Library Search Results - NonTarget Hits with Details

Dil.

Acq. Operator



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

240502 data.uaf **Analysis File Name**

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

File Name 3.D **Sample Name** 3

Acq. Method File 240501 scan Acq. Date-Time 5/1/2024 4:38:24 PM

Instrument Name GCMSD

44.3314

44.4701

Dodecanoic acid, methyl ester

Homovanillyl alcohol

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

1

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

Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
6.9703	Furfural	98-01-1	C5H4O2	450296.3	96.2	
7.3009	1,3-Propanediol	504-63-2	C3H8O2	1097042.1	96.2	
11.5953	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	1432320.7	79.7	
11.5963	2-[2-[2-(2- Methoxyethoxy)ethoxy]ethoxy]ethyl acetate	1000351-91-3	C13H26O7	1419277.9	80.0	
12.4083	Oxalic acid, diallyl ester	1000309-22-9	C8H10O4	4813942.9	79.7	
12.4089	Butyrolactone	96-48-0	C4H6O2	14306389.9	96.8	
12.8072	Acetoin	513-86-0	C4H8O2	980571.3	78.5	
13.2868	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	1026911.4	77.9	
15.8010	2-Furancarboxaldehyde, 5-methyl-	620-02-0	C6H6O2	292153.9	94.0	
16.4097	3-Ethoxy-1,2-propanediol	1874-62-0	C5H12O3	280460.6	83.4	
16.8677	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	484655.2	82.5	
17.4316	Silane, diethoxydimethyl-	78-62-6	C6H16O2Si	815498.8	76.6	
17.9921	Phenol	108-95-2	C6H6O	284126.1	96.6	
18.5412	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	900370.5	93.1	
18.6498	Diisoamyl ether	544-01-4	C10H22O	3594468.1	98.2	
19.7522	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	794895.0	93.6	
20.0475	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	1152241.2	95.8	
21.1633	Glycerin	56-81-5	C3H8O3	2695574.7	76.0	
21.1033			C5H12O3		76.3	
	Ethane, 1,1,1-trimethoxy-	1445-45-0 110-88-3		1615697.7 5205202.6		
21.3031	1,3,5-Trioxane		C3H6O3		78.6	
22.4395	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	192827.7	89.2	
22.8814	1-Propanol, 2-(2-hydroxypropoxy)-	106-62-7	C6H14O3	492680.9	80.8	
23.0386	1-Octanol	111-87-5	C8H18O	4277181.9	98.7	
23.5674	Phenol, 2-methoxy-	90-05-1	C7H8O2	8960638.9	98.5	
23.7030	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	3684388.4	90.2	
24.7460	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	4939024.9	87.1	
27.7237	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	1502763.0	79.7	
27.7238	1,2-Ethanediol, diacetate	111-55-7	C6H10O4	637837.2	76.7	
27.7248	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	1444941.4	79.8	
29.1672	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	1459982.0	98.3	
30.4760	1,3-Dioxane	505-22-6	C4H8O2	680492.2	85.2	
30.7891	Catechol	120-80-9	C6H6O2	1740133.5	85.8	
31.6067	5-Hydroxymethylfurfural	67-47-0	C6H6O3	723080.5	87.8	
32.0998	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	195350.8	89.5	
32.3003	3,3-Diethoxy-1-propanol	16777-87-0	C7H16O3	380525.2	78.2	
32.3041	Formic acid, TMS derivative	18243-21-5	C4H10O2Si	215413.1	76.3	
32.5057	2-Methoxyresorcinol	29267-67-2	C7H8O3	629212.3	94.0	
33.3390	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	4883338.0	90.3	
35.0748	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	24535793.6	77.9	
35.0871	4-Acetoxy-3-methoxystyrene	46316-15-8	C11H12O3	616701.8	79.3	
35.3937	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	22270698.5	78.6	
36.2405	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	5157489.4	82.3	
36.8119	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	18547258.5	99.0	
37.4174	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	586509.4	86.9	
37.9313	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	214515.3	81.6	
38.6060	Propanoic acid, 2-methyl-, anhydride	97-72-3	C8H14O3	483369.2	79.8	
38.8525	Propanoic acid, anhydride	123-62-6	C6H10O3	696532.3	85.4	
38.8609	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	2392865.7	75.7	
39.0077	Vanillin	121-33-5	C8H8O3	9170224.2	98.8	
39.8299	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	7436730.3	75.2	
39.8317	Propanoic acid, anhydride	123-62-6	C6H10O3	2289362.5	80.5	
40.6059	Sulfurous acid, 2-ethylhexyl isobutyl ester	1000309-18-7	C12H26O3S	272587.5	77.0	
40.8891	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	1412791.2	92.4	
41.1108	Phenol, 2-methoxy-4-(2-propenyl)-, acetate	93-28-7	C12H14O3	505697.8	91.9	
41.1112	Phenol, 2-methoxy-4-(1-propenyl)-	97-54-1	C10H12O2	496387.4	91.5	
41.4500	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	208193.9	77.8	
41.8128	Propanoic acid, 2-methyl-, anhydride	97-72-3	C8H14O3	202471.7	76.4	
41.8918	Propanoic acid, 2-methyl-, anhydride	97-72-3	C8H14O3	267604.8	75.2	
42.6238	Apocynin	498-02-2	C9H10O3	5830449.8	99.2	
44.0198	1,3-Dioxolane-2,2-diethanol	5694-95-1	C7H14O4	16986372.7	77.3	
44.0571	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	2650223.5	94.6	
44.3094	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	11591458.7	95.8	
AA 221A	Dodocanoic acid mothyl octor	111_02_0	C13H36O3	8E34387 U	04.0	

Page 1 of 102

C13H26O2

C9H12O3

111-82-0

2380-78-1

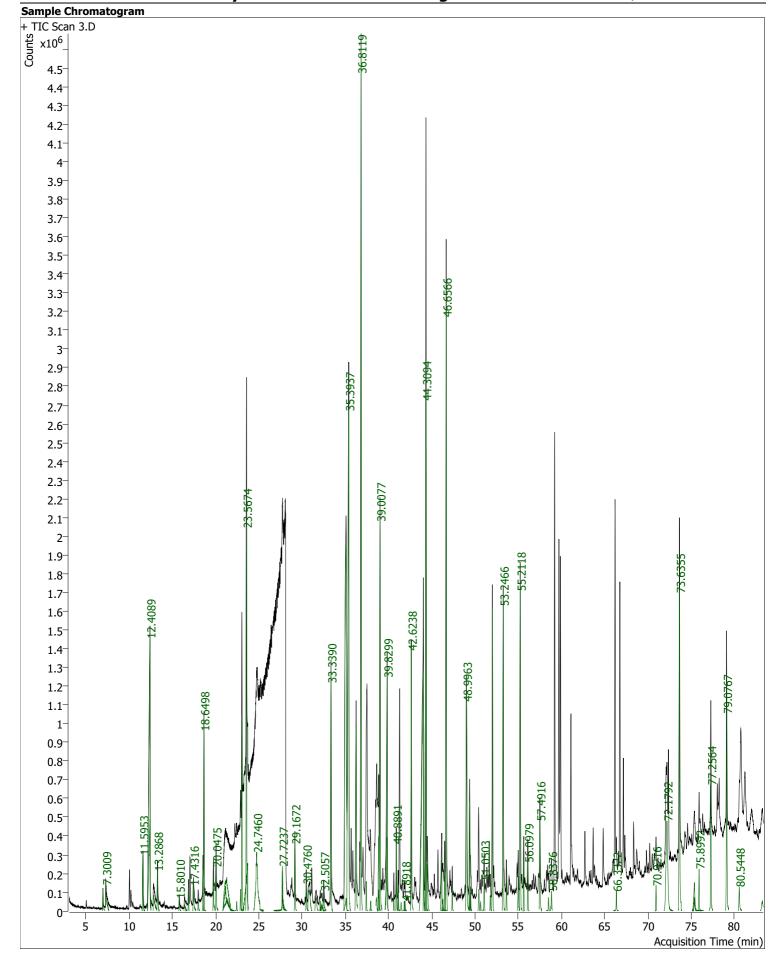
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8534287.0



Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc
46.1436	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	1666716.7	94.6	
46.2605	1,3-Dioxolane, 2-methyl-2-(4-methyl-3-methylenepentyl)-	66972-05-2	C11H20O2	538518.7	77.5	
46.4832	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	944602.6	88.2	
46.6566	Butyrovanillone	64142-23-0	C11H14O3	13234727.0	94.1	
47.3535	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	490621.7	88.1	
48.9963	Homovanillic acid	306-08-1	C9H10O4	7211167.7	90.9	
49.3647	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	2676765.8	97.0	
49.4184	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	425759.3	88.5	
49.4750	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	556119.4	85.4	
50.4463	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	644443.7	83.1	
50.6330	Phenylacetylformic acid, 4-hydroxy-3-methoxy-	1081-71-6	C10H10O5	191817.4	84.2	
51.0503	Butanoic acid, (tetrahydro-2-furanyl)methyl ester	2217-33-6	C9H16O3	732737.3	82.0	
51.7508	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-	4899-74-5	C10H12O4	324675.6	88.4	
52.0066	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	7085552.8	97.9	
53.2466	Syringylacetone	19037-58-2	C11H14O4	7069873.5	97.4	
3.6170	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	721353.6	83.0	
54.9886	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	926076.8	87.9	
55.2118	Butylsyringone	69271-91-6	C12H16O4	7647891.5	92.4	
55.6231	Acetyl syringic acid, ethyl ester	1000454-70-9	C13H16O6	887336.0	89.1	
56.0979	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	1055996.7	80.7	
57.4916	Dihydrosyringenin	20736-25-8	C11H16O4	2211690.8	93.6	
58.4886	Ethyl (E)-ferulate	28028-62-8	C12H14O4	300426.5	82.5	
58.8376	Isoelemicin	487-12-7	C12H16O3	499565.1	77.5	
6.3322	Ethyl Oleate	111-62-6	C20H38O2	428707.0	75.3	
70.9216	Methyl dehydroabietate	1235-74-1	C21H30O2	515632.6	77.6	
72.1792	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6988709.8	85.2	
73.6355	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	8879953.9	91.1	
75.3541	Octacosanol	557-61-9	C28H58O	1386569.7	79.3	
75.3660	Cyclopentane, 1-pentyl-2-propyl-	62199-51-3	C13H26	498755.1	75.3	
75.3663	1-Hexadecanol	36653-82-4	C16H34O	506670.6	75.2	
75.8992	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	960480.0	80.2	
77.2564	.alphaAmino-3'-hydroxy-4'-methoxyacetophenone	90765-44-9	C9H11NO3	3229251.6	77.0	
79.0767	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	5451907.2	92.1	
80.5448	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	775256.5	76.0	
83.2119	Carbonic acid, monoamide, N-(2-pentyl)-N- hexadecyl-, methyl ester	1000490-06-6	C23H47NO2	529240.2	76.1	



--- 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 6.9703 **Furfural** 450296.3 96.2 C5H4O2 Component RT: 6.9703 y x10² 0.9 95.0 0.8 0.7 0.6 39.0 0.5 0.4 0.3 0.2 67.0 82.0 0.1 53.0 10 15 20 25 30 35 45 50 60 65 70 75 80 85 90 100 105 Mass-to-Charge (m/z) Furfural (NIST20.L) St x10²_ 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 (6.9171-7.1481 min, 39 scans) 3.D st x10² 0.9 96.0 0.8 0.7 39.0 0.6 0.5 0.4^{-} 0.3 32.0 0.2 0.1 53.0 67.0 82.0 10 20 30 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: 6.9703 **EIC Peaks** Counts Counts 95.0 Component 95.0 96.0 0.8 2.5 96.0 39.0 0.7 2 38.0 0.6 39.0 0.5 37.0 38.0

7.1

Acquisition Time (min)

1.5

1-

0.5

37.0

7.1

Acquisition Time (min)

0.4

0.3

0.2

0.1 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 7.3009 1,3-Propanediol 1097042.1 96.2 C3H8O2 Component RT: 7.3009 y x10² 0.9 57.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 43.0 0.2 39.0 0.1 15 25 55 65 70 75 5 10 20 30 35 40 50 80 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10²_ 0.9 28.0 31.0 0.8 0.7 57.0 0.6 0.5 0.4 0.3 43.0 0.2 15.0 0.1 39.0 55.0 18.0 75.0 55 70 5 10 15 20 25 30 35 40 45 50 65 75 80 Mass-to-Charge (m/z) + Scan (7.2612-7.6594 min, 67 scans) 3.D st x10² 0.9 57.0 31.0 0.8 0.7 0.6 0.5 0.4^{-} 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) Component RT: 7.3009 **EIC Peaks** Counts Counts x10⁵ x10⁴ 57.0 Component 57.0 58.0 3 1 58.0 31.0 2.5 43.0 31.0 0.8 2

43.0

45.0

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Acquisition Time (min)

7.6

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7.6

Acquisition Time (min)

7.8

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 11.5953 4744-08-5 Propane, 1,1-diethoxy-1432320.7 79.7 C7H16O2 Component RT: 11.5953 v10² 0.9 103.0 43.0 87.0 0.8 0.7 0.6 57.0 31.0 0.5 0.4 0.3 0.2 117.0 0.1 0 40² 30 70 130 10 20 50 60 100 110 120 140 Mass-to-Charge (m/z) Propane, 1,1-diethoxy- (NIST20.L) st x10² 0.9 59.0 0.8 87.0 0.7 47.0 0.6 0.5 103.0 31.0 0.4 75.0 0.3 0.2 41.0 0.1 15.0 78.0 70.0 131.0 130 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.5071-11.8045 min, 50 scans) 3.D St x10² 0.9 87.0 0.8 43.0 103.0 0.7 31.0 0.6 0.5 57.0 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: 11.5953 EIC Peaks Counts Counts $x10^{4}$ 103.0 Component 103.0 43.0 4 3.5 43.0 87.0



11.6

11.7

Acquisition Time (min)

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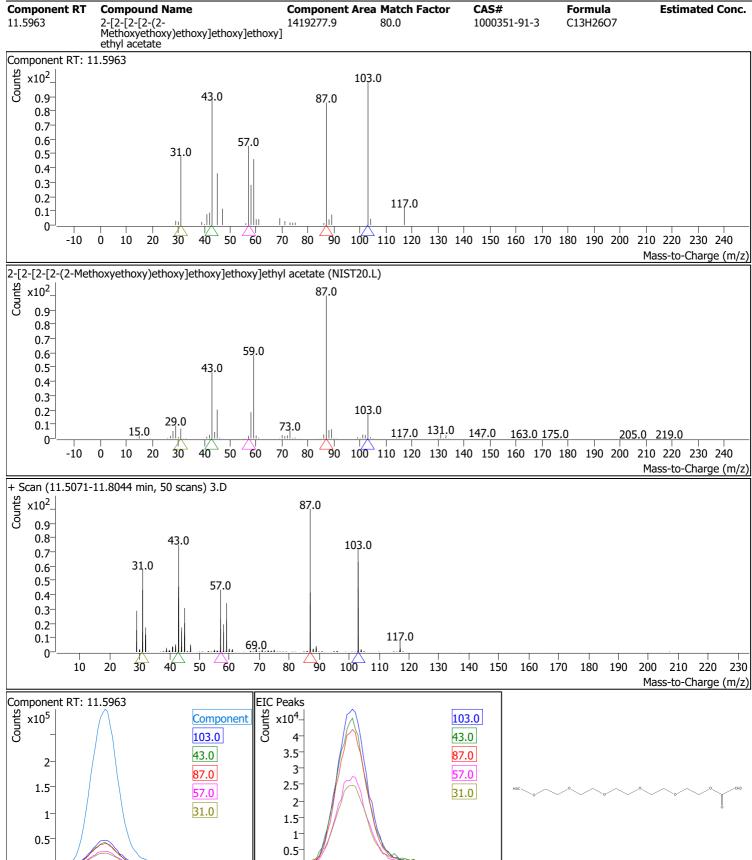
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Acquisition Time (min)

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Library Search Results - NonTarget Hits with Details



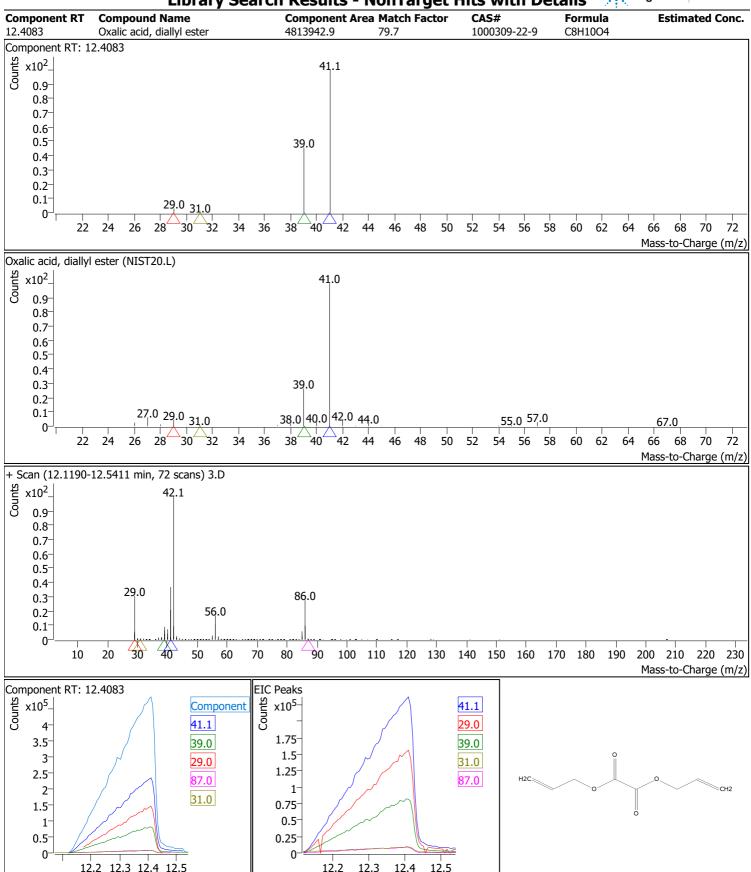
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Acquisition Time (min)

11.6

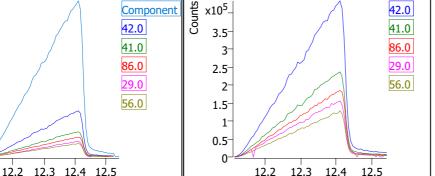
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Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 96-48-0 12.4089 Butyrolactone 14306389.9 96.8 C4H6O2 Component RT: 12.4089 v10² 0.9 42.0 0.8 0.7^{-} 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 0.1 70 75 10 15 20 25 30 35 40 50 55 60 65 80 85 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) st x10²_ 0.9-42.0 28.0 0.8 0.7 0.6 0.5 0.4 56.0 86.0 0.3 0.2 39.0 0.1 15.0_{18.0} 53.0 67.0 71.0 83.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.1139-12.5233 min, 69 scans) 3.D St x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 29.0 86.0 0.3 56.0 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) EIC Peaks Component RT: 12.4089 Counts stuno x10⁶ x10⁵-42.0 Component 42.0 41.0 1.2 3.5 41.0 86.0 3 1 0.8

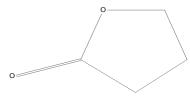


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Acquisition Time (min)



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 513-86-0 12.8072 Acetoin 980571.3 78.5 C4H8O2 Component RT: 12.8072 y x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 0.1 30.0 30 25 40 65 70 75 80 85 90 95 20 Mass-to-Charge (m/z) Acetoin (NIST20.L) St x10²_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 20 25 35 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.7736-13.2190 min, 75 scans) 3.D St x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 29.0 0.1 102.0 87.0 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: 12.8072 EIC Peaks Counts Counts x10⁴ x10⁴ 45.0 Component 45.0 43.0 6 43.0 46.0 5

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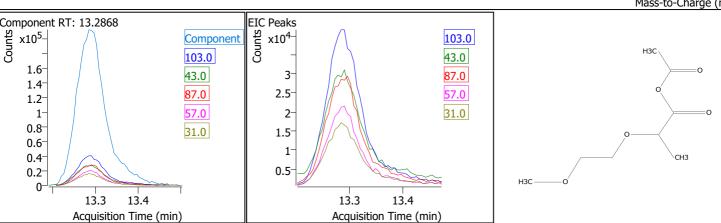
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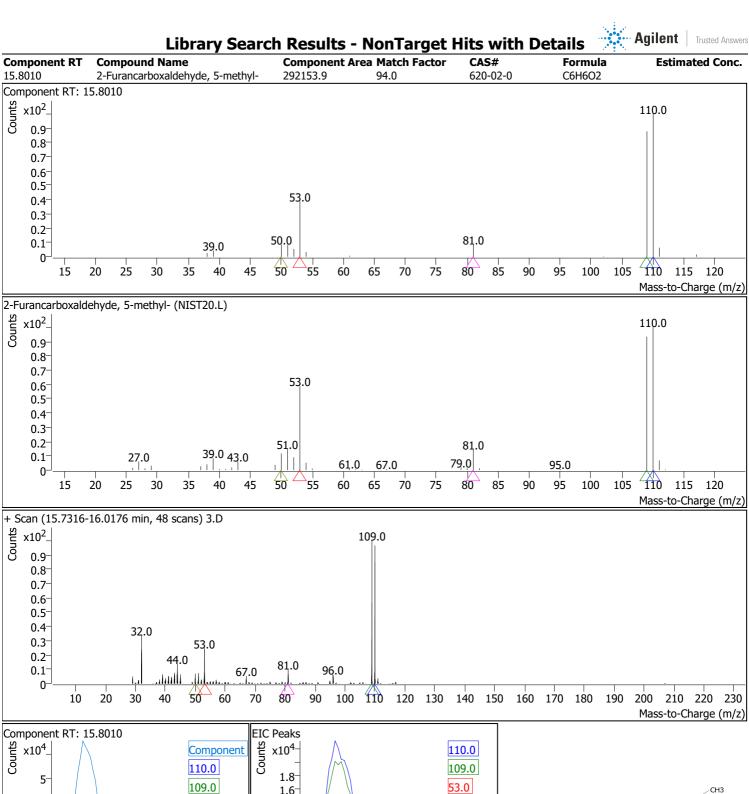
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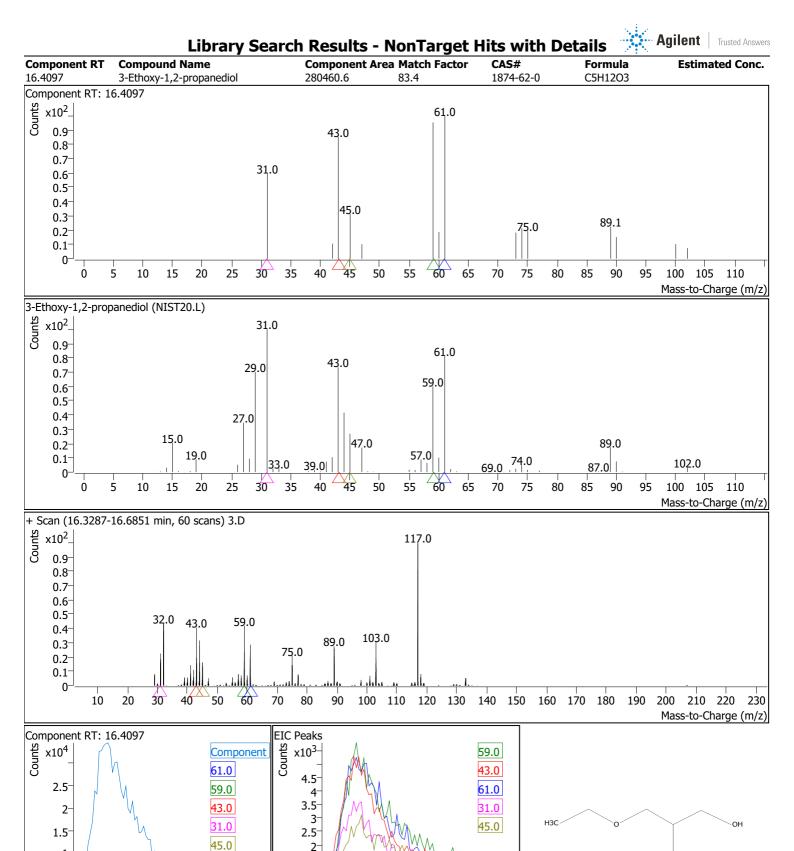
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--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-(2-methoxyethoxy)propanoic acid, O-acetyl-13.2868 1026911.4 77.9 1000506-61-7 C8H14O5 Component RT: 13.2868 x10². 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 0-30 140 0 10 20 40 50 70 80 90 100 110 120 130 150 160 Mass-to-Charge (m/z) 2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L) $x10^{2}$ 43.0 0.9 0.8 59.0 0.7 0.6 0.5 0.4 103.0 0.3 0.2 29.0 0.1 15.0 87.0 73.0 117.0 130.0 147.0 0 30 40 90 130 0 10 20 50 60 70 80 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (13.2037-13.4747 min, 46 scans) 3.D x10². 0.9 103.0 0.8 0.7 0.6 0.5 87.1 29.0 0.4 57.0 0.3 0.2 0.1 117.0 0 30 40 90 200 210 220 230 10 20 50 60 70 80 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) EIC Peaks Component RT: 13.2868 x10⁵x10⁴ 103.0 Component









16.5

Acquisition Time (min)

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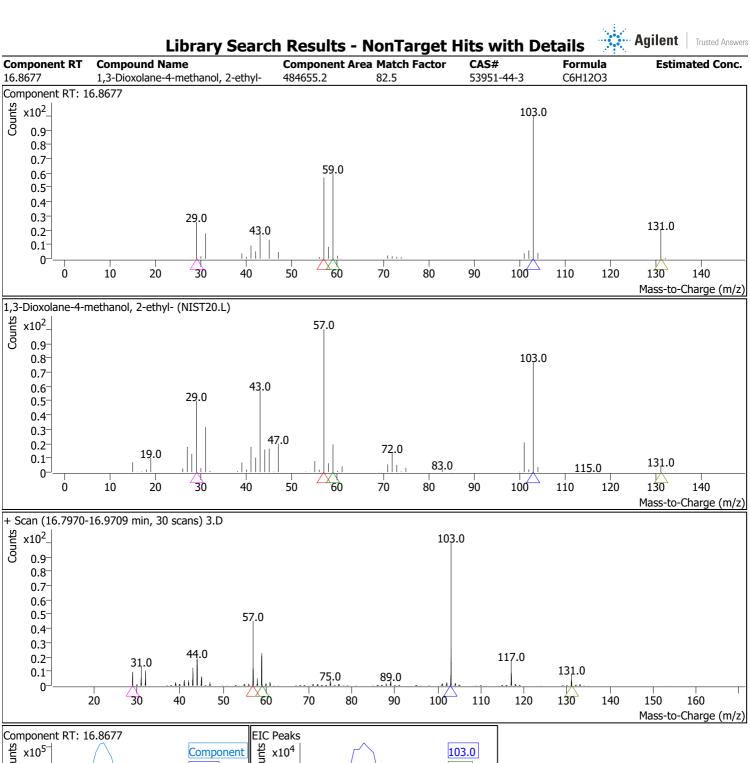
16.5

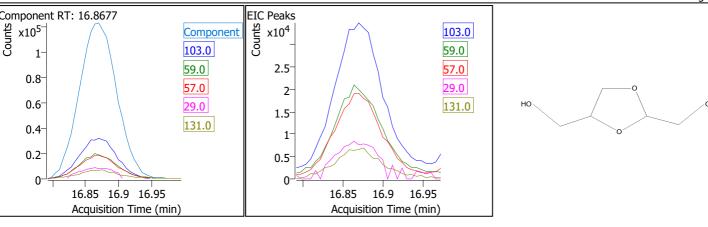
Acquisition Time (min)

16.6

0.5

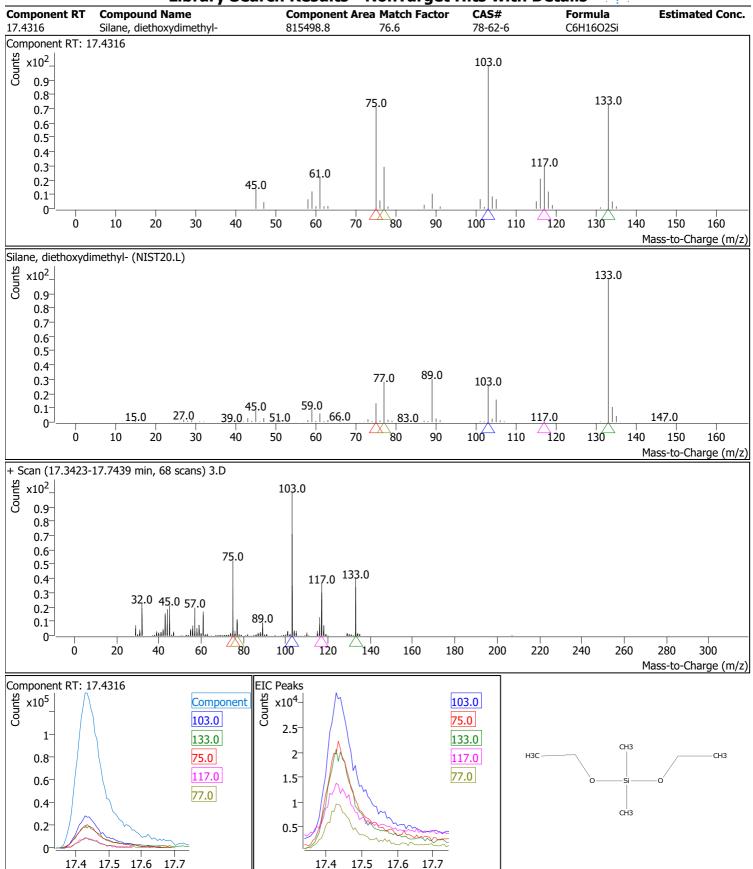
ОН





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.** 108-95-2 C6H6O 17.9921 Phenol 284126.1 96.6 Component RT: 17.9921 v10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 63.0 55.0 50.0 25 40 55 75 85 95 20 30 35 45 50 60 65 70 80 90 100 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10²_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 (17.9290-18.1779 min, 41 scans) 3.D St x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 0.3 61.0 43.0 32.0 0.2 103.1 117.0 75.0 0.1 132.9 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: 17.9921 Counts Counts x10⁴ x10⁴ 94.0 Component 94.0 66.0 5 2.25 66.0 65.0 1.75 39.0 65.0 1.5

18

18.1

Acquisition Time (min)

40.0

3

2

1-

39.0

40.0

18.1

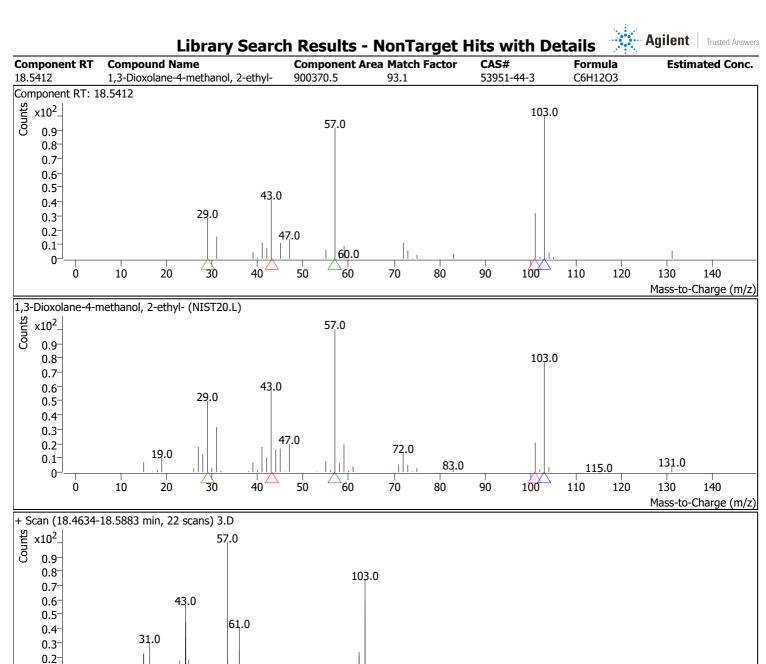
Acquisition Time (min)

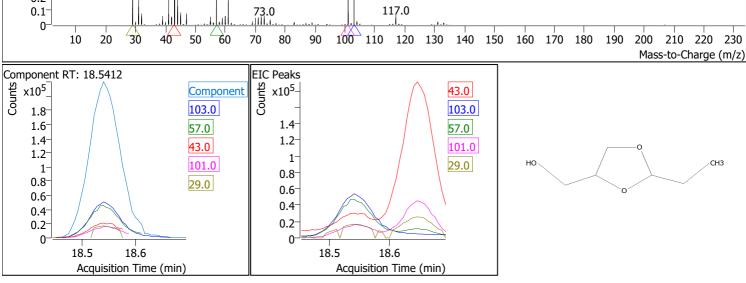
1.25

0.75 · 0.5

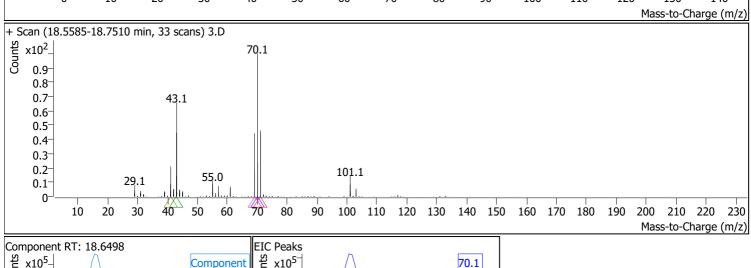
0.25

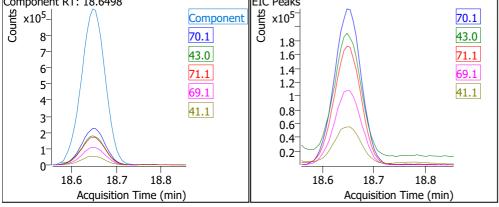
1

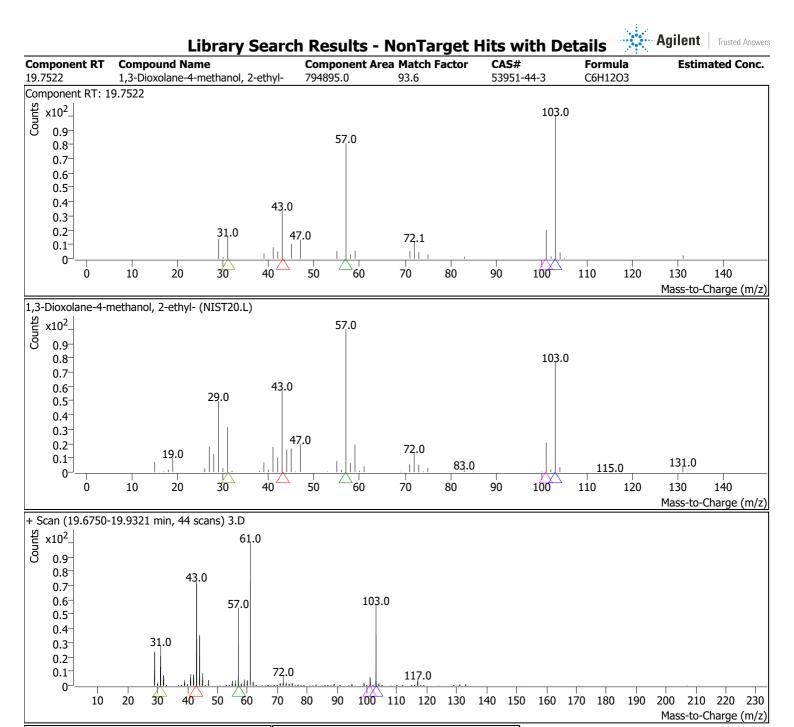




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 544-01-4 18.6498 Diisoamyl ether 3594468.1 98.2 C10H22O Component RT: 18.6498 v10² 0.9 70.1 43.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 55.0 101.0 0.2 29.0 0.1 100 10 20 30 40 50 60 80 90 110 120 130 140 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) St x10² 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 + Scan (18.5585-18.7510 min, 33 scans) 3.D









19.8

Acquisition Time (min)

19.9

103.0

57.0

43.0

31.0

101.0

EIC Peaks

3.5

3

2

1

19.7

2.5

1.5

0.5

Counts

Component 103.0

57.0

43.0

101.0

31.0

Component RT: 19.7522

x10⁵ 1.4

1.2

0.8

0.6

0.4

0.2

19.7

19.8

Acquisition Time (min)

19.9

1

--- 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 20.0475 2-Cyclopenten-1-one, 2-hydroxy-3-1152241.2 95.8 C6H8O2 methyl-Component RT: 20.0475 x10² 112.0 0.9 8.0 0.7 0.6 0.5 69.1 0.4 55.0 0.3 41.1 83.1 0.2^{-} 43.0 0.1 29.0 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 (19.9476-20.3007 min, 60 scans) 3.D st x10² 43.0 0.8 0.7^{-} 0.6 0.5 112.0 0.4 0.3 31.0 0.2 69.0 84.1 103.0 0.1 0 Ó 20 40 60 100 200 260 80 120 140 160 180 220 240 280 300 Mass-to-Charge (m/z) Component RT: 20.0475 EIC Peaks Counts Counts x10⁵x10⁴-112.0 Component 112.0 55.0 1.8 4.5 69.1 69.1 1.6 1.4 55.0 3.5 83.1 1.2 3 83.1 41.1 нзс 2.5 1

41.1

2⁻ 1.5⁻

1

20

20.1

20.2

Acquisition Time (min)

0.5

0.8

0.6⁻ 0.4⁻

0.2

20

20.1

20.2

Acquisition Time (min)

ОН

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2695574.7 21.1633 Glycerin 76.0 56-81-5 C3H8O3 Component RT: 21.1633 v10² 0.9 61.0 0.8 43.0 0.7 0.6 0.5 0.4 0.3 29.0 0.2 0.1 47.0 91.0 __30 90 10 15 20 25 35 50 55 65 75 85 95 100 Mass-to-Charge (m/z) Glycerin (NIST20.L) x10²_ 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 85 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 100 Mass-to-Charge (m/z) + Scan (21.0856-21.2164 min, 22 scans) 3.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 89.0 31.0 0.2 0.1 55.0 117.0 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: 21.1633 **EIC Peaks** Counts Counts x10⁵-Component 61.0 61.0 43.0 1 43.0 0.8 0.8 29.0 29.0



21.4

Acquisition Time (min)

21.2

21.6

31.0

60.0

21.2 21.4 21.6

Acquisition Time (min)

0.6

0.4

0.2

0.6

0.4

0.2

60.0

ОН

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1445-45-0 21.2320 Ethane, 1,1,1-trimethoxy-1615697.7 76.3 C5H12O3 Component RT: 21.2320 v10² 0.9 43.0 89.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 15 20 25 35 40 55 60 65 70 80 95 100 105 110 115 Mass-to-Charge (m/z) Ethane, 1,1,1-trimethoxy- (NIST20.L) st x10² 0.9 43.0 0.8 0.7 89.0 0.6 0.5 0.4 0.3 0.2 105.0 29.0 0.1 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (20.8122-22.1427 min, 223 scans) 3.D St x10² 0.9 61.0 0.8 0.7 0.6 43.0 0.5 0.4^{-} 0.3 0.2 31.0 89.0 0.1 117.0 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.2320 **EIC Peaks** Counts Counts x10⁴ Component 43.0 43.0 89.0 H3C 6 89.0 3.5 5 90.0 3

21.5

Acquisition Time (min)

22

4

3

2

1

21

2.5

2⁻ 1.5⁻

1

21

21.5

Acquisition Time (min)

22

0.5

CH3

H3C

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 21.3031 1,3,5-Trioxane 5205202.6 78.6 110-88-3 C3H6O3 Component RT: 21.3031 v10² 0.9 61.0 0.8 0.7 0.6 89.1 0.5 0.4 0.3 0.2 43.0 0.1 31.0 57.0 85.0 0 __90 25 30 55 10 15 20 35 40 60 65 75 80 85 95 100 Mass-to-Charge (m/z) 1,3,5-Trioxane (NIST20.L) Counts x10²_ 0.9 31.0 0.8 61.0 89.0 0.7 0.6 0.5 29.0 0.4 0.3 0.2 0.1 44.0 14.0 56.0 90 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (21.4437-21.5494 min, 18 scans) 3.D st x10² 0.9 0.8 0.7 0.6 0.5 43.0 0.4^{-} 0.3 0.2 31.0 89.0 0.1 117.0 90 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) Component RT: 21.3031 **EIC Peaks** Counts Counts x10⁵-61.0 Component 61.0 w^w 43.0 1.4 89.1 89.1 1.2 0.8 43.0 31.0 1

21.25 21.5 21.75

Acquisition Time (min)

60.0

31.0

21.5

Acquisition Time (min)

0.8

0.6

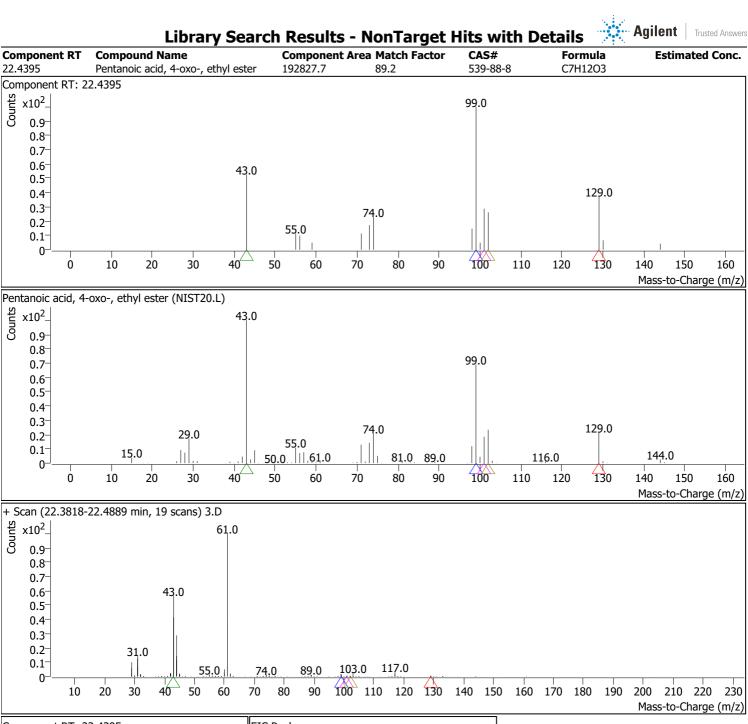
0.4

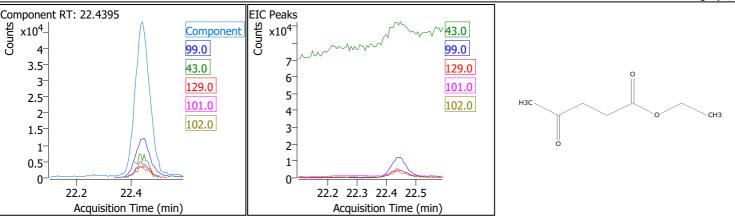
0.2

21

0.6

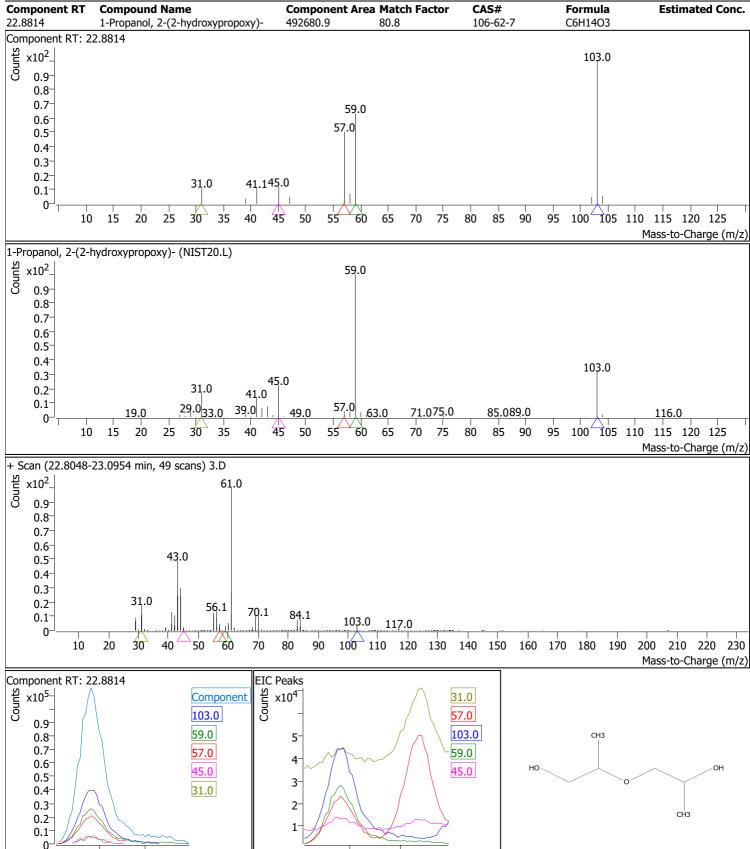
0.4











22.9

23

Acquisition Time (min)

22.9

23

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0386 1-Octanol 4277181.9 98.7 111-87-5 C8H18O Component RT: 23.0386 v10² 0.9 56.0 70.1 0.8 41.1 0.7 84.1 0.6 0.5 0.4 0.3 0.2 0.1 55 100 105 110 115 120 125 130 135 140 45 65 70 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10²_ 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 (22.9527-23.1667 min, 37 scans) 3.D St x10²_ 0.9 0.8 0.7 0.6 43.0 0.5 0.4^{-} 0.3 31.0 0.2 56.1 70.1 84.1 0.1 103.0 117.0 0 10 20 30 40 50 60 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: 23.0386 Counts Counts x10⁵ 56.0 Component 56.0 55.0 0.8 1 55.0 70.1 0.7 0.8 70.1 69.1 0.6

23.1

Acquisition Time (min)

23.2

41.1

 0.5^{-}

 0.4^{-}

0.3⁻ 0.2⁻

0.1

69.1

41.1

23.1

Acquisition Time (min)

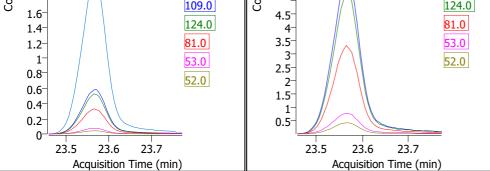
23

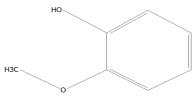
23.2

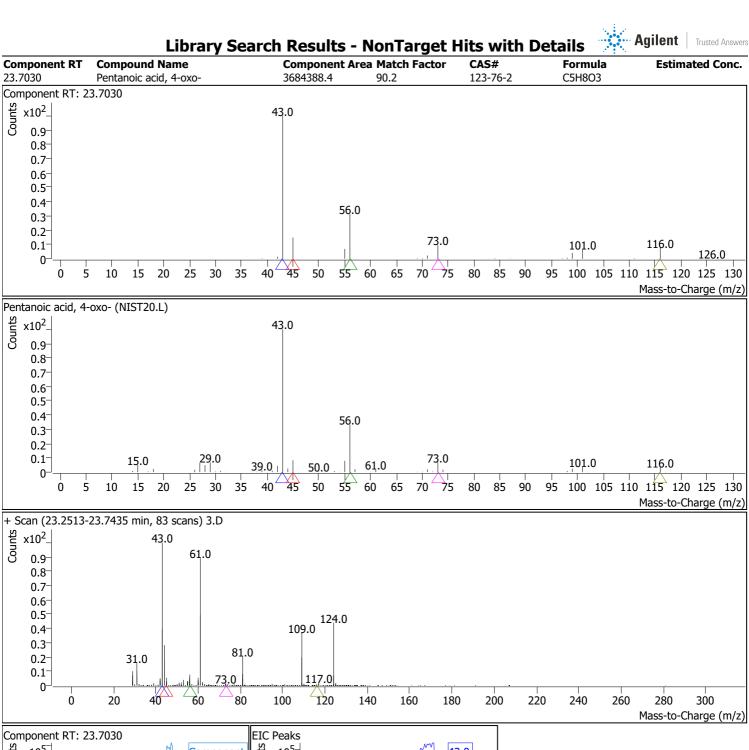
 0.6^{-}

0.4

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 8960638.9 90-05-1 23.5674 Phenol, 2-methoxy-98.5 C7H8O2 Component RT: 23.5674 v10² 0.9 109.0 124.0 0.8 0.7 0.6 81.0 0.5 0.4 0.3 0.2 53.0 0.1 29.0 39.0 80 110 50 10 20 30 40 60 70 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) St x10²_ 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 77.0 95.0 15.0 110 50 10 20 30 40 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4581-23.7732 min, 54 scans) 3.D st x10² 0.9 43.0 0.8 61.0 0.7 0.6 109.0 0.5 0.4^{-} 81.0 0.3 0.2 31.0 0.1 117.0 73.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.5674 Counts Counts x10⁵-109.0 Component 109.0 124.0 1.6 4.5 124.0 81.0 1.4

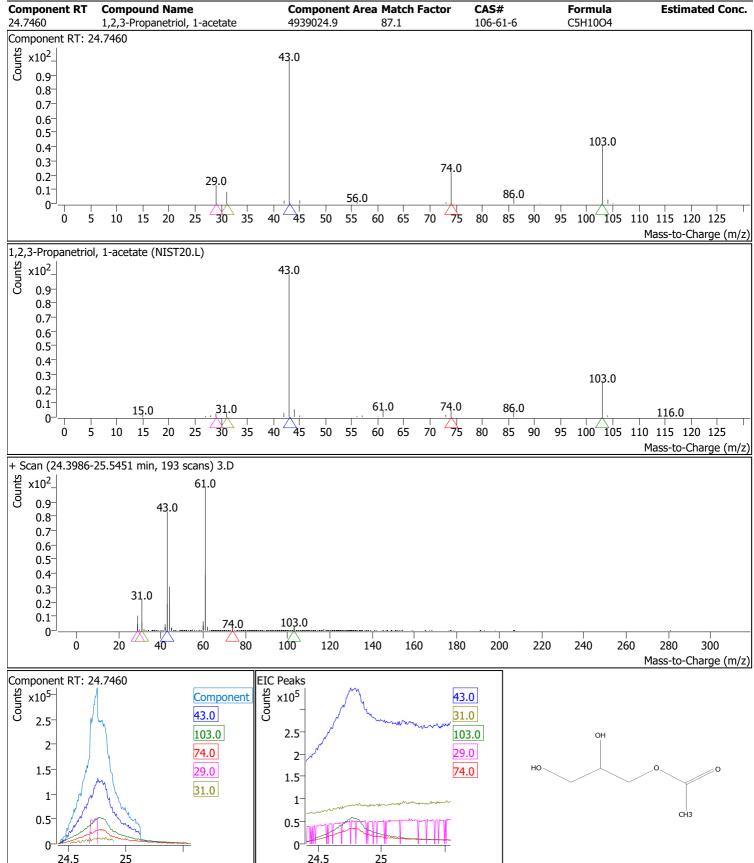






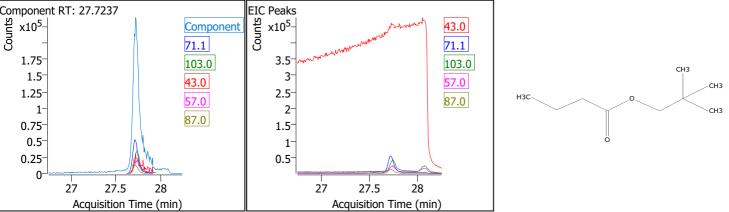


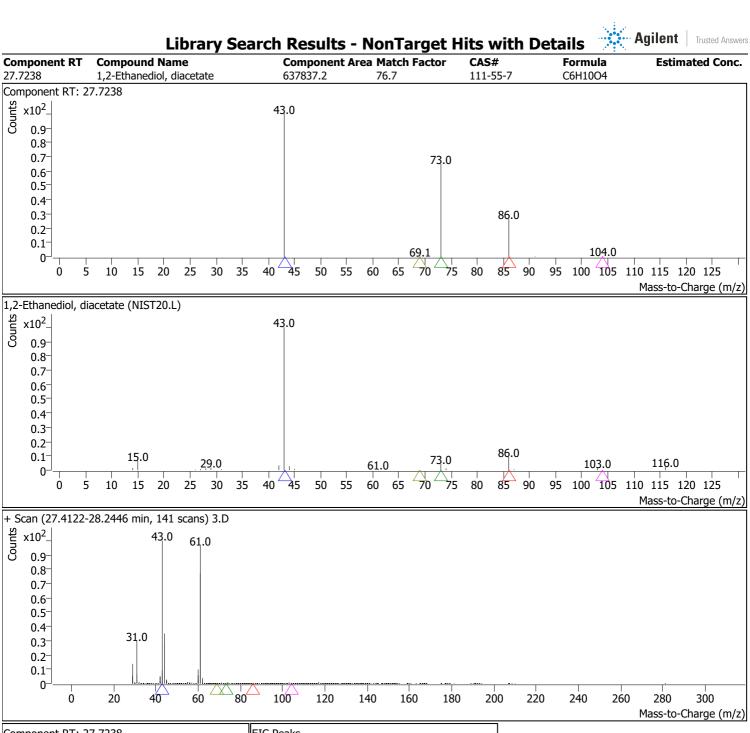


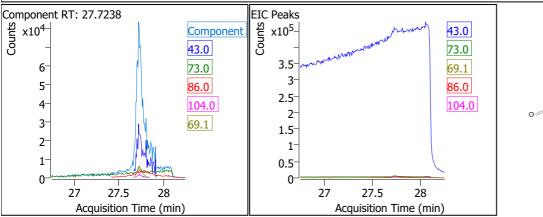


Acquisition Time (min)

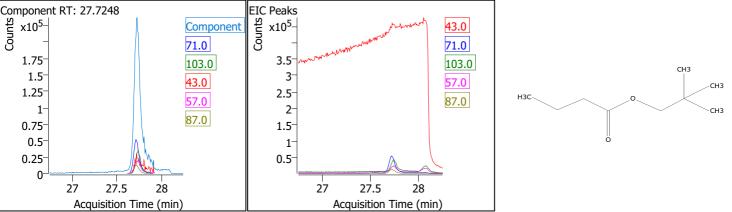
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7237 Butanoic acid, 2,2-dimethylpropyl 1502763.0 79.7 23361-69-5 C9H18O2 ester Component RT: 27.7237 x10²_ 71.1 0.9 8.0 0.7 103.0 0.6 43.0 0.5 0.4 57.0 0.3 87.0 0.2^{-} 31.0 0.1 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 _{93.0} 36.0 0.1 27.0 49.0 130.0 143.0 66.0 0 90 100 10 20 30 40 50 60 70 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6490-27.7987 min, 26 scans) 3.D x10². 61.0 0.9 0.8 0.7 0.6 0.5 0.4 31.0 0.3 0.2 0.1 103.0 0 70 100 110 120 130 190 200 210 220 230 10 20 30 40 50 60 80 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 27.7237 **EIC Peaks** Counts Counts x10⁵x10⁵. 43.0 Component 71.1 71.1

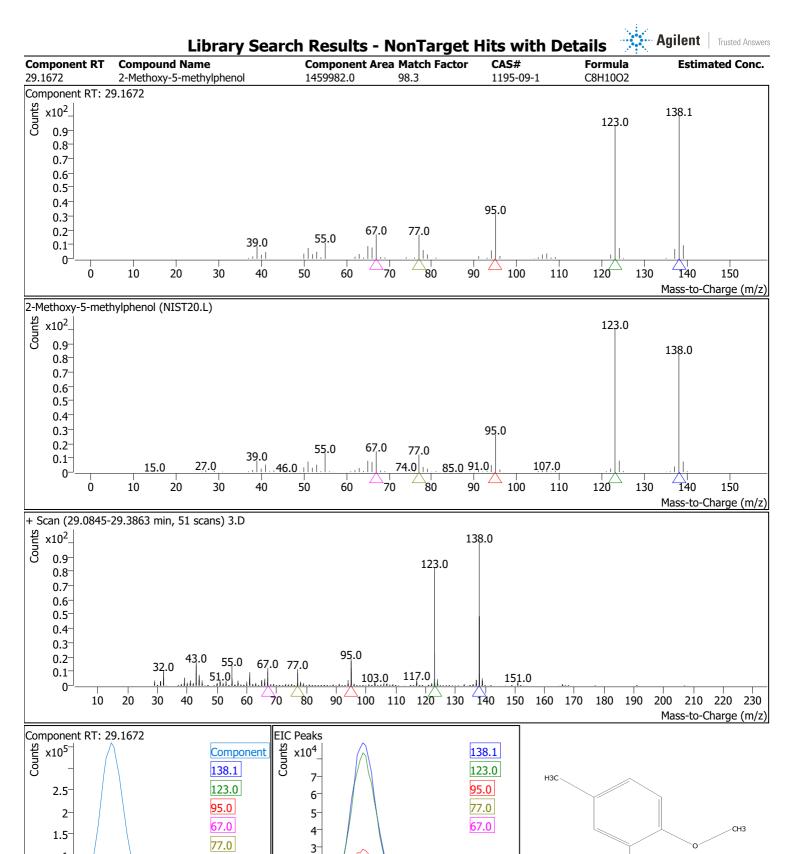






--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.7248 Butanoic acid, 2,2-dimethylpropyl 1444941.4 79.8 23361-69-5 C9H18O2 Component RT: 27.7248 x10²_ 71.0 0.9 8.0 0.7 103.0 0.6 43.0 0.5 57.0 0.4 0.3 87.0 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) x10². 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 _{93.0} 36.0 0.1 27.0 49.0 130.0 143.0 66.0. 0 90 100 10 20 30 40 50 60 70 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6498-27.7987 min, 26 scans) 3.D x10². 61.0 0.9 0.8 0.7 0.6 0.5 0.4 31.0 0.3 0.2 0.1 103.0 0 70 100 110 120 130 190 200 210 220 230 10 20 30 40 50 60 80 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 27.7248 **EIC Peaks** x10⁵x10^{5.} 43.0 Component





29.2

29.3 Acquisition Time (min)

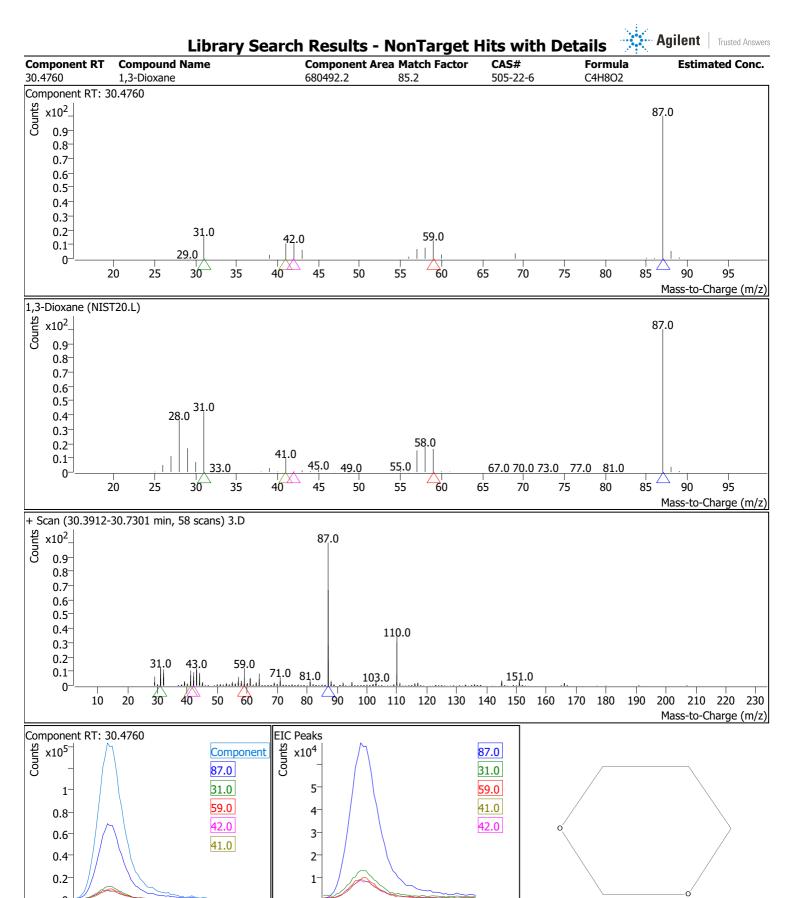
2-

1-

29.2

29.3

Acquisition Time (min)



30.5

30.6

Acquisition Time (min)

30.7

30.5

30.6

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.** 120-80-9 30.7891 Catechol 1740133.5 85.8 C6H6O2 Component RT: 30.7891 y x10² 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 0.1 123.0 100 105 110 115 120 125 10 35 55 80 85 90 Mass-to-Charge (m/z) Catechol (NIST20.L) st x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 65 10 15 25 30 35 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.6266-31.0749 min, 76 scans) 3.D St x10²_ 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 64.0 0.2 43.0 32.0 92.0 103.0 0.1 81.0 69.1 0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 30.7891 Counts 0.9x10⁴-110.0 Component 110.0 81.0 3.5 0.9 0.8 64.0 3 64.0 0.7 63.0 2.5 63.0 0.6



30.7 30.8 30.9

31

Acquisition Time (min)

81.0

92.0

0.5

0.3

0.2

0.1

30.8

31

Acquisition Time (min)

2-

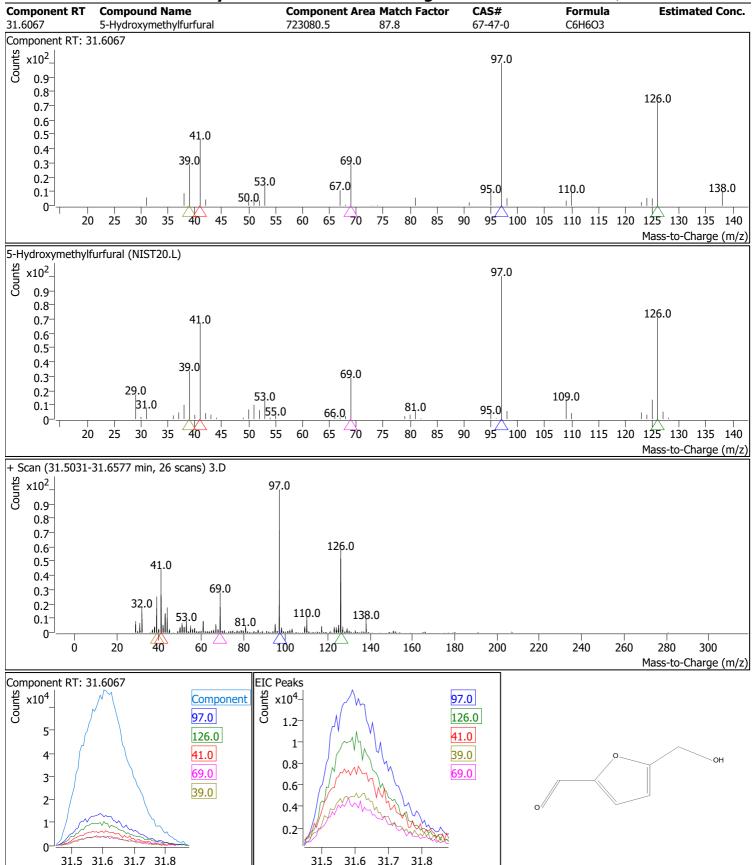
1.5

0.5

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.** 1450-72-2 32.0998 Ethanone, 1-(2-hydroxy-5-195350.8 89.5 C9H10O2 methylphenyl)-Component RT: 32.0998 x10²_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 0.3 77.0 0.2^{-} 0.1 107.0 51.0 131.0 0-80 150 0 10 20 30 40 50 60 70 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 150.0 0.5 0.4 0.3 107.0 0.2 77.0 43.0 51.0 0.1 27.0 63.0 131.0 85.091.0 121.0 0 130 150 10 20 30 40 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0268-32.2166 min, 32 scans) 3.D x10². 135.0 0.9 0.8 43.0 0.7 0.6 150.0 0.5 32.0 0.4 103.0 0.3 77.0 55.0 0.2 96.0 39.0 0.1 عاليطاناستمات ماميستوناياك 120 130 140 150 160 170 180 190 200 210 220 230 10 20 30 40 50 60 70 80 90 100 110 Mass-to-Charge (m/z) Component RT: 32.0998 **EIC Peaks** Counts Counts x10⁴ x10⁴-135.0 Component НО 150.0 135.0 4 1.8 150.0 77.0 3.5 1.6 **Н3С** 1.4 77.0 136.0 3-1.2 2.5 136.0 79.0



32.1

32.2

Acquisition Time (min)

2

1

32.1

32.2

Acquisition Time (min)

1.5

0.5

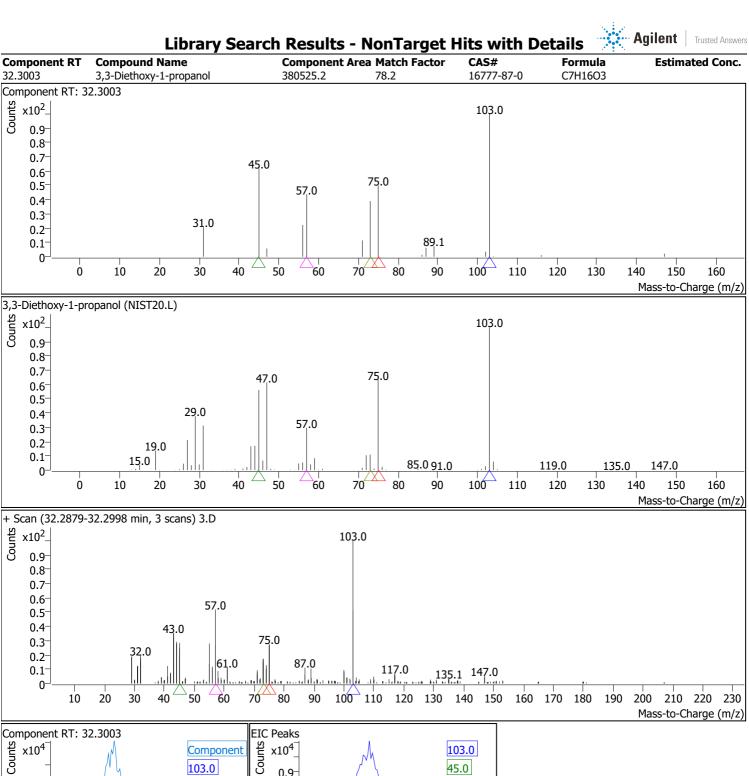
79.0

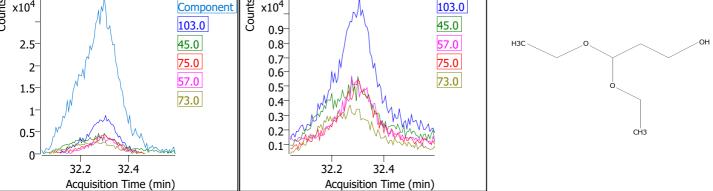
0.8

0.6

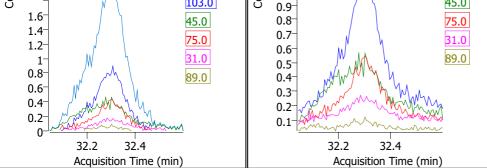
0.4

0.2





··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 18243-21-5 32.3041 Formic acid, TMS derivative 215413.1 76.3 C4H10O2Si Component RT: 32.3041 v10² 0.9 103.0 0.8 0.7^{-} 45.0 0.6 75.0 0.5 0.4 0.3 31.0 0.2 89.0 0.1 90 100 105 10 15 30 35 55 65 70 110 115 Mass-to-Charge (m/z) Formic acid, TMS derivative (NIST20.L) Counts x10²_ 0.9 103.0 75.0 0.8 0.7 0.6 0.5 0.4 45.0 0.3 0.2 73.0 0.1 15.0 45 90 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (32.2879-32.2998 min, 3 scans) 3.D st x10² 0.9 103.0 0.8 0.7 0.6 57.0 0.5° 0.4^{-} 43.0 75.0 0.3 0.2 61.0 87.0 117.0 0.1 70 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 32.3041 **EIC Peaks** Counts Counts x10⁴ 103.0 Component 103.0 45.0 0.9 1.6 CH3 45.0 0.8 75.0 1.4 0.7



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2-Methoxyresorcinol 32.5057 629212.3 94.0 29267-67-2 C7H8O3 Component RT: 32.5057 v10² 0.9 140.0 125.0 0.8 0.7^{-} 0.6 97.0 0.5 0.4 0.3 0.2 51.0 79.0 107.0 0.1 39.0 80 140 10 20 30 40 50 60 70 90 100 110 120 150 Mass-to-Charge (m/z) 2-Methoxyresorcinol (NIST20.L) st x10²_ 0.9-125.0 0.8 140.0 0.7 0.6 97.0 0.5 0.4 0.3 51.0 0.2 79.0 107.0 0.1 39.0 68.0 76.0 93.0 27.0 80 140 10 20 30 50 60 70 90 100 110 120 130 150 Mass-to-Charge (m/z) + Scan (32.4137-32.7636 min, 59 scans) 3.D st x10² 0.9 140.0 0.8 0.7 0.6 125.0 0.5 0.4^{-} 97.0 0.3 44.0 32.0 0.2 103.0 51.0 61.0 79.0 91.0 0.1 0 90 100 110 10 20 30 40 50 60 70 80 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 32.5057 **EIC Peaks** Counts Counts x10⁴ 140.0 Component 140.0 125.0 2.5 8.0 125.0 97.0 0.7^{-1} 2 97.0 51.0 0.6

32.6

Acquisition Time (min)

32.7

79.0

H₃C

1.5

1-

32.5

0.5

51.0

79.0

 0.5^{-}

0.4

0.3⁻ 0.2⁻

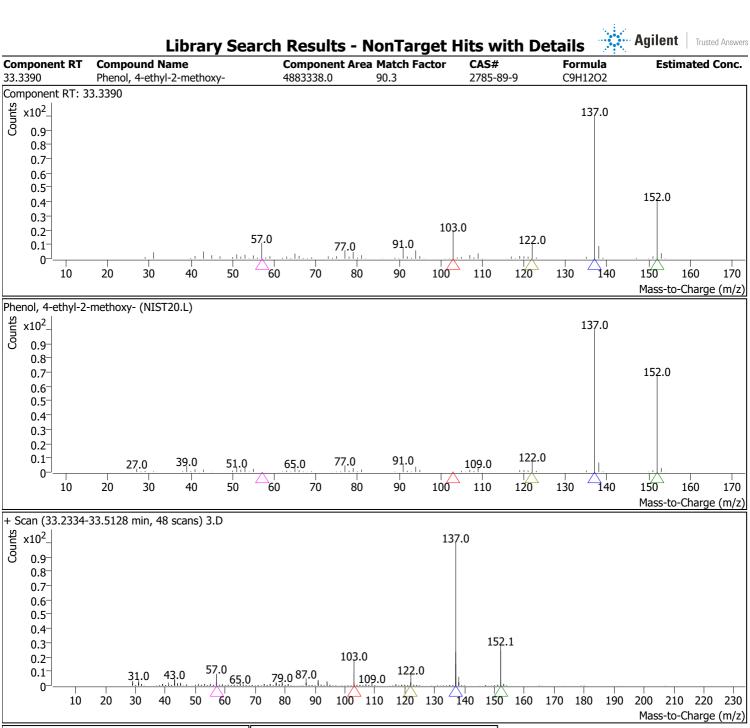
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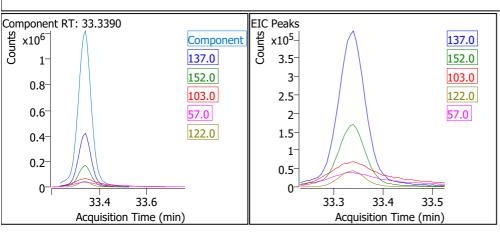
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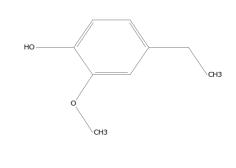
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Acquisition Time (min)

32.7

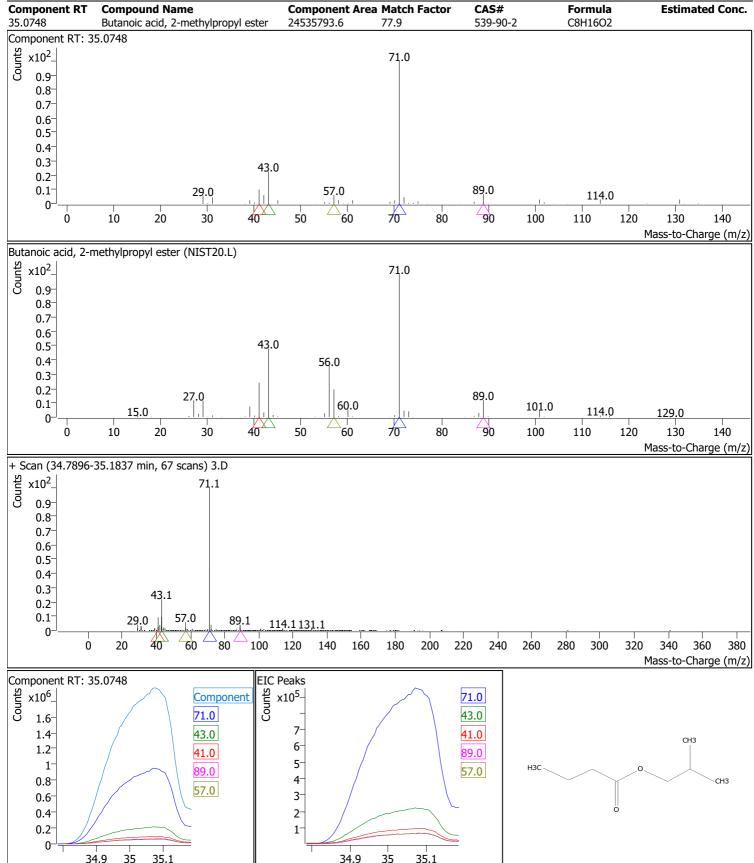






Library Search Results - NonTarget Hits with Details

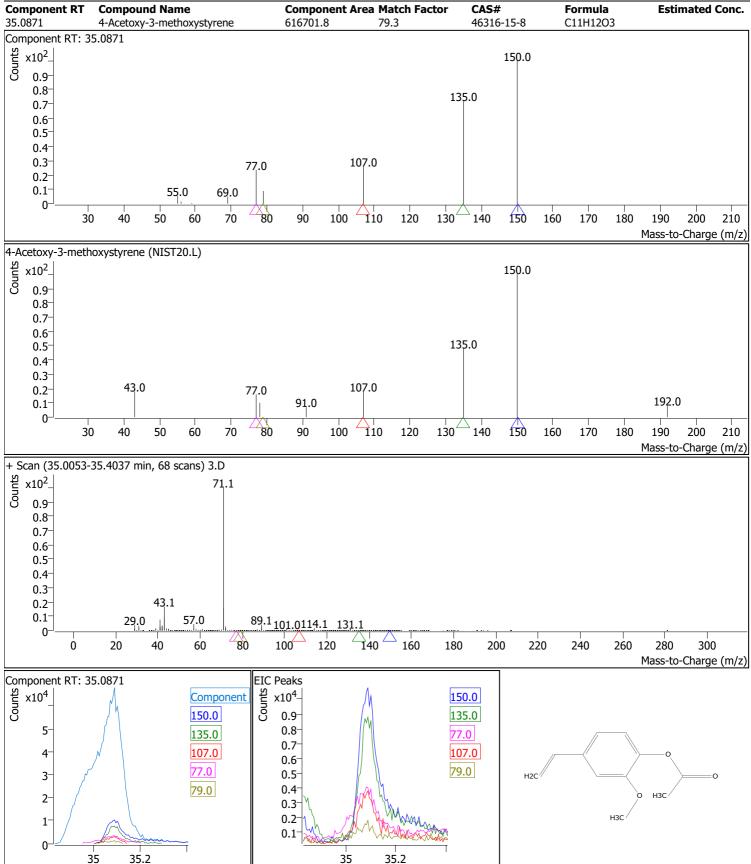




Acquisition Time (min)







--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 35.3937 2-Furanmethanol, tetrahydro-22270698.5 78.6 C5H10O2 Component RT: 35.3937 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 57.0 0.1 89.0 29.0 100 10 25 30 40 55 60 65 85 90 105 110 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts x10²_ 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 45 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (35.1837-35.5702 min, 66 scans) 3.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 3,1.0 57.0 89.1_{101.1114.1} 131.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.3937 Counts Counts x10⁶ x10⁶ 71.0 Component 71.0 43.0 2 1 43.0 41.0 1.75 <u>57.0</u> 41.0 0.8

42.0



57.0

42.0

35.3 35.4 35.5

Acquisition Time (min)

0.6

0.4

0.2

35.3

35.4

Page 44 of 102

Acquisition Time (min)

35.5

1.5

1.25

0.75 0.5

0.25

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.2405 2-Furanmethanol, tetrahydro-5157489.4 97-99-4 C5H10O2 Component RT: 36.2405 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 0.1 57.0 100 105 110 10 55 60 65 90 Mass-to-Charge (m/z) 2-Furanmethanol, tetrahydro- (NIST20.L) Counts x10²_ 0.9 71.0 0.8 0.7 0.6 43.0 0.5 0.4 41.0 0.3 0.2 39.0 0.1 53.0,57.0 61.0 67.0 102.0 10 20 35 40 50 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.1088-36.4264 min, 54 scans) 3.D st x10² 0.9 71.1 0.8 0.7 0.6 0.5 0.4^{-} 0.3 43.1 0.2 0.1 57.0 131.1 10 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 36.2405 **EIC Peaks** Counts Counts x10⁵ x10⁵ 71.0 Component 71.0 43.0 8 4.5 4 7 43.0 41.0 3.5

131.0

31.0

36.4

6

5

4

3

2

1

36.2

36.3

Acquisition Time (min)

36.4

41.0

131.0

31.0

3

2

1

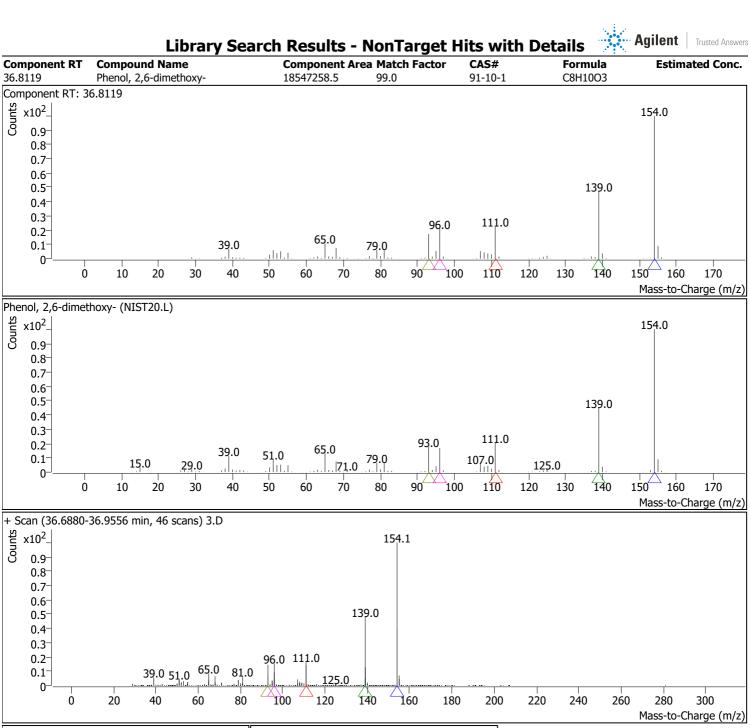
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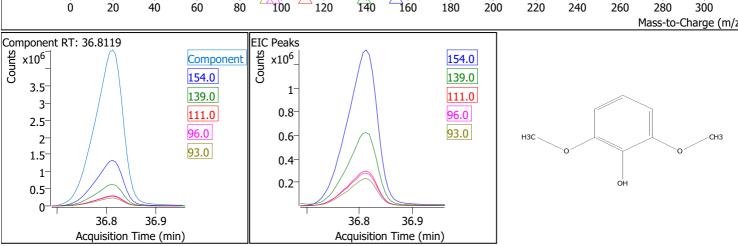
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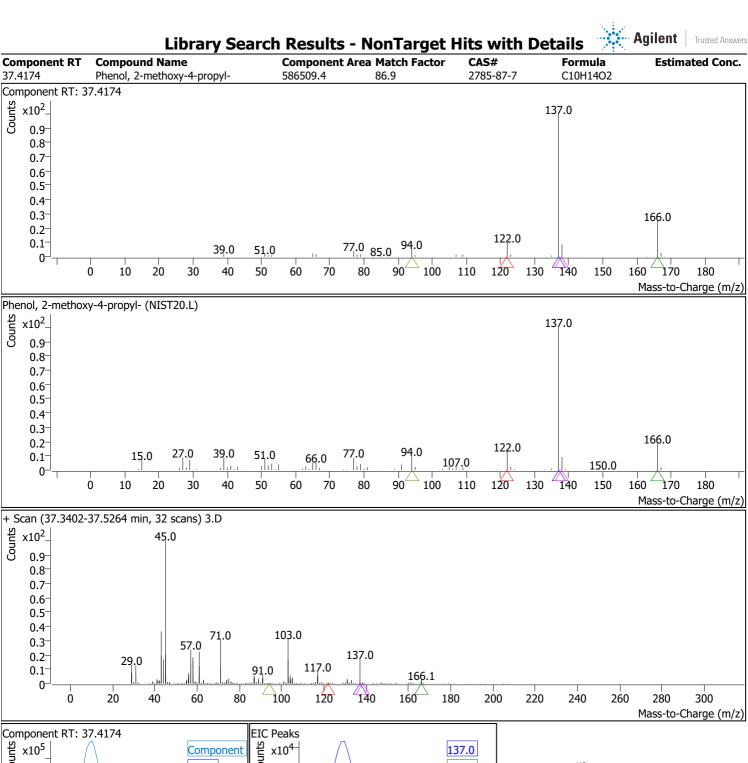
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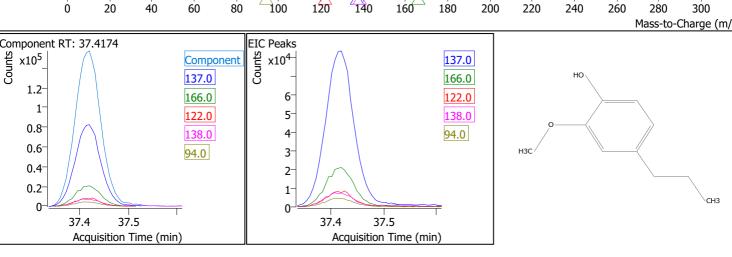
2.5

1.5



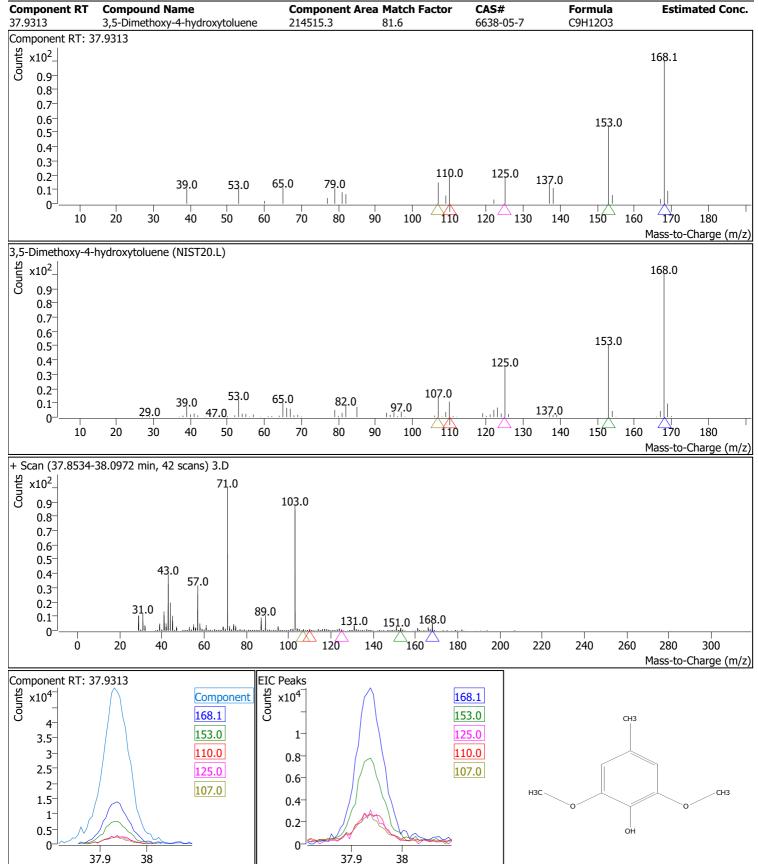






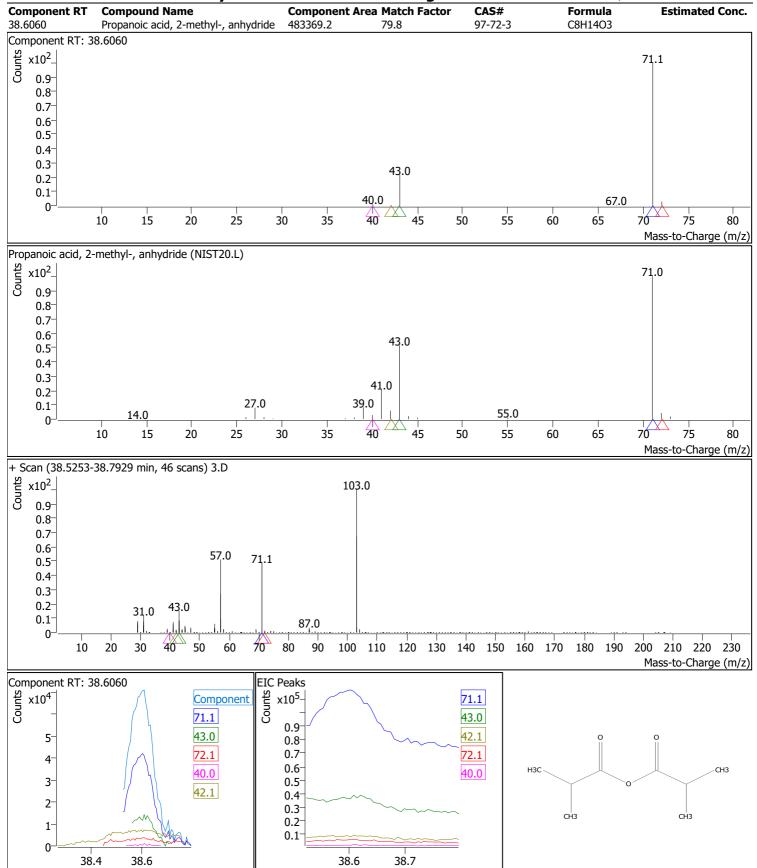






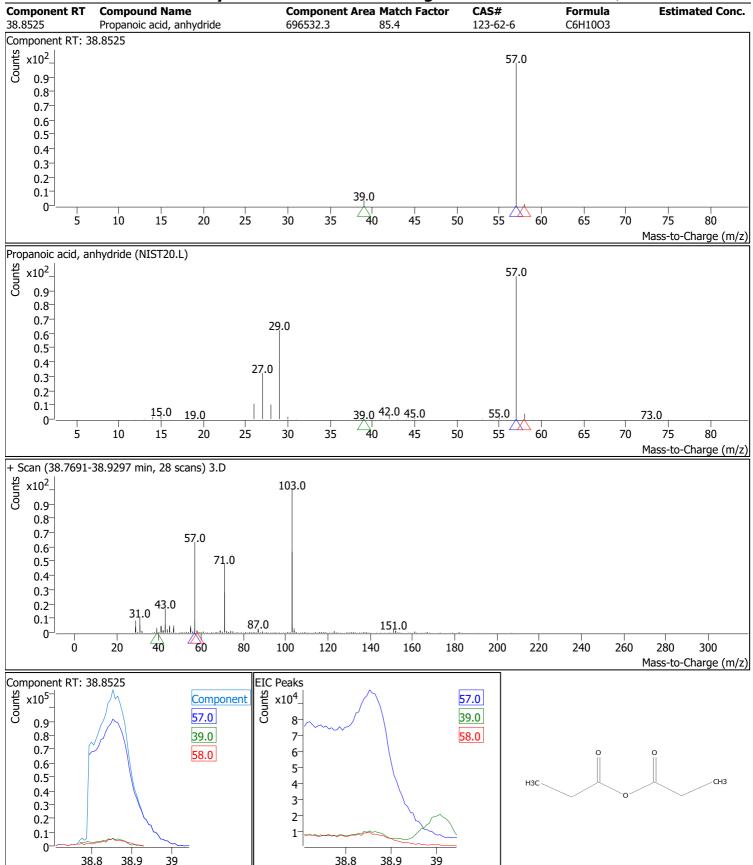






Library Search Results - NonTarget Hits with Details





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.** 38.8609 Butanoic acid, 2,2-dimethylpropyl 2392865.7 75.7 23361-69-5 C9H18O2 Component RT: 38.8609 x10²_ 71.0 57.0 0.9 8.0 0.7 103.0 0.6 0.5 0.4 0.3 0.2^{-} 47.0 31.0 0.1 39.0 0-70 10 20 30 50 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Butanoic acid, 2,2-dimethylpropyl ester (NIST20.L) St x10² 71.0 0.8 0.7 0.6 0.5 0.4 43.0 57.0 0.3 103.0 0.2 87.0 _{93.0} 36.0 0.1 27.0 49.0 130.0 143.0 66.0 0 10 20 30 40 50 60 70 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (38.8108-38.9455 min, 23 scans) 3.D st x10² 0.9 103.0 0.8 0.7 57.0 0.6 0.5 71.0 0.4 0.3 31.0 43.0 0.2 0.1 151.0 87.0 123.0 0 60 40 80 100 260 Ó 20 120 140 160 180 200 220 240 280 300 Mass-to-Charge (m/z) Component RT: 38.8609 EIC Peaks Counts Counts x10⁵ x10⁵ 103.0 Component 71.0 71.0 1.6 3 57.0 57.0 1.4 СНЗ 2.5 55.0 103.0 1.2



38.9

Acquisition Time (min)

47.0

1

0.8

0.6

0.4

0.2

38.8

47.0

55.0

2

1

0-

38.8

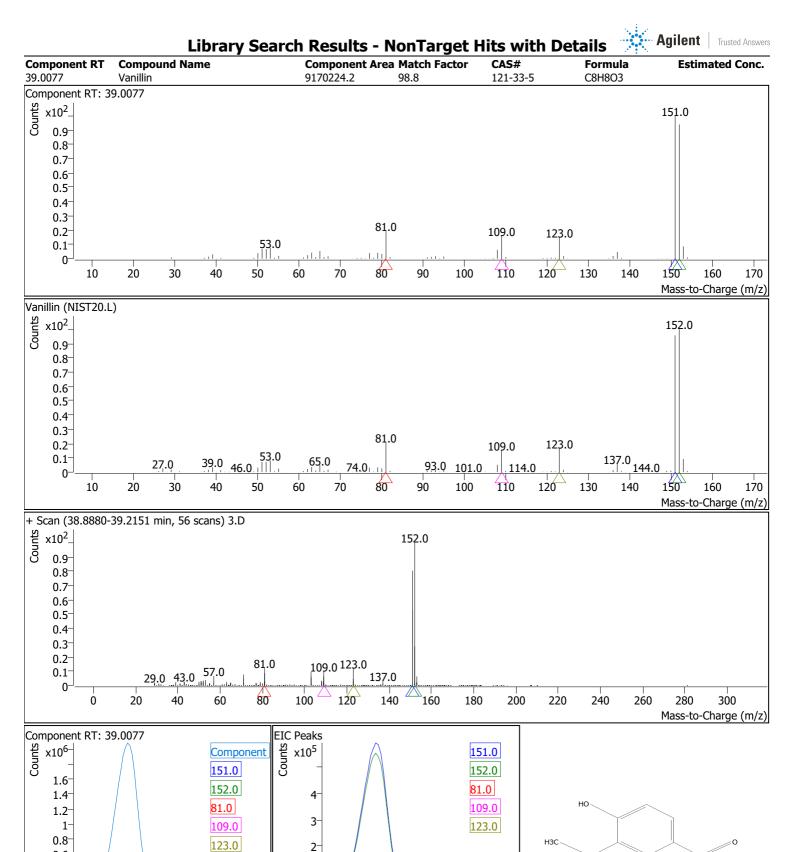
38.9

Acquisition Time (min)

1.5

0.5

-CH3





1

39.1

Acquisition Time (min)

Page 52 of 102

0.6⁻ 0.4⁻

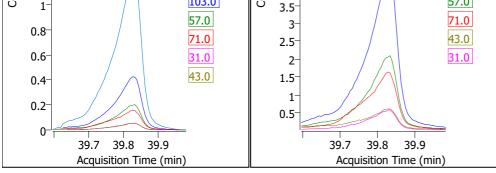
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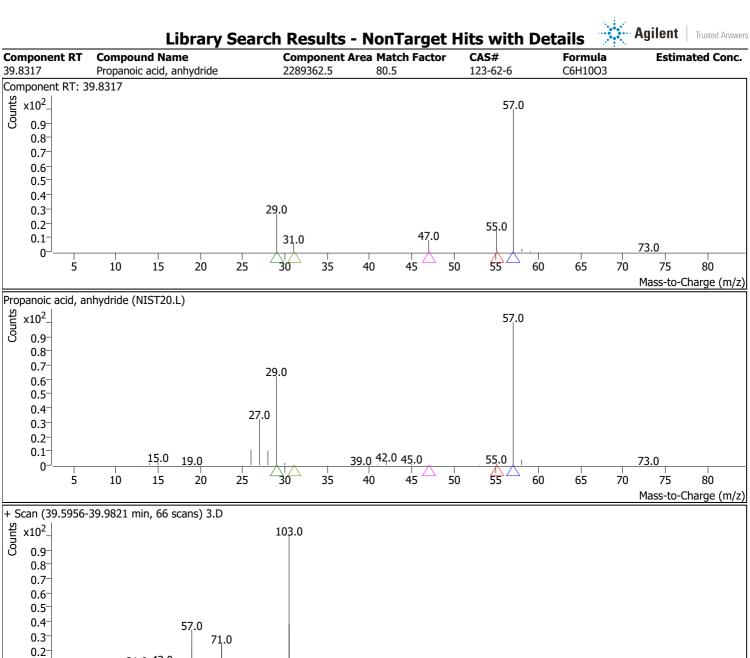
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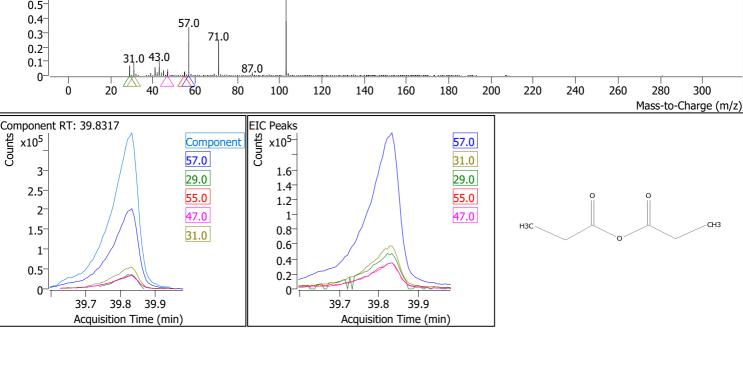
39

39.1

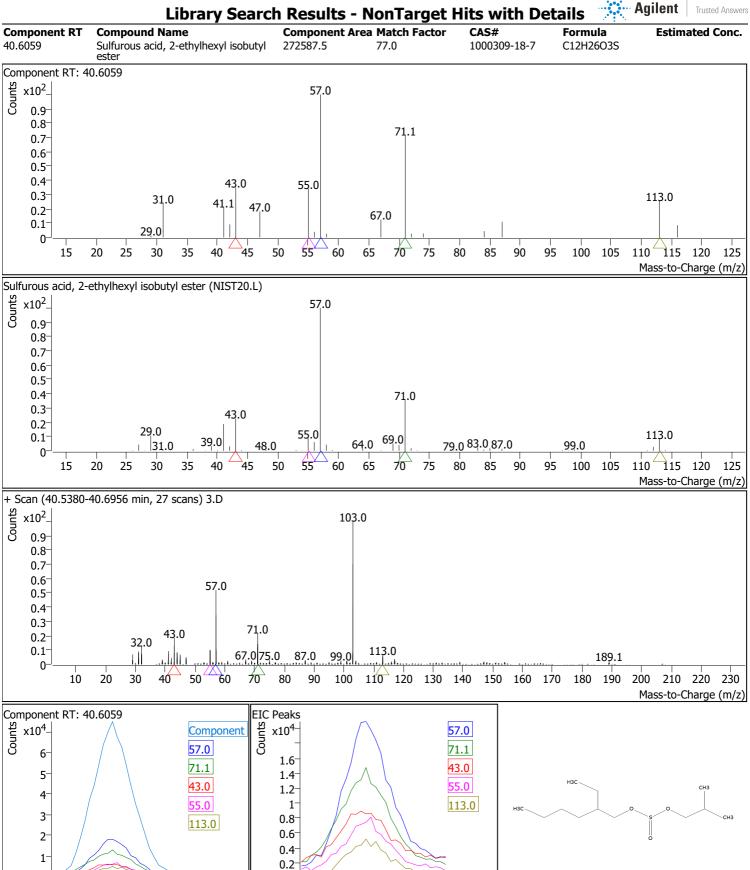
-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 39.8299 1,3-Dioxolane-4-methanol, 2-ethyl-7436730.3 C6H12O3 Component RT: 39.8299 v10² 0.9 103.0 0.8 0.7 0.6 57.0 0.5 71.0 0.4 0.3 0.2 31.0 43.0 0.1 70 120 130 Ó 10 20 30 50 80 90 100 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10²_ 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 (39.6254-39.9804 min, 60 scans) 3.D st x10² 0.9 103.0 0.8 0.7 0.6 0.5 0.4^{-} 57.0 0.3 71.0 0.2 31.0 43.0 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: 39.8299 Counts Counts x10⁶ x10⁵ 103.0 Component 103.0 57.0 1 3.5







Library Search Results - NonTarget Hits with Details



0

40.55

40.6

40.65

Acquisition Time (min)

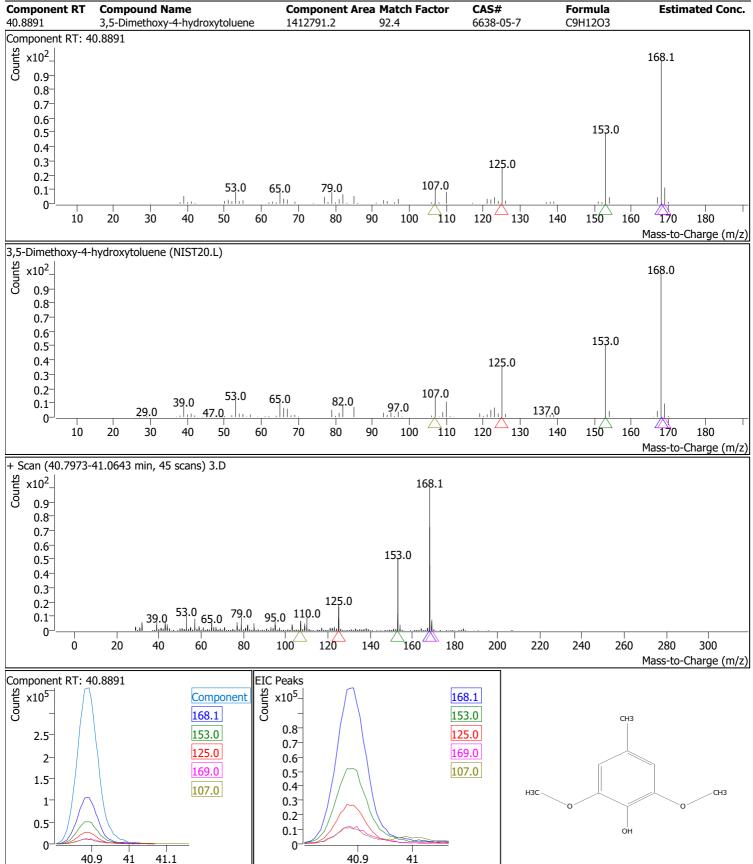
40.55

40.6

40.65







--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 93-28-7 41.1108 Phenol, 2-methoxy-4-(2-propenyl)-, 505697.8 91.9 C12H14O3 acetate Component RT: 41.1108 x10²_ 164.0 0.9 8.0 0.7 0.6 0.5 0.4 149.0 0.3 103.0 77.0 91.0 0.2^{-} 131.0 121.0 0.1 0-90 **15**0 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-(2-propenyl)-, acetate (NIST20.L) Counts $x10^{2}$ 164.0 0.9 0.8 0.7 0.6 0.5 149.0 0.4 77.0 0.3 55.0 103.0 91.0 131.0 0.2 51.0 121.0 65.0 137.0 0.1 43.0 82.0 70.0 59.0 0 150 90 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (41.0329-41.2843 min, 43 scans) 3.D st x10² 103.0 0.8 0.7 71.0 0.6 0.5 0.4 43.0 57.0 0.3 0.2 31.0 89.1 164.1 0.1 116.0 131.0 0 Ó 20 100 120 160 220 260 40 60 80 140 180 200 240 280 300 Mass-to-Charge (m/z) Component RT: 41.1108 **EIC Peaks** Counts Counts x10⁵x10⁵ 103.0 Component 164.0 164.0 2 1 149.0 149.0 1.75 103.0 77.0 8.0 1.5

41.2

Acquisition Time (min)

77.0

91.0

41.2

Acquisition Time (min)

0.6

0.4

0.2

1.25

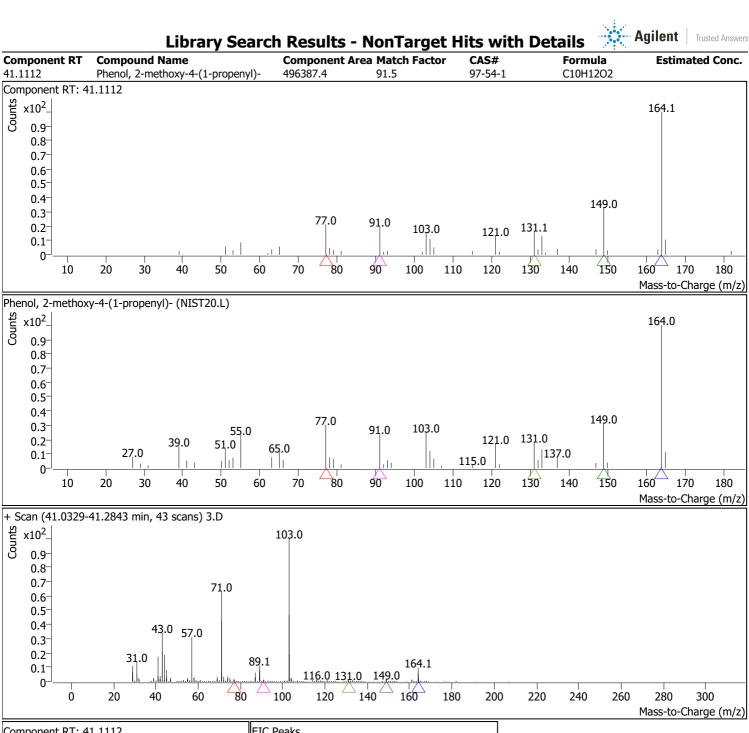
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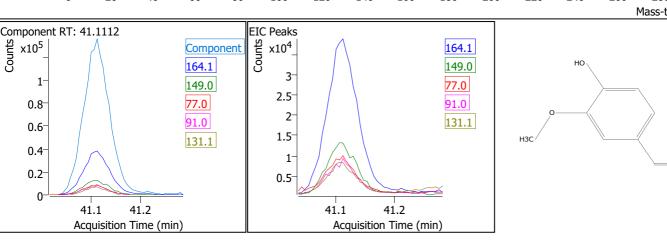
0.25

41.1

1

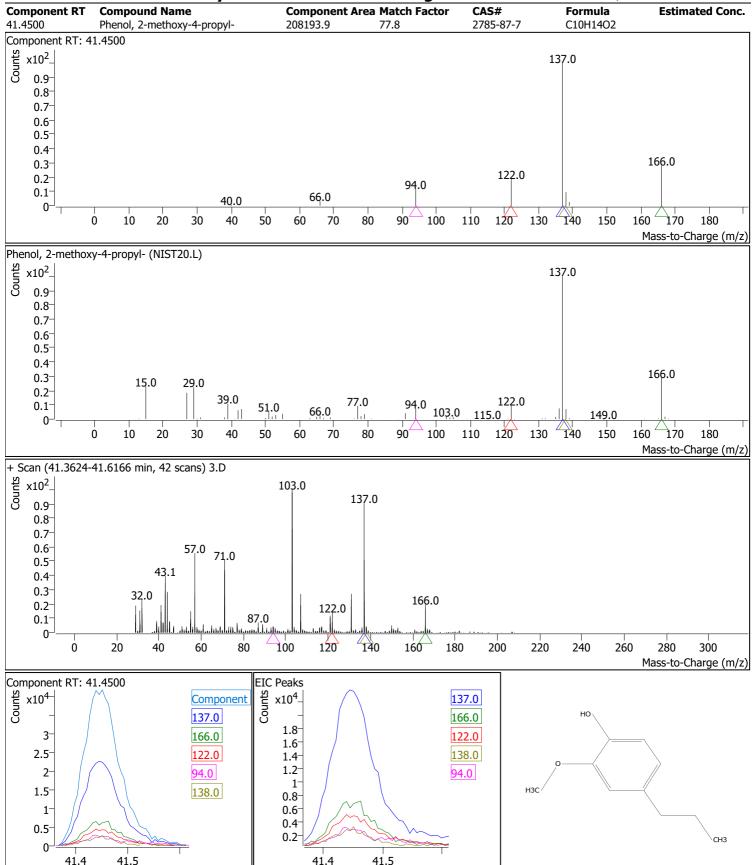
91.0





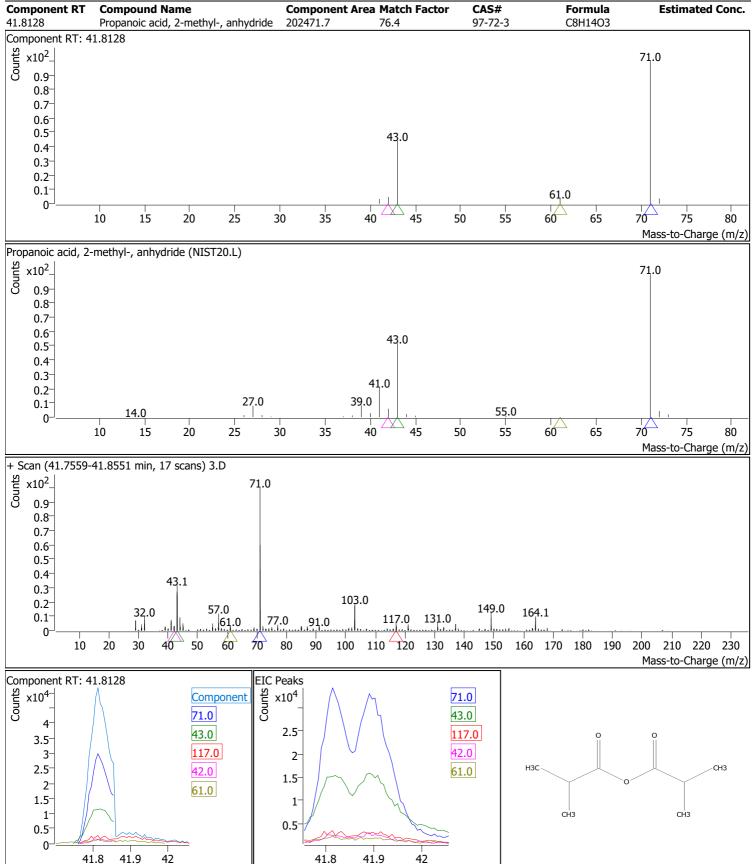






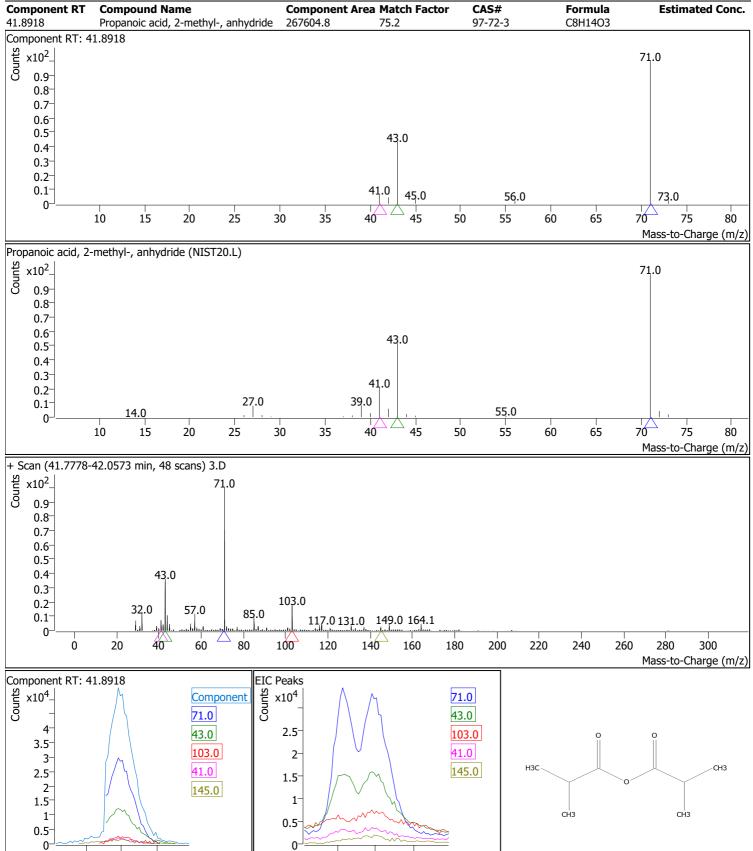






Library Search Results - NonTarget Hits with Details





41.9

Acquisition Time (min)

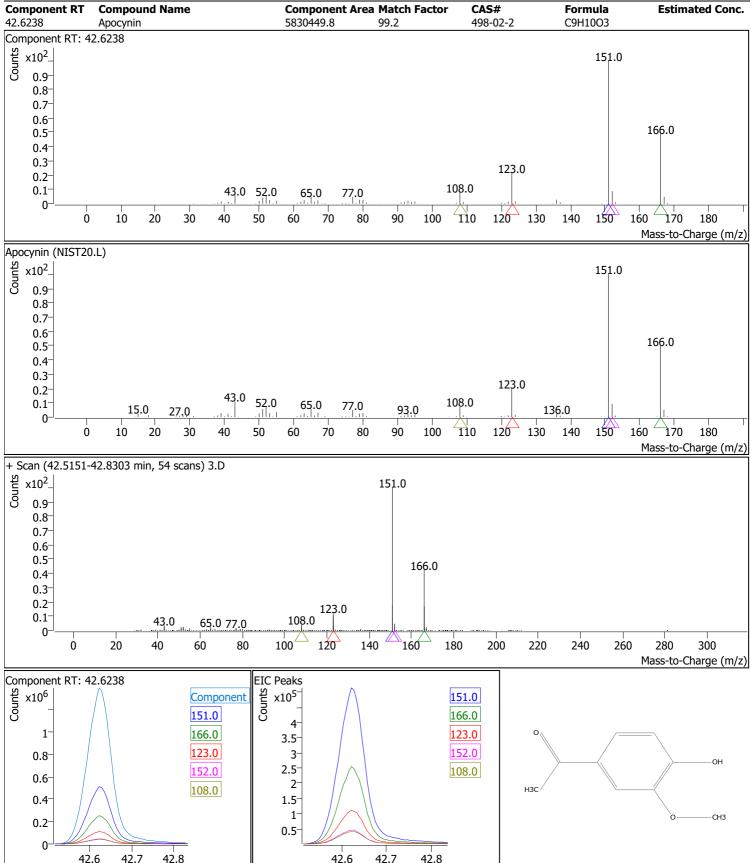
42

41.8

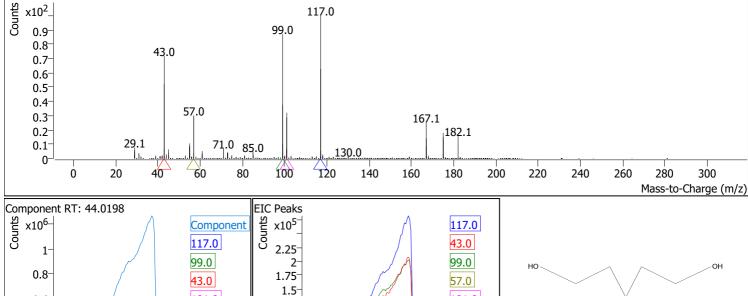
41.8

41.9





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5694-95-1 44.0198 1,3-Dioxolane-2,2-diethanol 16986372.7 C7H14O4 Component RT: 44.0198 v10² 0.9 117.0 99.0 0.8 43.0 0.7^{-} 0.6 0.5 57.0 0.4 0.3 0.2 61.0 0.1 100 10 20 30 40 50 60 70 80 90 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) 1,3-Dioxolane-2,2-diethanol (NIST20.L) Counts x10²_ 0.9 117.0 0.8 0.7 0.6 0.5 99.0 0.4 0.3 0.2 87.0 31.0 73.0 0.1 127.0 162.0 **100** 10 20 30 40 50 70 80 90 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) + Scan (43.5547-44.1622 min, 103 scans) 3.D 117.0



101.0

0.6

0.4

0.2

43.6

43.8

44

Acquisition Time (min)

101.0

57.0

1.25

0.75

0.25

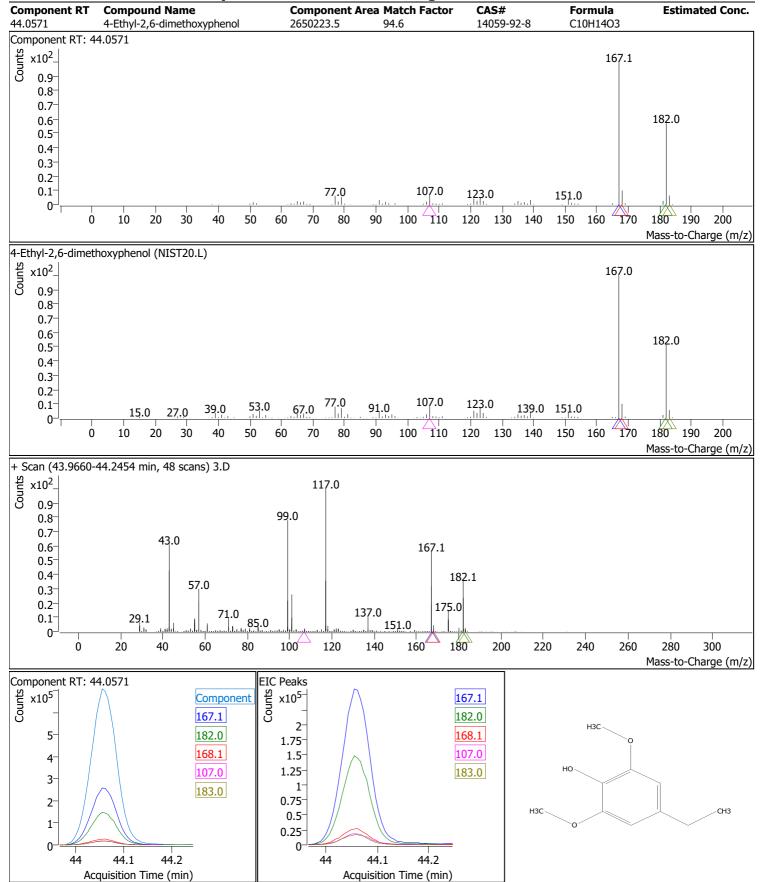
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43.6

43.8







--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 44.3094 2-Propanone, 1-(4-hydroxy-3-11591458.7 95.8 2503-46-0 C10H12O3 methoxyphenyl) Component RT: 44.3094 Counts x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2 122.0 0.1 0-120 180 20 30 70 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 131.0 147.0 164.0 173.0 0 100 180 20 30 60 80 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.1919-44.3941 min, 35 scans) 3.D x10². 137.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 87.0 0.3 180.1 43.0 0.2 122.0 0.1 55.1 94.0 171.1 115.1 129.1 214.2 0 100 140 180 Ó 20 40 60 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 44.3094 Counts Counts x10⁶ x10⁶. 137.0 Component 180.0 137.0 2.25 0.9 2 0.8 180.0 122.0 1.75 0.7 122.0 138.0 1.5 0.6



44.3

44.4

Acquisition Time (min)

94.0

138.0

94.0

0.5

 0.4°

0.3

0.2

0.1

1.25

0.75

0.5

44.3

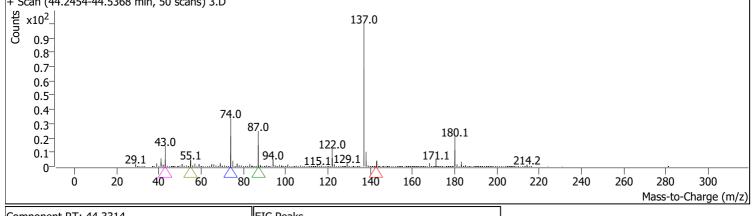
44.4

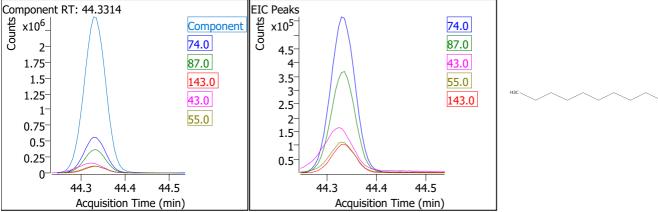
Acquisition Time (min)

0.25

1

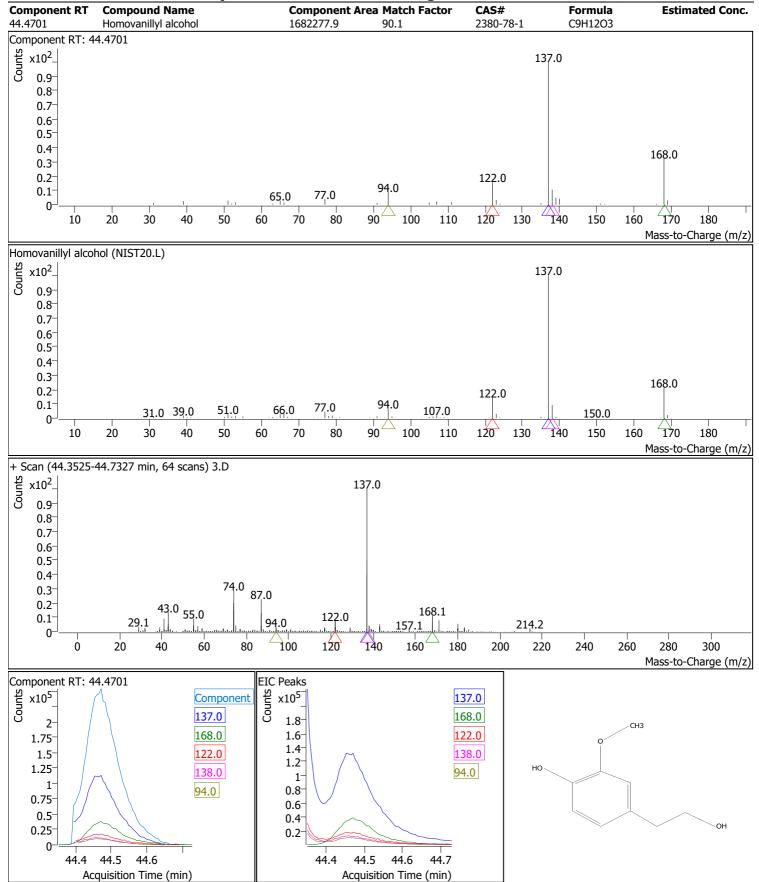
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3314 Dodecanoic acid, methyl ester 8534287.0 111-82-0 C13H26O2 Component RT: 44.3314 Counts $x10^{2}$ 74.0 0.9 0.8 0.7^{-} 87.0 0.6 0.5 0.4 0.3 43.0 55.0 143.0 0.2 69.0 0.1 130 140 150 160 170 180 190 200 210 220 230 240 70 100 110 120 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10²_ 0.9 74.0 0.8 87.0 0.7 0.6 0.5 0.4 0.3 55.0 43.0 0.2 69.0 101.0 115.0 0.1 __90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 -10 10 20 30 40 50 60 70 80 Mass-to-Charge (m/z) + Scan (44.2454-44.5368 min, 50 scans) 3.D





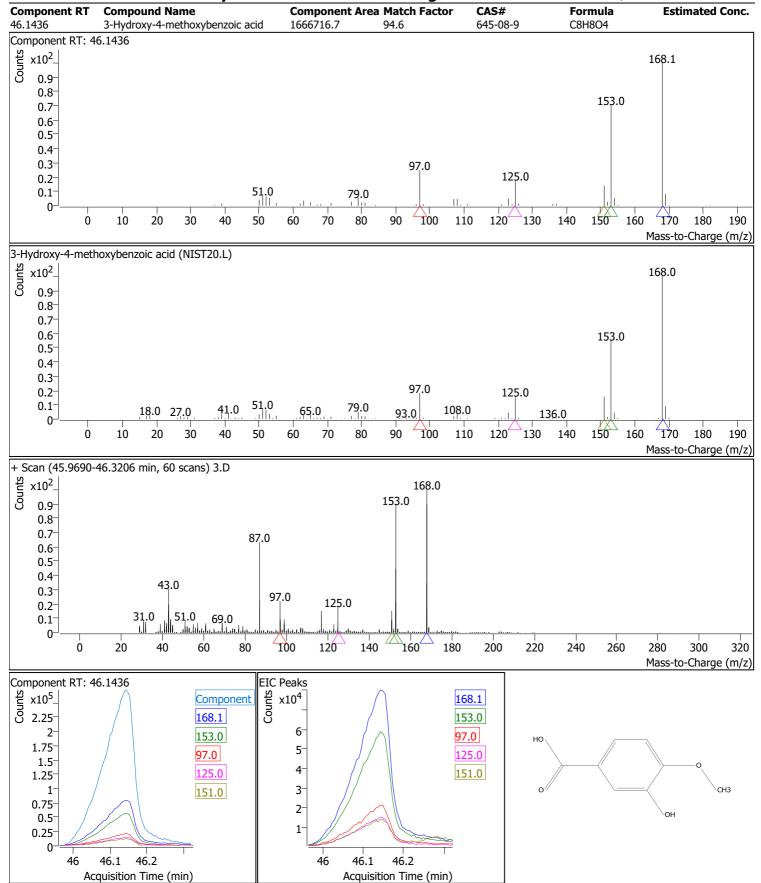




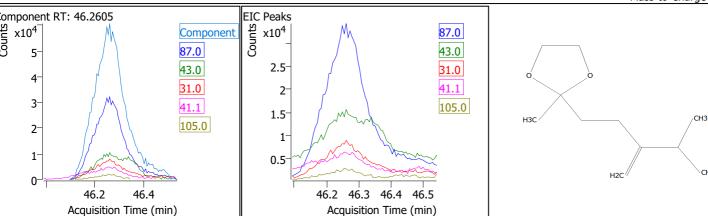


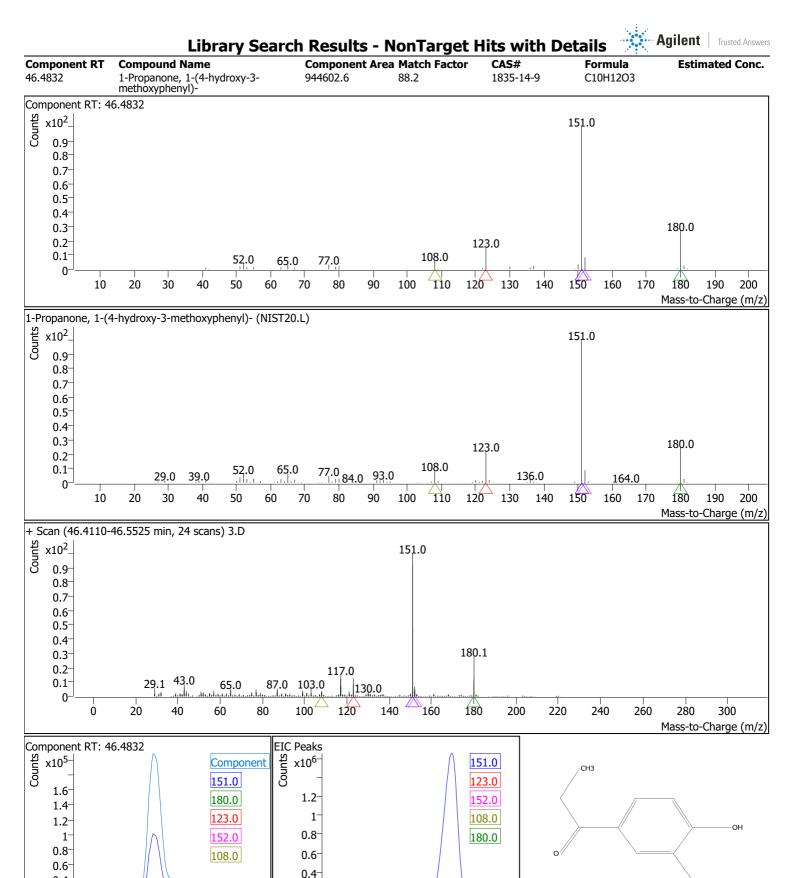






--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1,3-Dioxolane, 2-methyl-2-(4-methyl-3-methylenepentyl)-46.2605 538518.7 66972-05-2 C11H20O2 Component RT: 46.2605 x10²_ 87.0 0.9 8.0 0.7 0.6 0.5 0.4 43.0 0.3 0.2 41.1 0.1 105.0 100.0 0-55 65 70 75 85 95 105 35 40 50 60 80 90 100 Mass-to-Charge (m/z) 1,3-Dioxolane, 2-methyl-2-(4-methyl-3-methylenepentyl)- (NIST20.L) $x10^{2}$ 87.0 0.9 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 41.0 0.1 99.0 105 85 100 35 40 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (46.0898-46.5453 min, 76 scans) 3.D x10². 151.0 0.9 168.0 0.8 87.0 0.7 0.6 0.5 0.4 43.0 117.0 0.3 180.1 97.0 0.2 51.0 69.0 0.1 0 20 40 80 260 300 60 100 120 140 160 180 200 220 240 280 320 Mass-to-Charge (m/z) Component RT: 46.2605 **EIC Peaks** Counts Counts x10⁴ x10⁴ 87.0 Component 87.0 43.0 5 2.5 43.0 31.0 31.0 41.1 2





46.4

Acquisition Time (min)

46.6

0.2

46.2

0.4

0.2

46.2

46.4

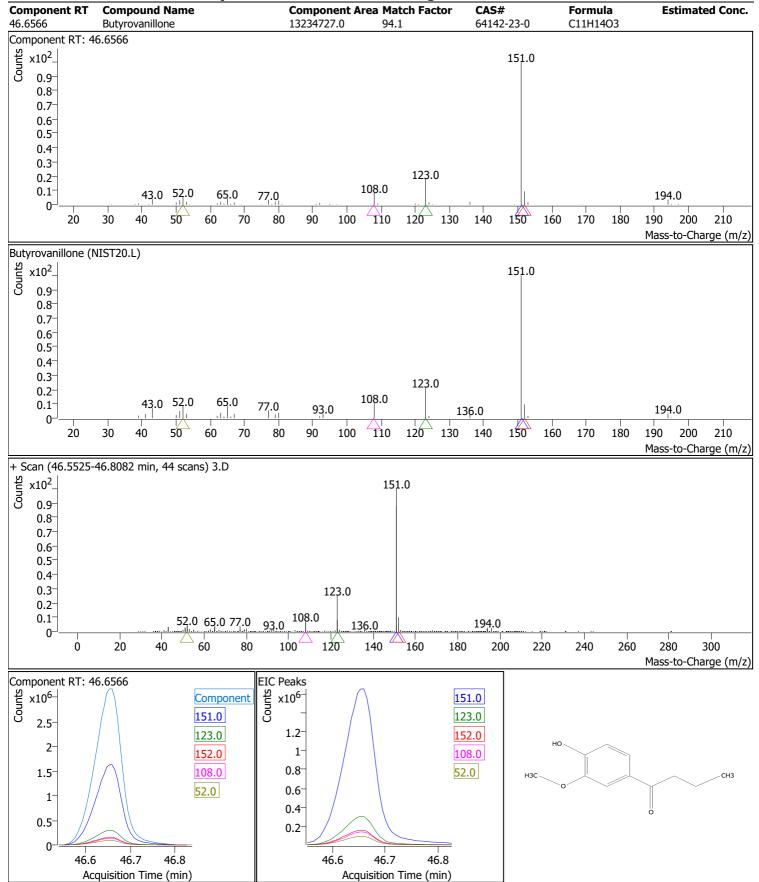
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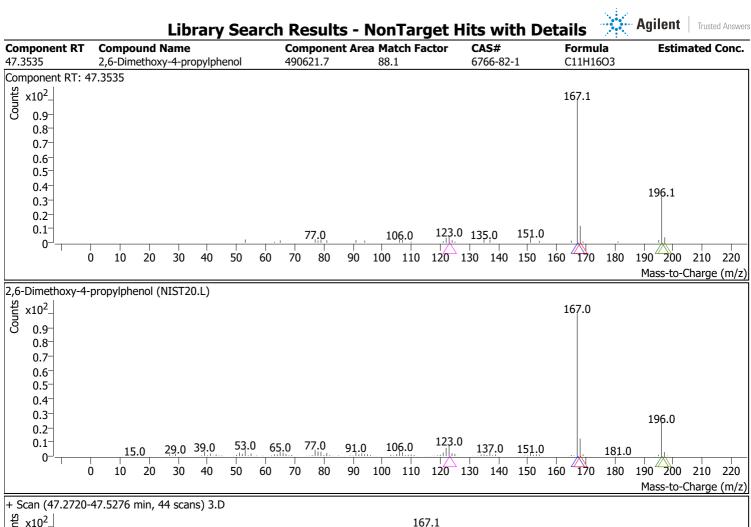
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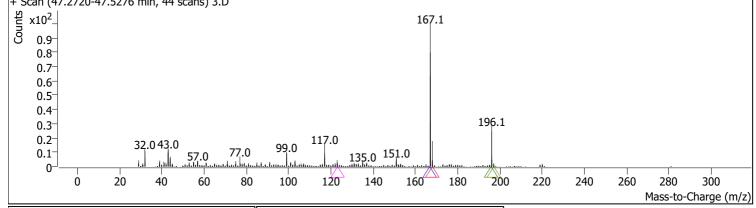
нзс

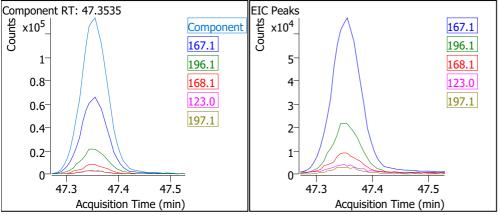


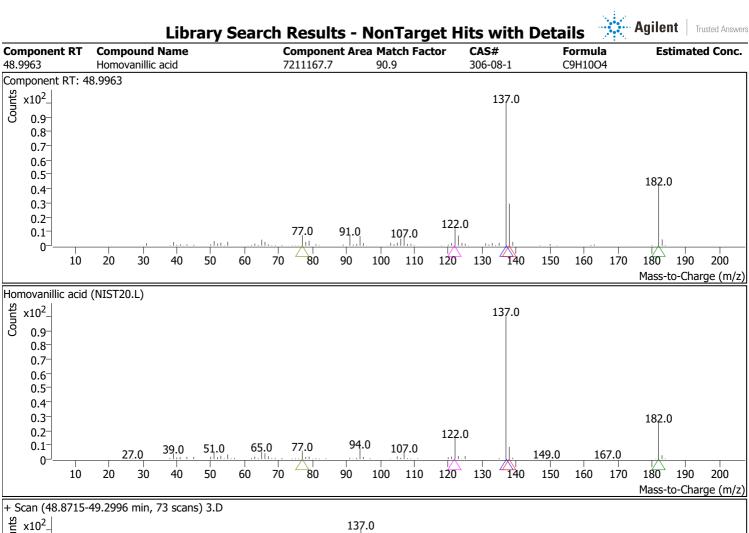


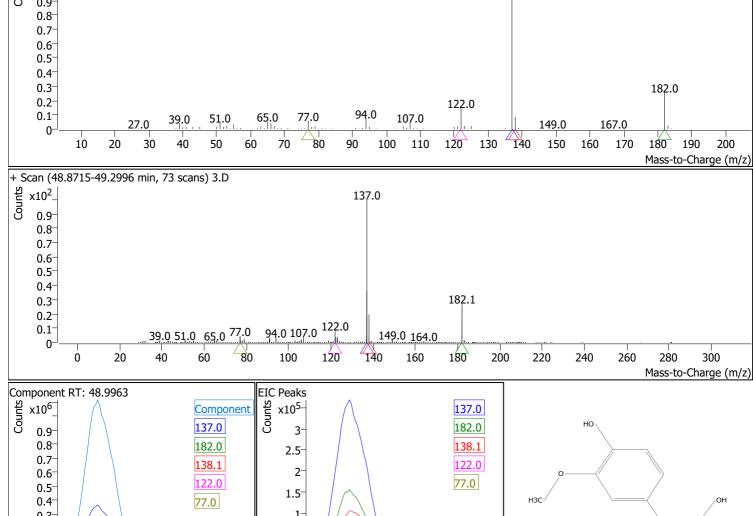


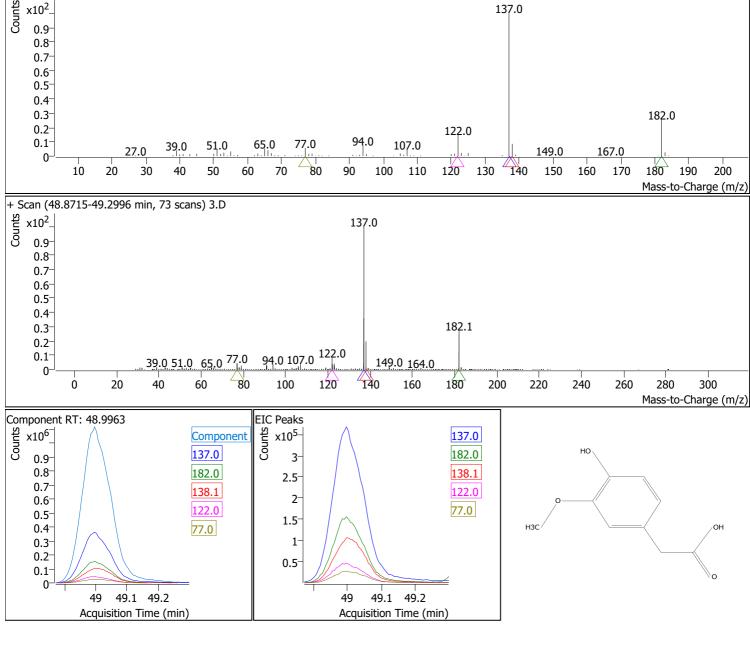




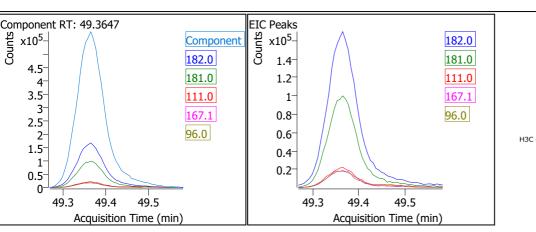


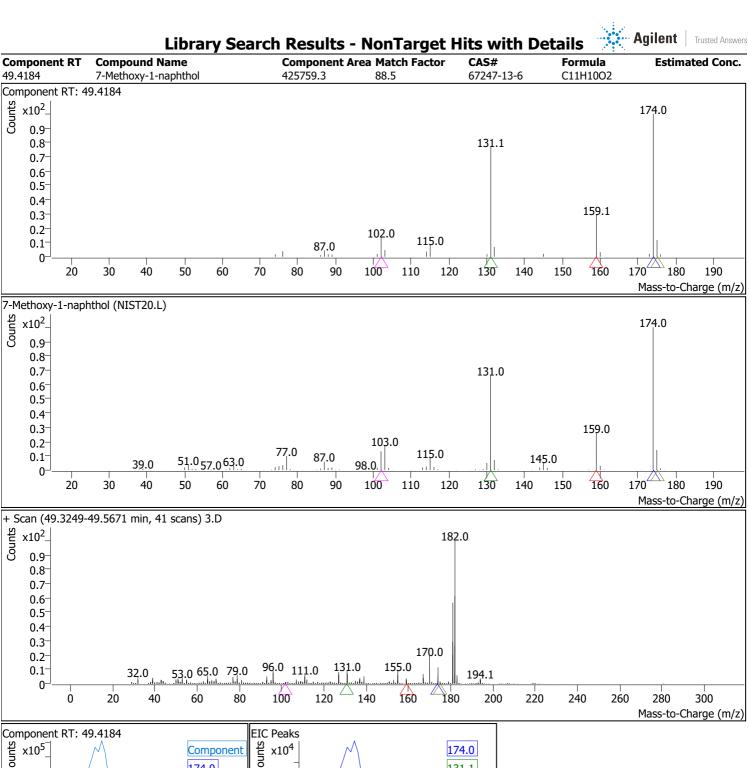


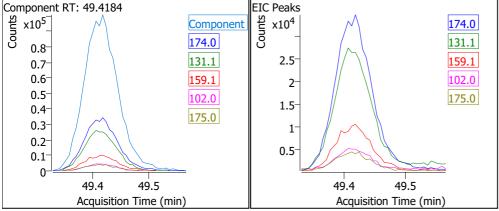




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.3647 Benzaldehyde, 4-hydroxy-3,5-2676765.8 97.0 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3647 x10²_ 182.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 111.0 96.0 139.0 167.1 65.0 79.0 0.1 Titil 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 0.2 167.0 139.0 65.0 93.0 39.0 51.0 79.0 0.1 29.0 153.0 15.0 123.0 0 160 170 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2698-49.5790 min, 53 scans) 3.D x10². 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 170.0 0.2 53.0 65.0 79.0 96.0 111.0 155.0 0.1 32.0 194.1 0 40 100 200 0 20 60 80 120 140 160 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3647 **EIC Peaks** Counts Counts x10⁵x10⁵-182.0 Component 0 181.0 182.0 1.4 4.5 181.0 111.0 1.2 3.5 111.0 1 167.1

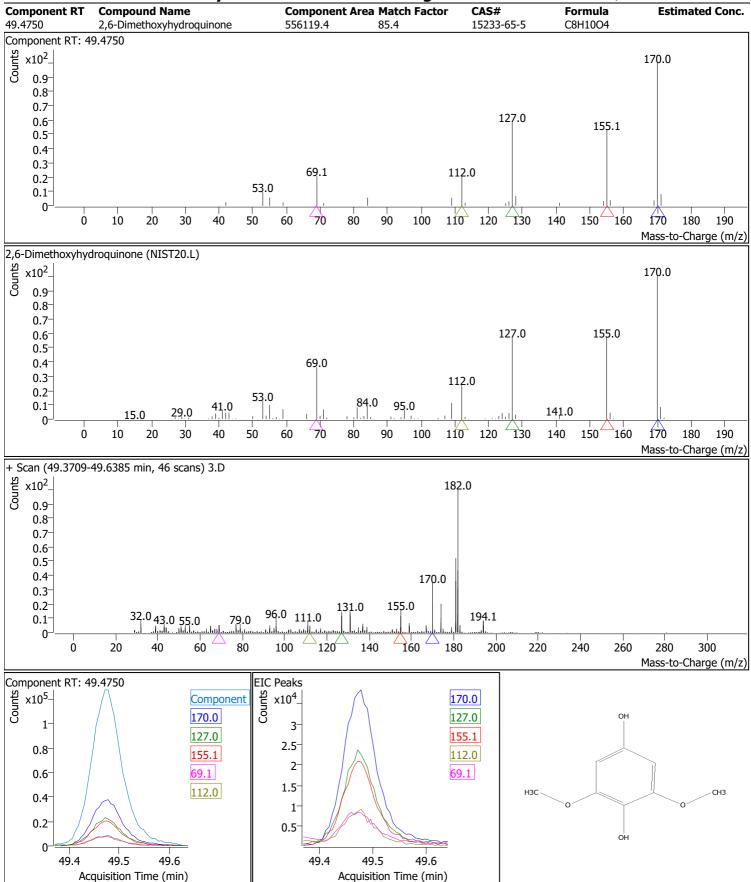


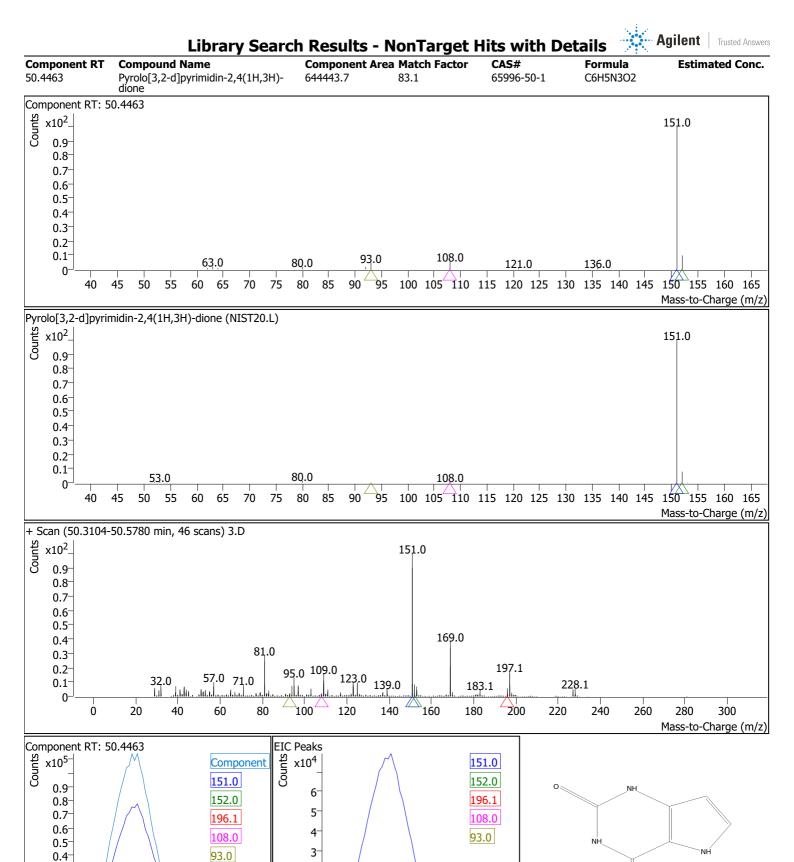












50.5

Acquisition Time (min)

2

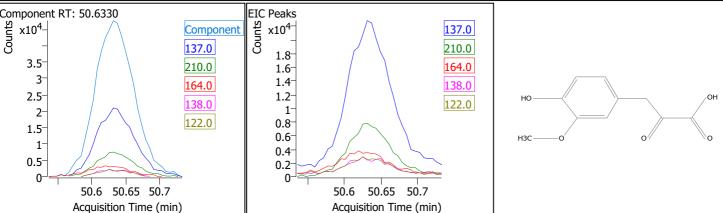
0.3

0.2⁻ 0.1⁻

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.** 50.6330 Phenylacetylformic acid, 4-hydroxy-3- 191817.4 1081-71-6 C10H10O5 methoxy-Component RT: 50.6330 Counts x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 210.0 0.3 164.0 0.2^{-} 122.0 77.0 149.0 0.1 91.0 100 110 120 130 140 150 160 170 180 190 200 210 220 230 -10 10 20 30 50 60 70 80 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 0.2 164.0 122.0 0.1 51.0 65.0 77.0 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 (50.5603-50.7316 min, 28 scans) 3.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 210.1 151.0 71.0 0.3 43.1 0.2 164.0 77.0 91.0 55.0 0.1 181.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 50.6330 **EIC Peaks** Counts Counts 137.0 x10⁴. x10⁴ Component 137.0 210.0 1.8



··· 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 51.0503 732737.3 82.0 C9H16O3 Component RT: 51.0503 x10²_ 71.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 43.0 0.2^{-} 0.1 57.0 87.0 0-10 15 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 x10² 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 95 100 105 110 115 120 125 90 Mass-to-Charge (m/z) + Scan (50.9466-51.1607 min, 37 scans) 3.D st x10² 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 153.0 169.0 0.1 32.0 97.0 127.0 57.0 194.1 81.0 40 20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 51.0503 **EIC Peaks** Counts Counts x10⁵ x10⁵ 71.0 Component 71.0 43.0 0.8 1.2 43.0 41.0 0.7 41.0 1 0.6 70.0

72.0

51.1

Acquisition Time (min)

0.5

 0.4^{-}

0.3

0.2

0.1

50.9

70.0

72.0

0.8

0.6

0.4

0.2

50.9

51

Acquisition Time (min)

51.1

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor Component RT** CAS# **Formula Estimated Conc.** 2-Propanone, 1-hydroxy-3-(4-hydroxy- 324675.6 3-methoxyphenyl)-51.7508 88.4 4899-74-5 C10H12O4 Component RT: 51.7508 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 196.0 0.2^{-} 122.0 94.0 0.1 77.0 66.0 51.0 39.0 0-140 190 200 120 10 20 30 40 50 60 70 80 90 100 110 130 150 160 170 180 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) x10². 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 60 70 80 90 100 110 120 130 140 150 160 170 180 210 Mass-to-Charge (m/z) + Scan (51.6661-51.9039 min, 41 scans) 3.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 196.0 0.2 169.0 71.1 32.0 103.0 122.0 0.1 51.0_{اأيانا} 81.0 151.0 0 200 20 40 60 80 100 120 140 160 180 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 51.7508 **EIC Peaks** Counts Counts x10⁴ $x10^{4}$ 137.0 Component 137.0 196.0 4 H₃C 6 196.0 122.0 3.5 5 3-122.0 138.0 4 2.5 138.0

51.8

Acquisition Time (min)

2

1

51.7

1.5

0.5

94.0

3

2-

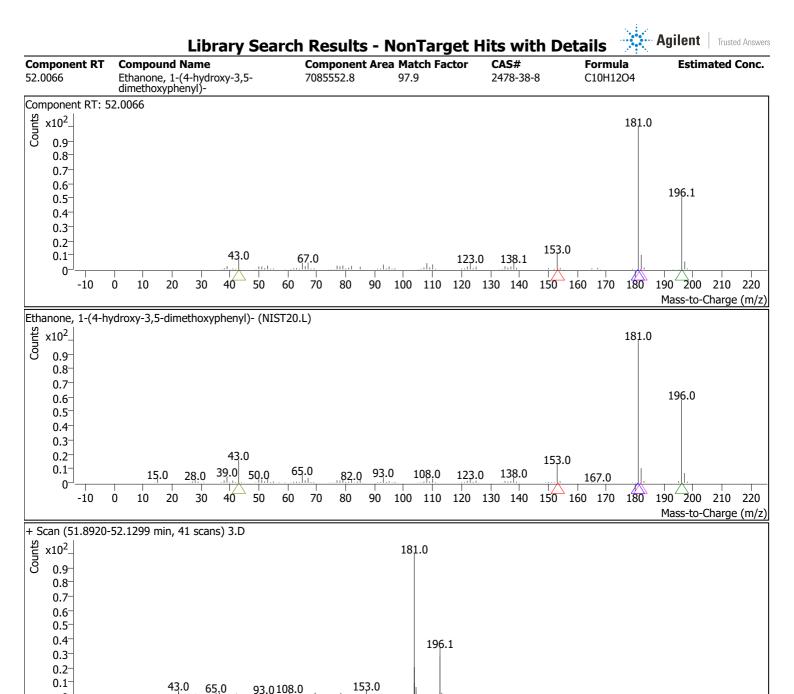
1

51.7

51.8

Acquisition Time (min)

94.0



200

220

181.0

196.1

153.0

182.0

43.0

240

260

280

300

320

ОН

340

СНЗ

360

Mass-to-Charge (m/z)

380

180

160

52

52.1

Acquisition Time (min)

140

0

x10⁶

1.2

8.0

0.6

0.4

0.2

1

Counts

Component RT: 52.0066

20

52

52.1

Acquisition Time (min)

60

80

Component

181.0

196.1

153.0

182.0

43.0

100

Counts x10⁵

120

4.5

3.5

2.5

4

3

2 1.5

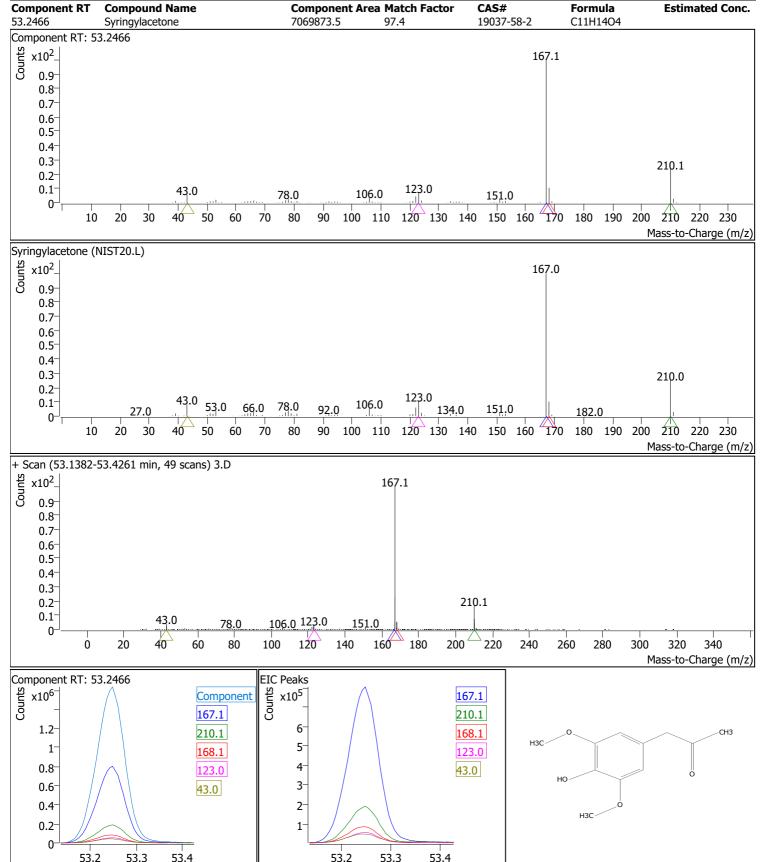
1

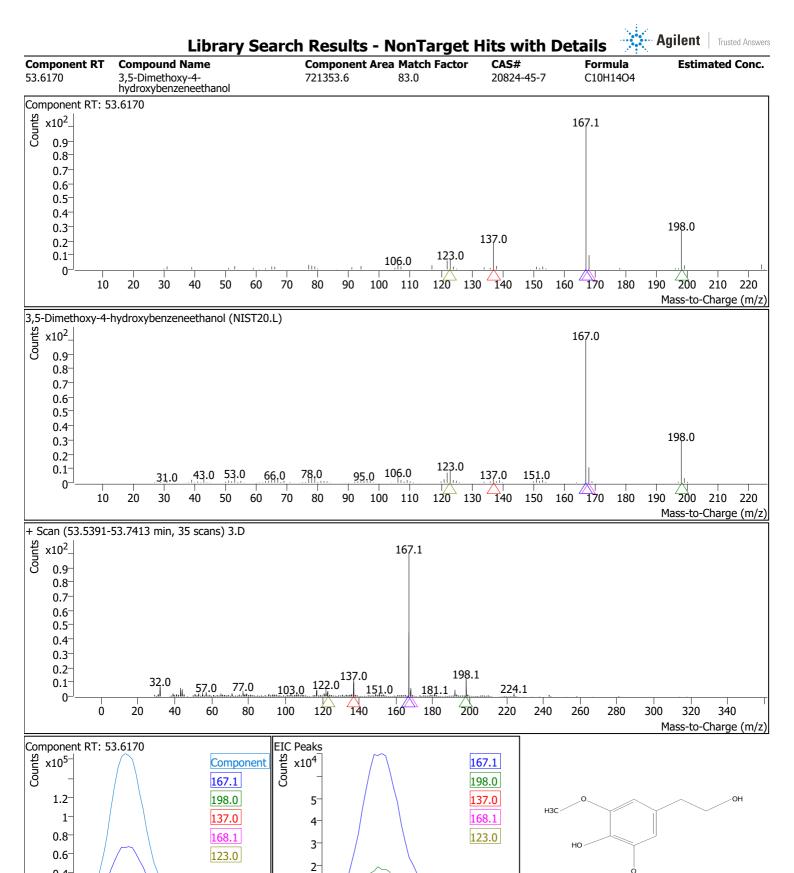
0.5

EIC Peaks









53.6 53.65 53.7

Acquisition Time (min)

0.4

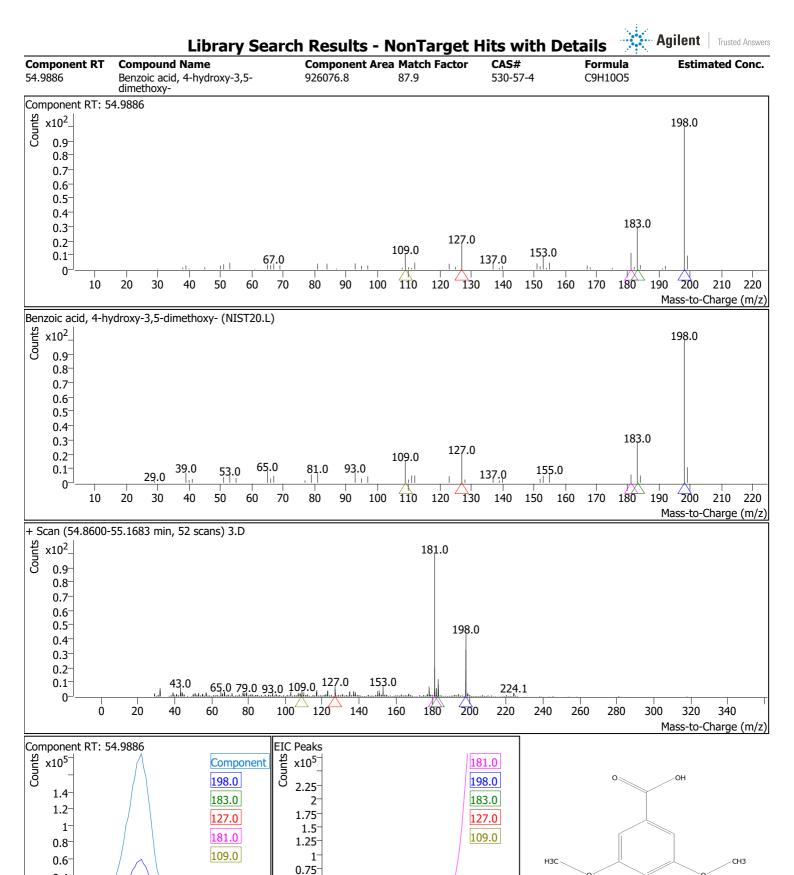
0.2

53.6

53.7

Acquisition Time (min)

H3C



55

55.1

Acquisition Time (min)

0.5

0.25

54.9

0.4

0.2

0

54.9

55

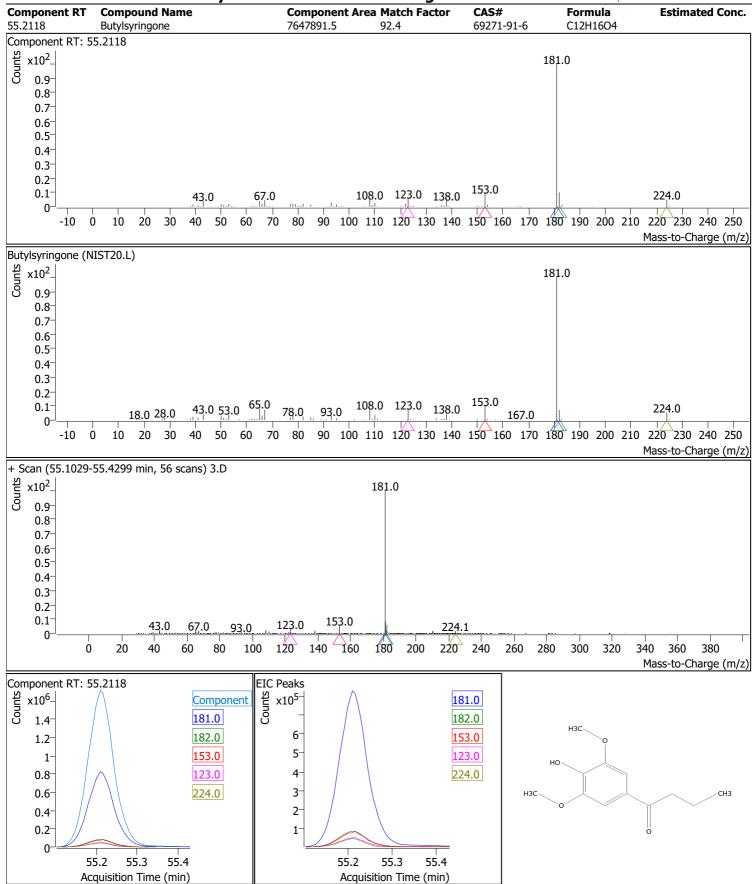
Acquisition Time (min)

55.1

ОН

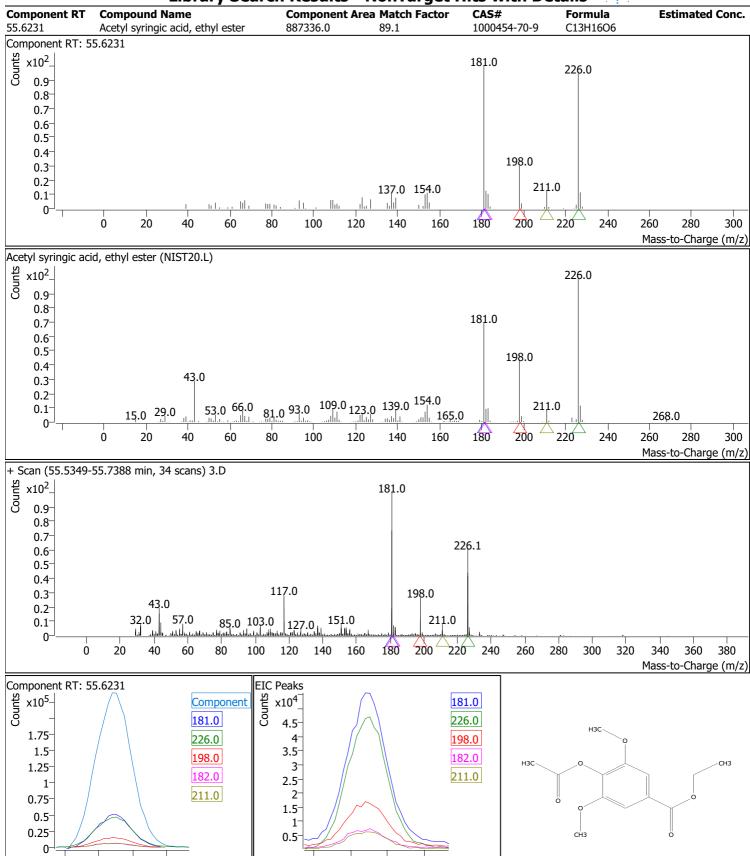












55.6 55.65

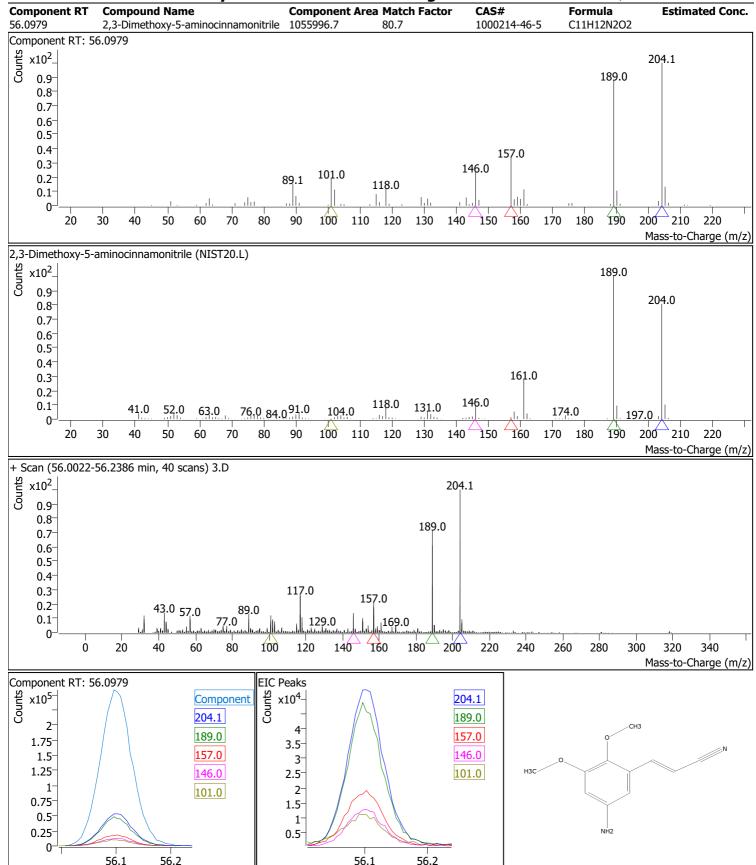
Acquisition Time (min)

55.7

55.6 55.65 55.7

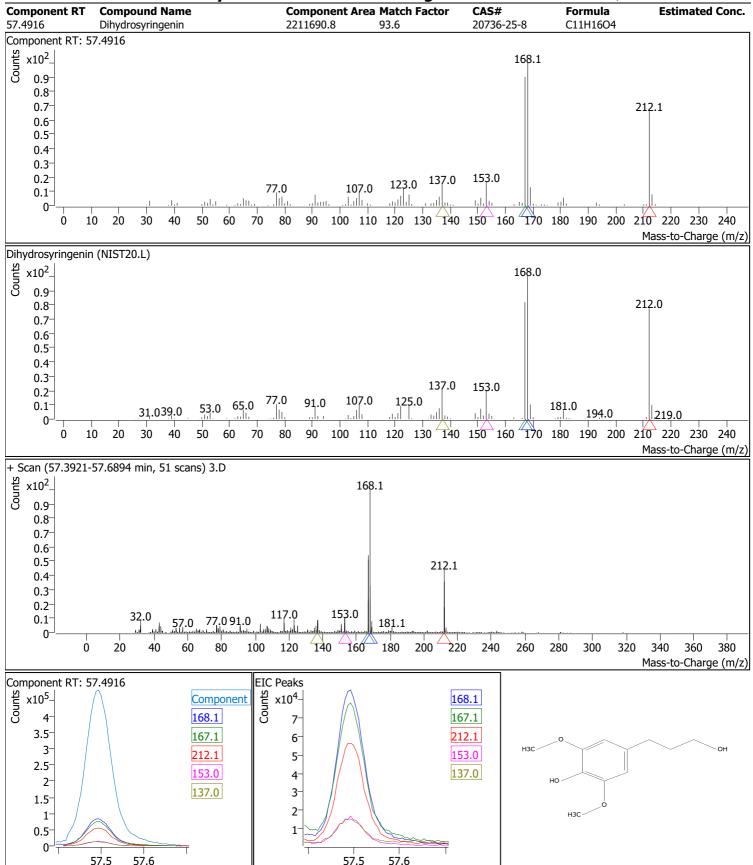






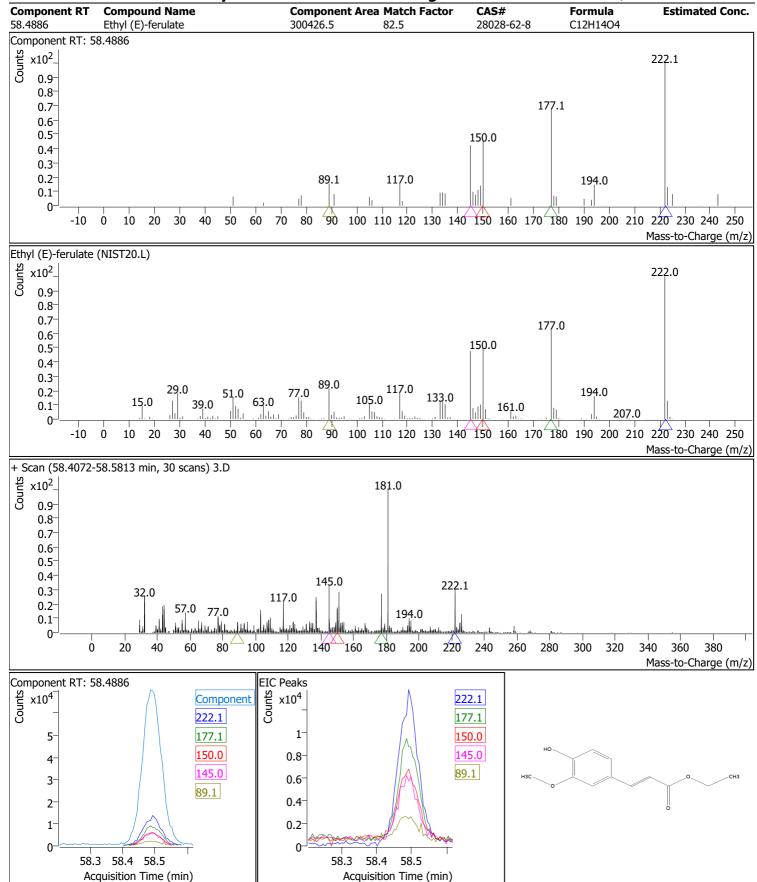






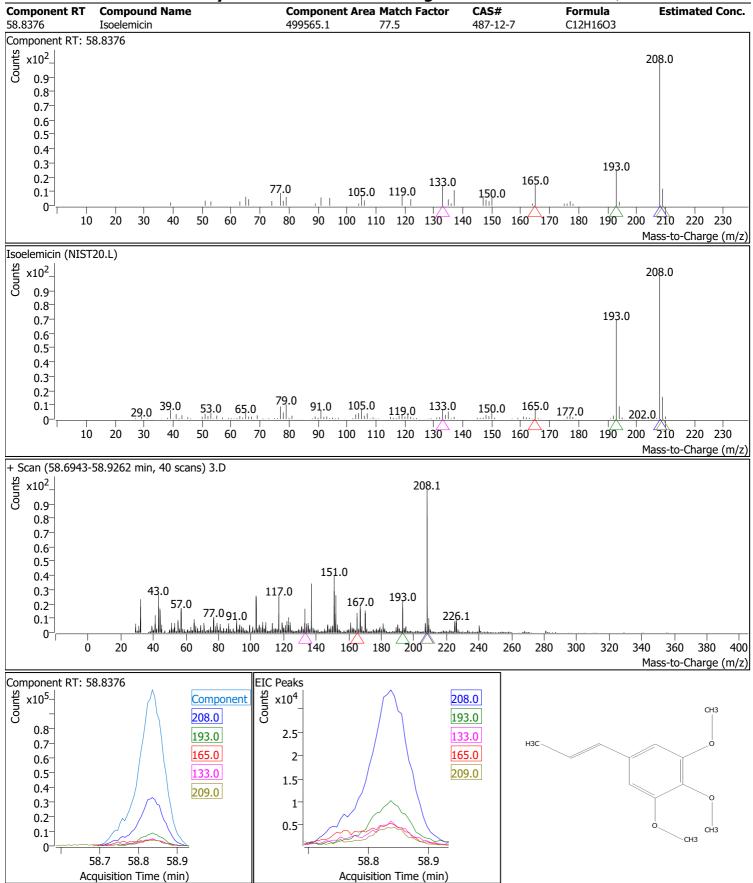


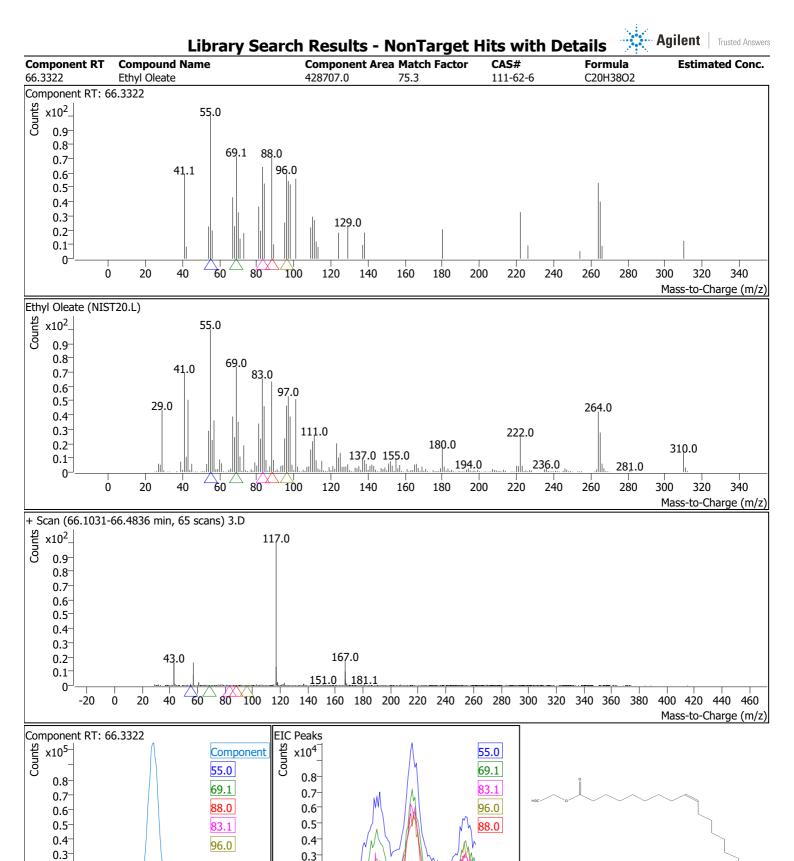












66.4

Acquisition Time (min)

0.2

66

0.2

0.1

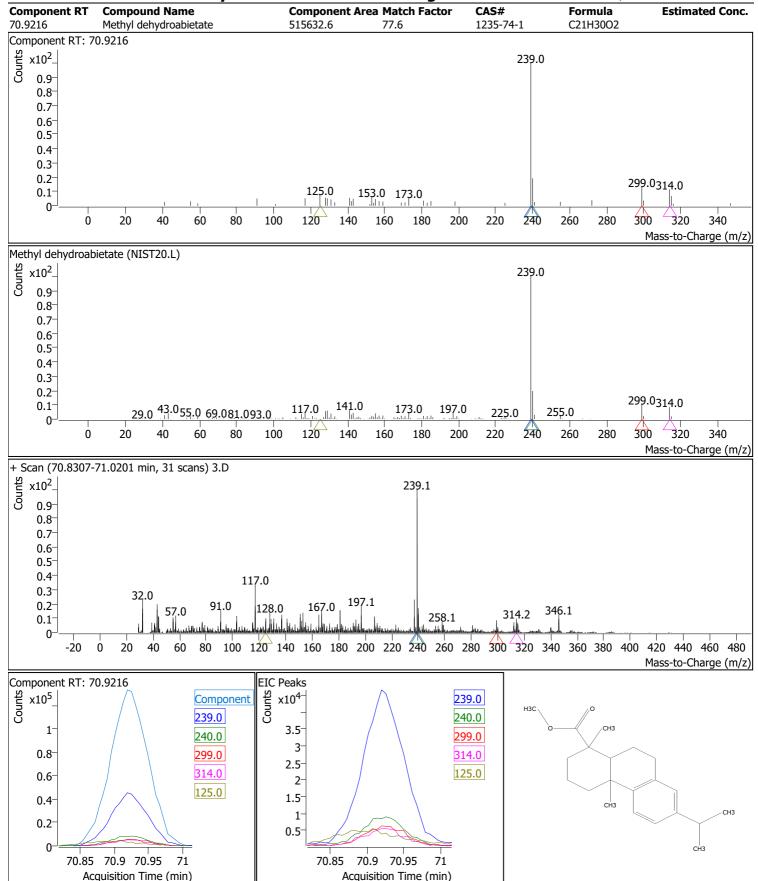
66

66.2

66.4

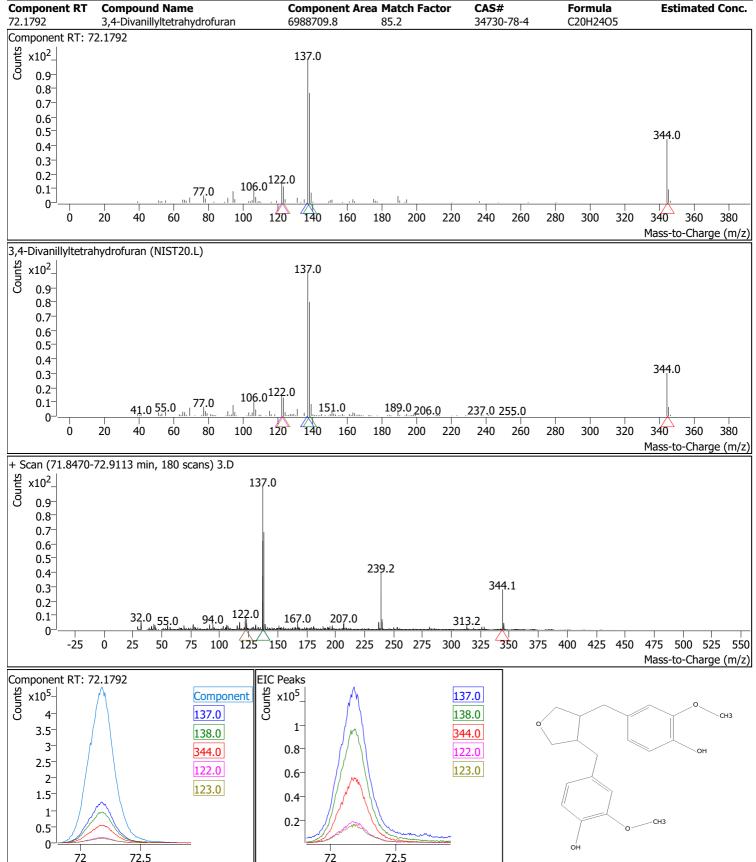












Compound Name Component Area Match Factor Component RT CAS# **Formula Estimated Conc.** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6355 8879953.9 5155-70-4 C20H28O2 Component RT: 73.6355 $x10^{2}$ 285.1 239.2 0.9 0.8 0.7 0.6 0.5 197.1 0.4^{-} 300.2 0.3 141.0 0.2 0.1 300 200 240 280 320 0 20 40 60 80 100 120 140 160 180 220 260 Mass-to-Charge (m/z) 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.)]- (NIST20.L) Counts x10²_ 285.0 0.9 0.8 239.0 0.7° 0.6 0.5 0.4 300.0 0.3 197.0 43.0 0.2 141.0 55.0 _{69.0} 91.0 183.0 0.1 225.0 255.0 240 280 300 0 20 40 60 80 100 120 140 160 180 200 220 260 320 Mass-to-Charge (m/z) + Scan (73.4881-73.8210 min, 57 scans) 3.D 돌 x10². 239.2 0.9 0.8 285.2 0.7 0.6 0.5 197.1 0.4 300.2 0.3 117.0 141.0 0.2 43.1 183.1 0.1 91.0 175 200 225 250 275 25 50 100 300 325 350 375 400 425 450 475 500 525 550 -25 75 125 Mass-to-Charge (m/z) Component RT: 73.6355 EIC Peaks St x10⁶. x10⁵-239.2 Component 285.1 1.8 285.1 СНЗ 1.6 239.2 197.1 1.2 1.4 197.1 300.2 1 1.2 300.2 141.0 0.8^{-} 1 0.8 141.0

73.7

Acquisition Time (min)

73.6

73.8

0.6

0.4

0.2

0.6

0.4

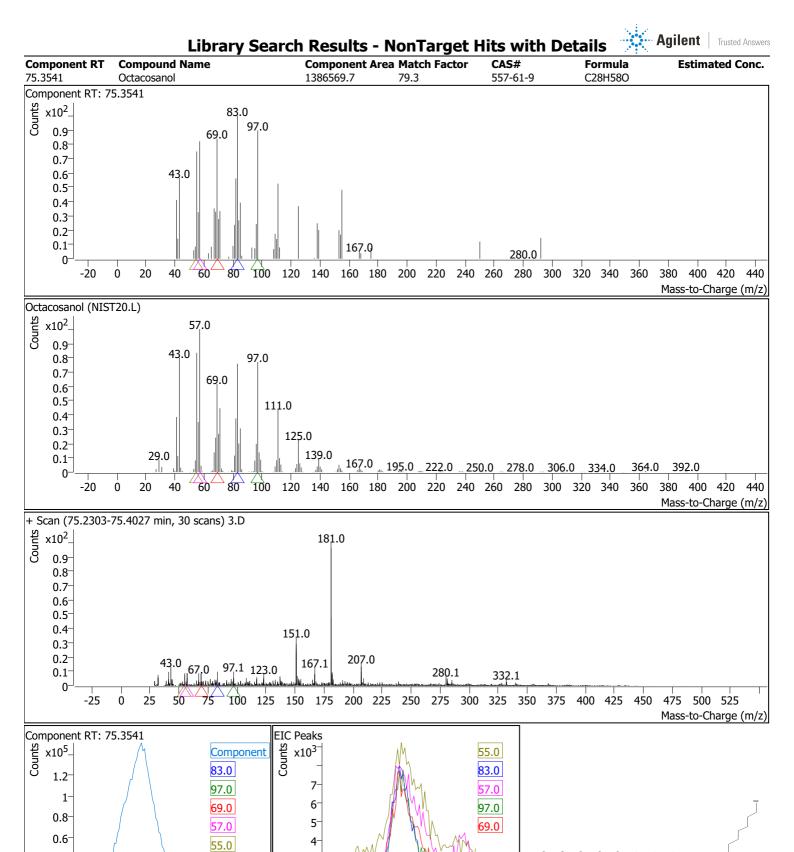
0.2

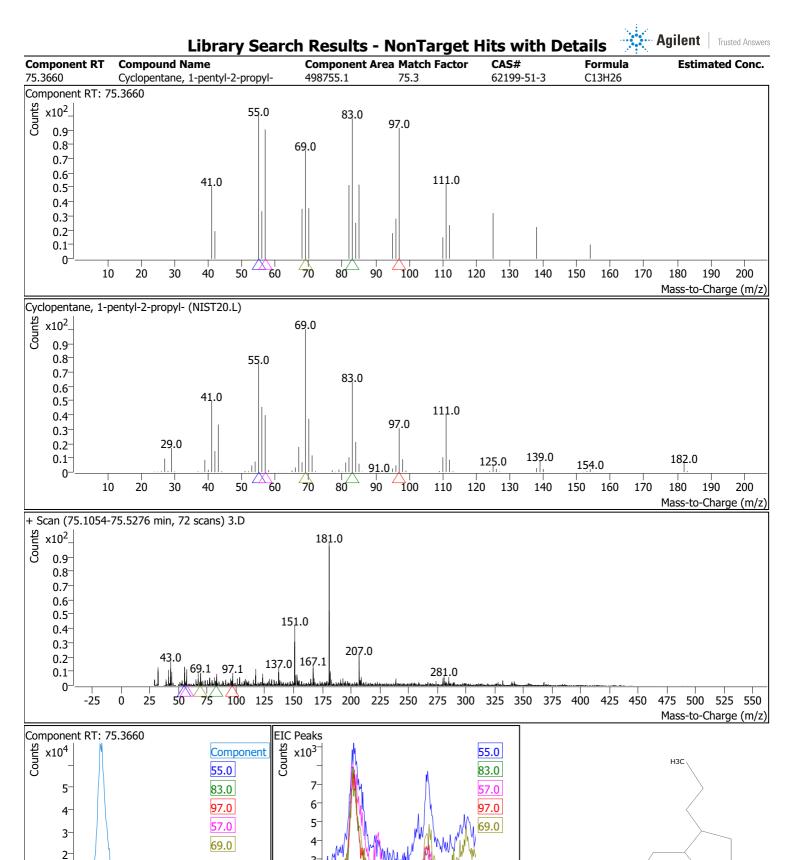
73.6 73.7

Acquisition Time (min)

73.8

СНЗ





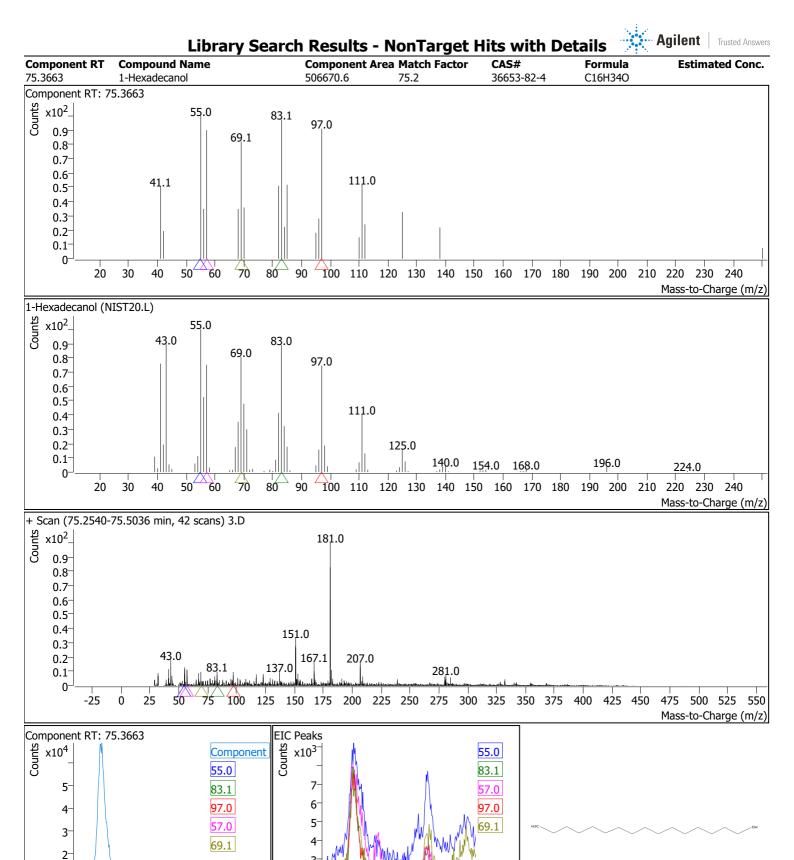
76

Acquisition Time (min)

1

75.5

76

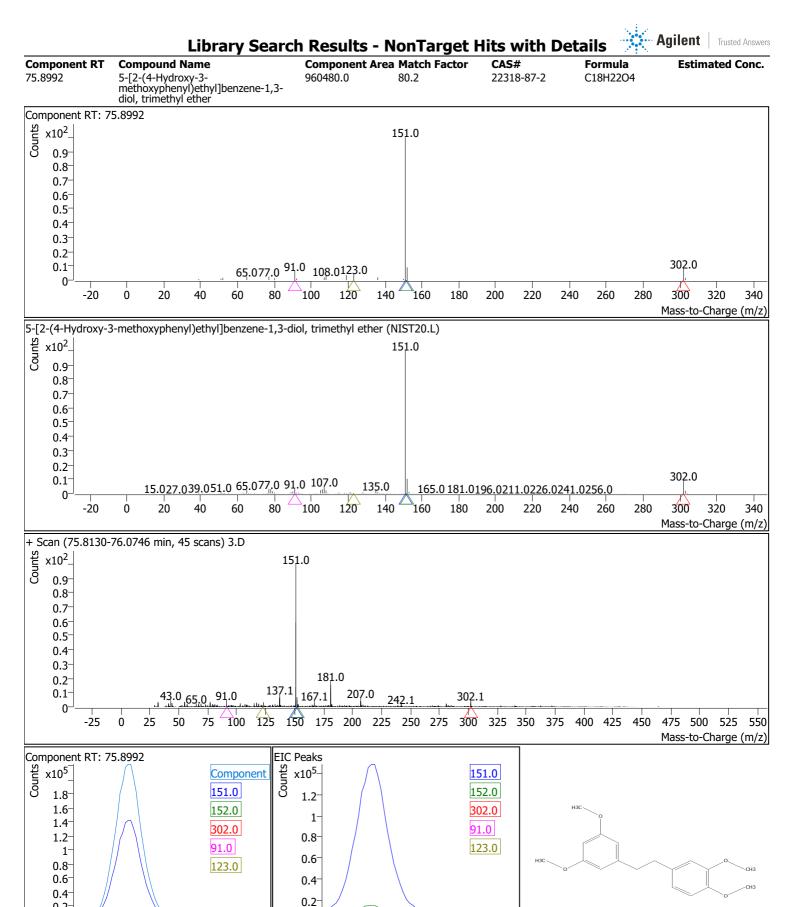


76 Acquisition Time (min)

1

75.5

76



76

Acquisition Time (min)

0.2

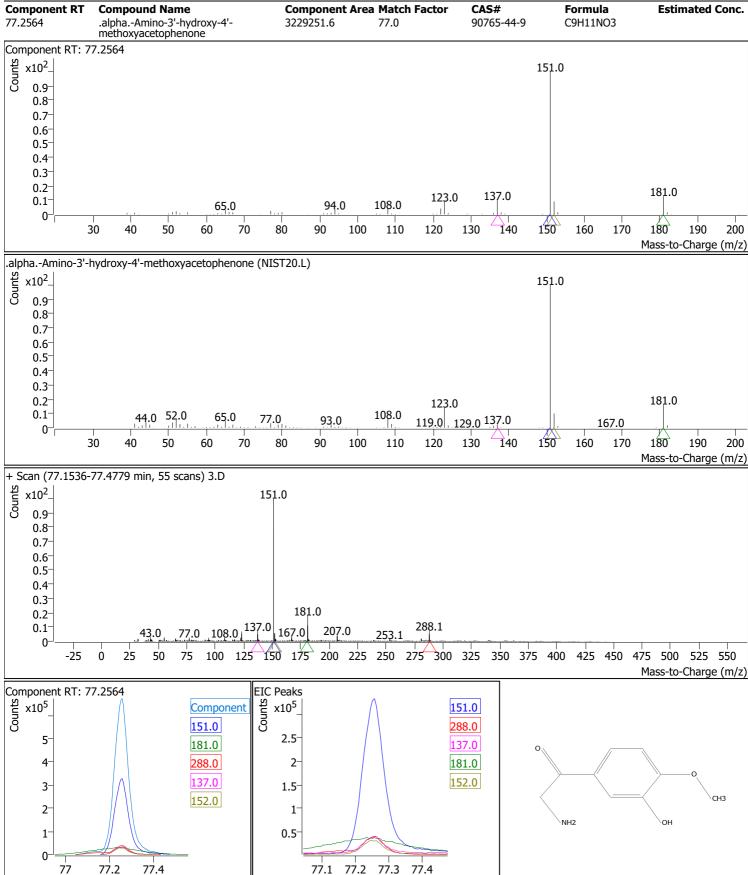
75.8

75.9

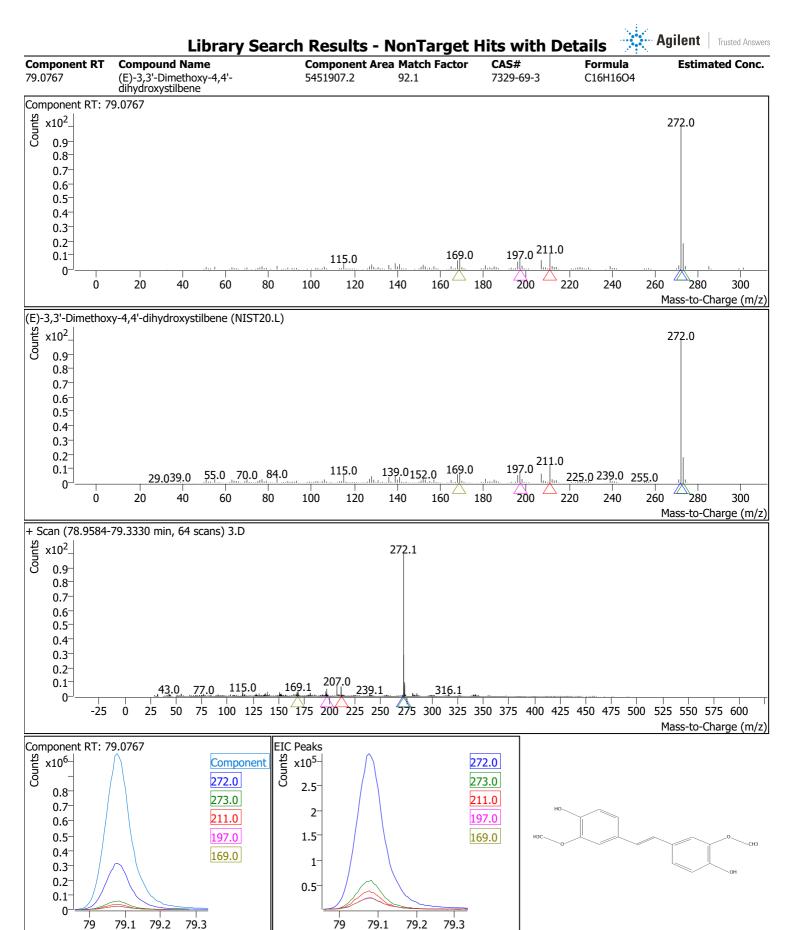
76

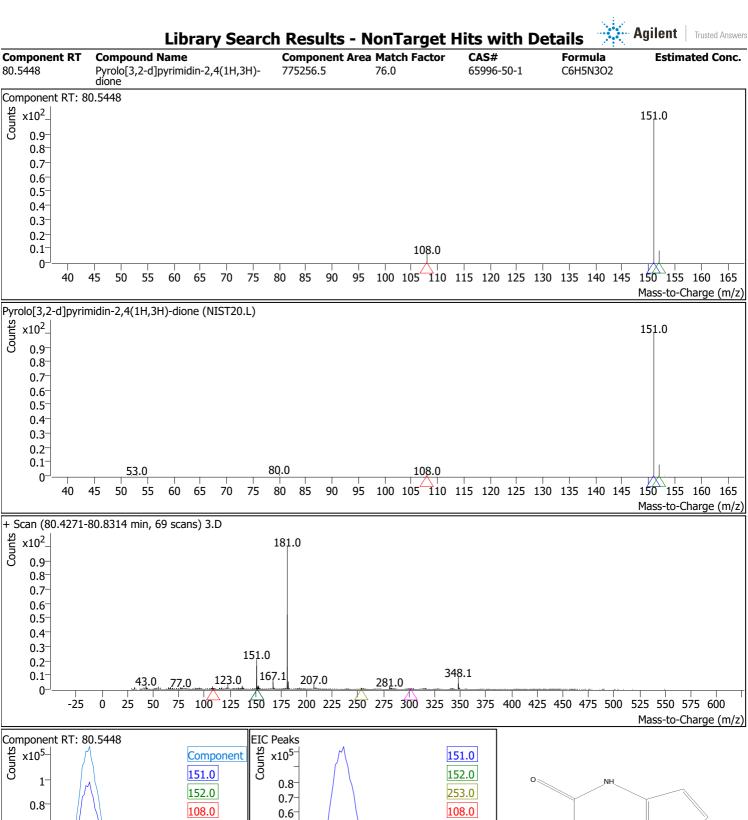
Library Search Results - NonTarget Hits with Details

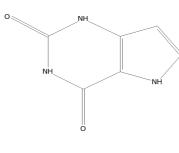




Acquisition Time (min)







··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Carbonic acid, monoamide, N-(2-pentyl)-N-hexadecyl-, methyl ester 83.2119 529240.2 76.1 1000490-06-6 C23H47NO2 Component RT: 83.2119 Counts x10²_ 326.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 0.1 163.1 76.0 125.0 0-320 340 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 360 380 400 Mass-to-Charge (m/z) Carbonic acid, monoamide, N-(2-pentyl)-N-hexadecyl-, methyl ester (NIST20.L) Counts x10² 326.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 116.0 29.043.0 354.0 71.0 310.0 268.0 0 340 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 360 380 400 Mass-to-Charge (m/z) + Scan (83.1861-83.2217 min, 7 scans) 3.D x10²_ 326.1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 207.0 0.2 137.0, 167.1 281.0 32.0 55.0 77.0 225.0251.0 0.1 370.0 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 50 75 Mass-to-Charge (m/z) Component RT: 83.2119 **EIC Peaks** Counts Counts x10⁴ x10⁴ 326.1 Component 326.1 327.1 3 327.1 125.0 3.5 2.5 152.0 163.1 3 2-163.1 2.5

1.5

1-

0

83

83.1

83.2

Acquisition Time (min)

125.0

2

1⁻ 0.5⁻

83

83.1

83.2

Acquisition Time (min)

1.5