.0 212.1 2.5

57.5

57.6

Acquisition Time (min)

153.0

153.0

137.0

3-

2-

2

0.5

57.4

57.5

57.6

Acquisition Time (min)

1.5

# ··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 63.6296 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-592568.4 76.5 65996-50-1 C6H5N3O2 Component RT: 63.6296 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 93.0 0.1 120.0 90 <sup>∠</sup> 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 90 <sup>∠</sup> 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (63.5413-63.8429 min, 50 scans) 1.D x10<sup>2</sup>. 151.0 0.9 0.8 225.1 0.7 0.6 0.5 0.4 0.3 0.2 93.0 57.0 77.0 204.0 0.1 100 60 80 360 380 20 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 63.6296 Counts Counts x10<sup>5</sup> x10<sup>4</sup>-151.0 Component 151.0 93.0 8 7 1 93.0 152.0 6 57.0 152.0 8.0

63.7

Acquisition Time (min)

63.8

77.0

5

4

3-

2-

63.6

77.0

57.0

63.8

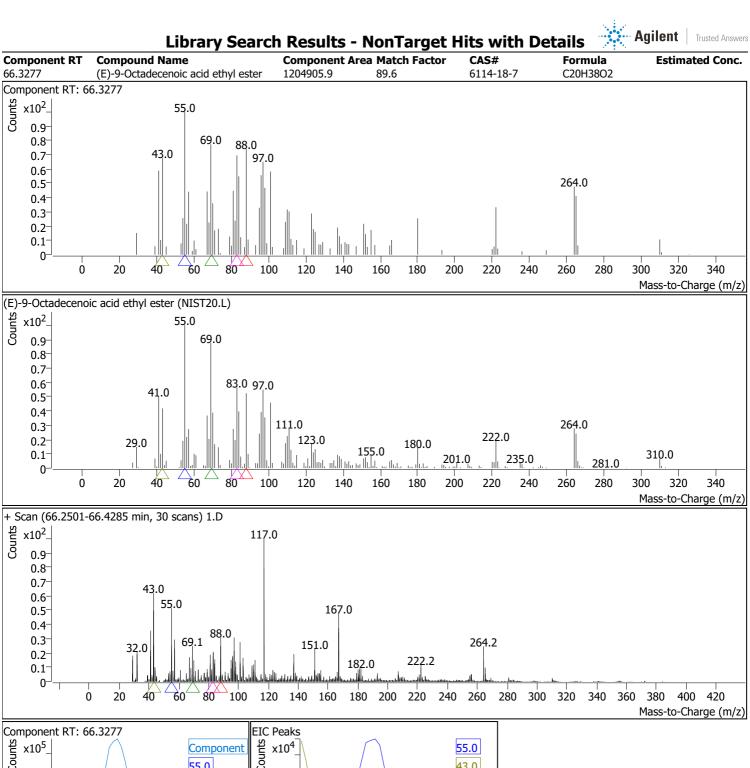
0.6

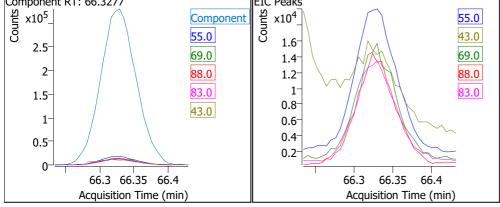
0.4

0.2

63.6

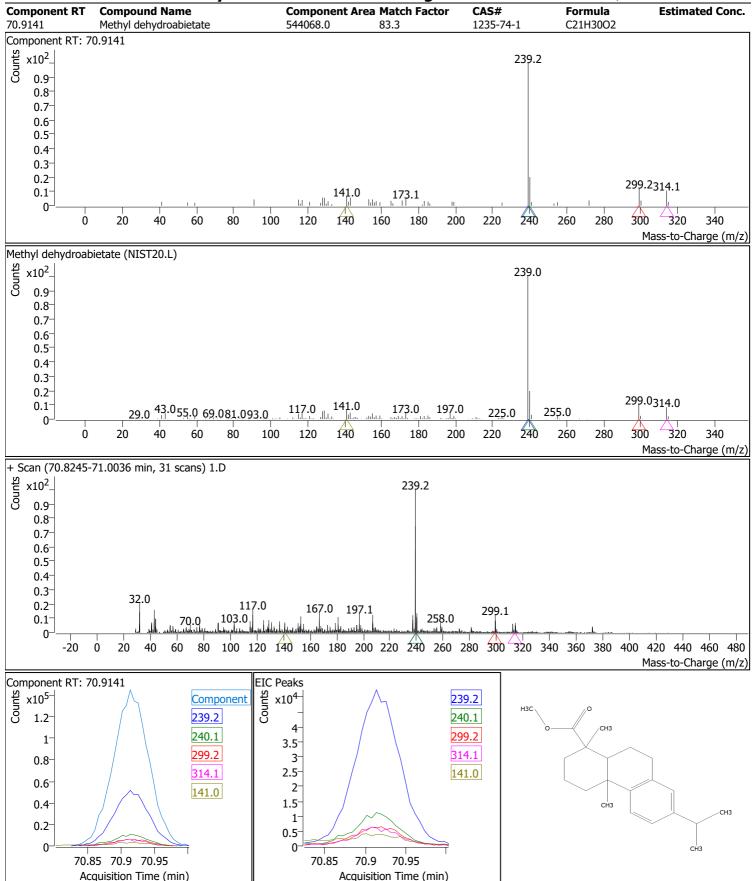
63.7





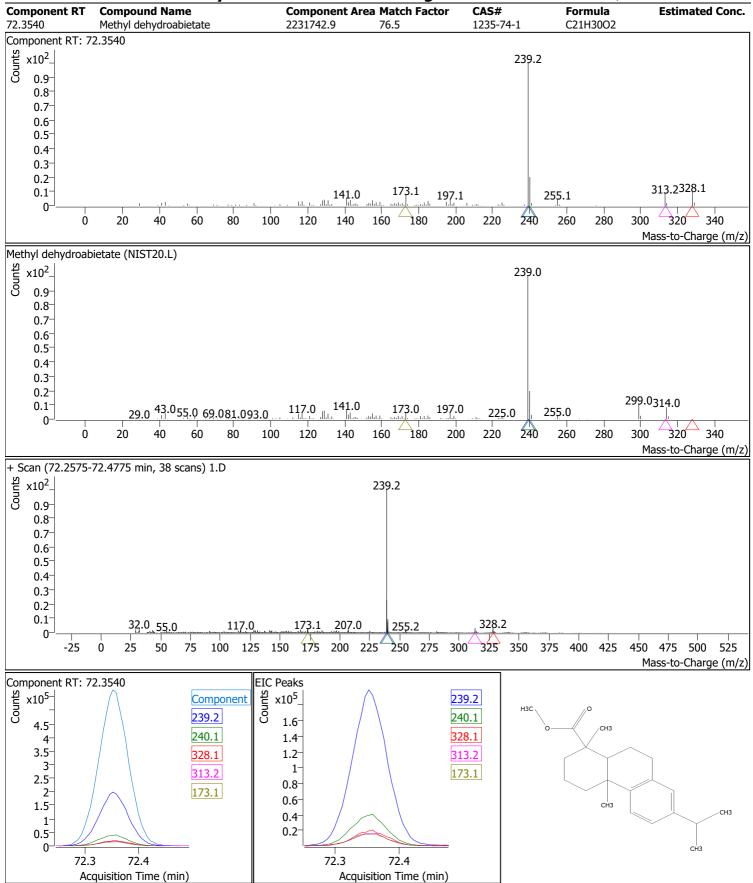




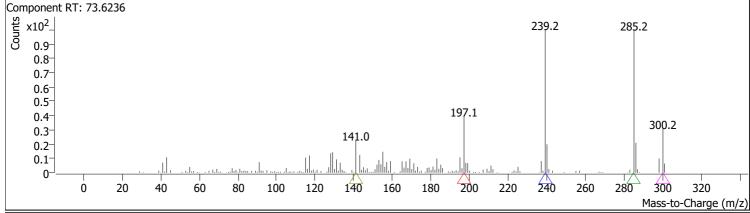


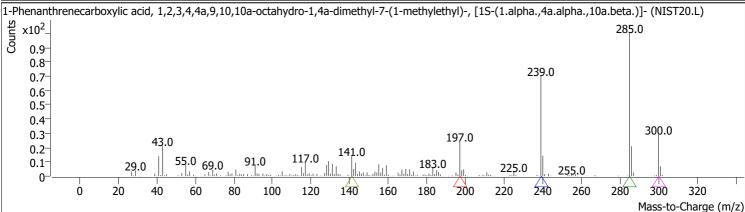


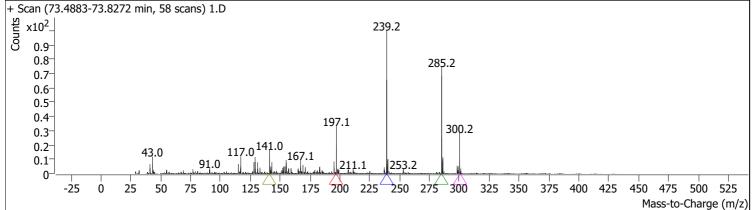


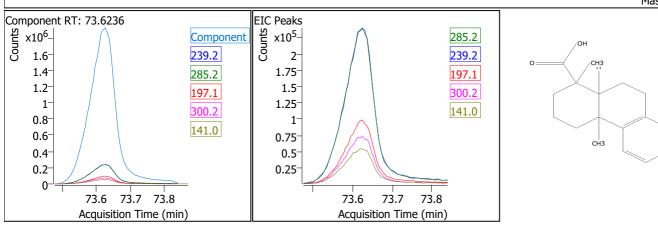


--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor Component RT** CAS# **Formula Estimated Conc.** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6236 10413462.8 93.3 5155-70-4 C20H28O2 Component RT: 73.6236 239.2 285.2









СНЗ

### --- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 75.3528 Cyclotetradecane 268574.4 295-17-0 C14H28 Component RT: 75.3528 v10<sup>2</sup> 0.9 83.0 97.0 57.0 69.0 43.0 0.8 $0.7^{-}$ 111.0 0.6 0.5 0.4 0.3 0.2 0.1 200 10 20 30 40 50 90 100 110 120 130 140 150 160 170 180 190 210 220 Mass-to-Charge (m/z) Cyclotetradecane (NIST20.L) Counts x10<sup>2</sup>\_ 0.9 55.0 41.0 0.8 69.0 0.7 83.0 0.6 0.5 97.0 0.4 29.0 0.3 111.0 0.2 125.0 0.1 139.0 168.0 196.0 10 20 30 40 50 70 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) + Scan (75.2743-75.4743 min, 34 scans) 1.D St x10<sup>2</sup> 0.9 207.0 55.1 0.8 167.0 0.7 43.0 0.6 0.5 280.0 97.1 137.0 181.0 $0.4^{-}$ 0.3 0.2 0.1 -25 $^{-1}$ 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 Mass-to-Charge (m/z) EIC Peaks Component RT: 75.3528 Counts Counts x10<sup>3</sup> 57.0 Component 97.0 55.0 5.5 83.0 97.0 3.5 4.5 57.0 83.0

4

3.5 3

2.5

1.5

75.3

75.4 Acquisition Time (min)

69.0

55.0

3

2.5

1.5

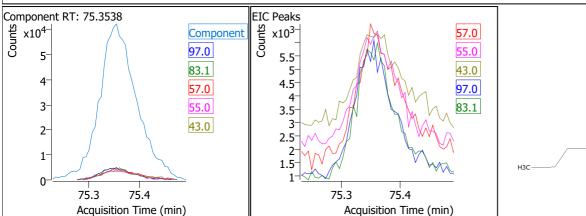
0.5

1

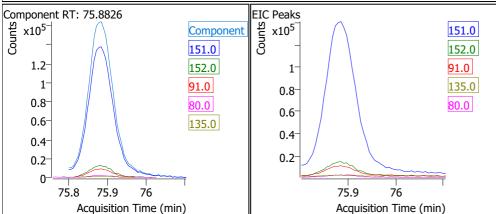
75.3

75.4

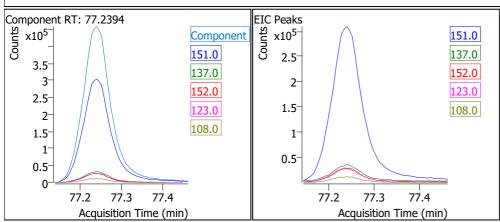
# --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 75.3538 Undecane, 4-cyclohexyl-316799.7 84.8 13151-79-6 C17H34 Component RT: 75.3538 St x10<sup>2</sup>. 83.1 97.0 57.0 43.0 69.1 0.8 $0.7^{-}$ 111.0 0.6 0.5 155.1 0.4 0.3 0.2 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 70 Mass-to-Charge (m/z) Undecane, 4-cyclohexyl- (NIST20.L) st x10<sup>2</sup> 0.9 83.0 57.0 0.8 0.7 43.0 0.6 0.5 71.0 97.0 0.4 0.3 29.0 0.2 0.1 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 20 60 70 Mass-to-Charge (m/z) + Scan (75.2743-75.4743 min, 34 scans) 1.D st x10<sup>2</sup> 0.9 207.0 55.1 0.8 167.0 $0.7^{-}$ 43.0 0.6 0.5 280.0 97.1 137.0 181.0 $0.4^{-}$ 0.3 0.2 0.1 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 -25 Mass-to-Charge (m/z) Component RT: 75.3538 **EIC Peaks** Si x10<sup>4</sup> Counts x10<sup>3</sup> Component 57.0 97.0 5 5.5

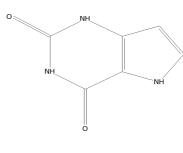


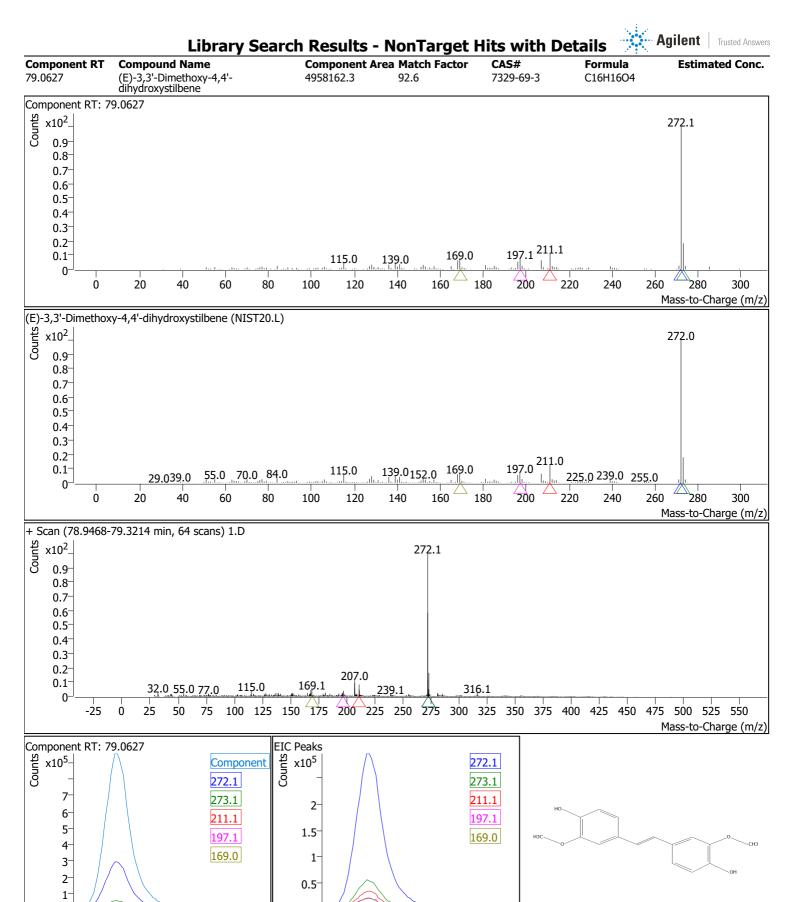
# · Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 75.8826 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-771065.1 92.0 65996-50-1 C6H5N3O2 dione Component RT: 75.8826 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 91.0 0.1 80.0 100 105 110 115 120 125 130 135 140 145 40 50 55 65 70 75 80 85 90 95 150 155 160 165 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 50 55 65 70 75 80 85 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 60 Mass-to-Charge (m/z) + Scan (75.8013-76.1046 min, 52 scans) 1.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 302.1 167.0 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 Mass-to-Charge (m/z) Component RT: 75.8826 **EIC Peaks** Counts Counts x10<sup>5</sup> x10<sup>5</sup> 151.0 Component 152.0 151.0 1.2 152.0 91.0 1



# --- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 77.2394 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-2195585.6 76.2 65996-50-1 C6H5N3O2 Component RT: 77.2394 x10<sup>2</sup>\_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 $0.2^{-}$ 123.0 137.0 0.1 94.0 108.0 77.0 50 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 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 50 55 65 70 75 80 85 90 60 Mass-to-Charge (m/z) + Scan (77.1405-77.4602 min, 54 scans) 1.D x10<sup>2</sup>. 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 402.1 0.1 207.0 288.1 167.0 100 125 <sup>1</sup>50 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 -25 Mass-to-Charge (m/z) Component RT: 77.2394 **EIC Peaks** Counts Counts x10<sup>5</sup> 151.0 x10<sup>5</sup> Component 137.0 151.0 2.5 3.5 137.0 152.0







79.1

79.2

Acquisition Time (min)

79.1

79.2