Library Search Results - NonTarget Hits with Details



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

D:\MassHunter\GCMS\1\data\RBEL\240501 scan **File Name** 8.D **Path Name Sample Name** 8 **Sample Type** Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

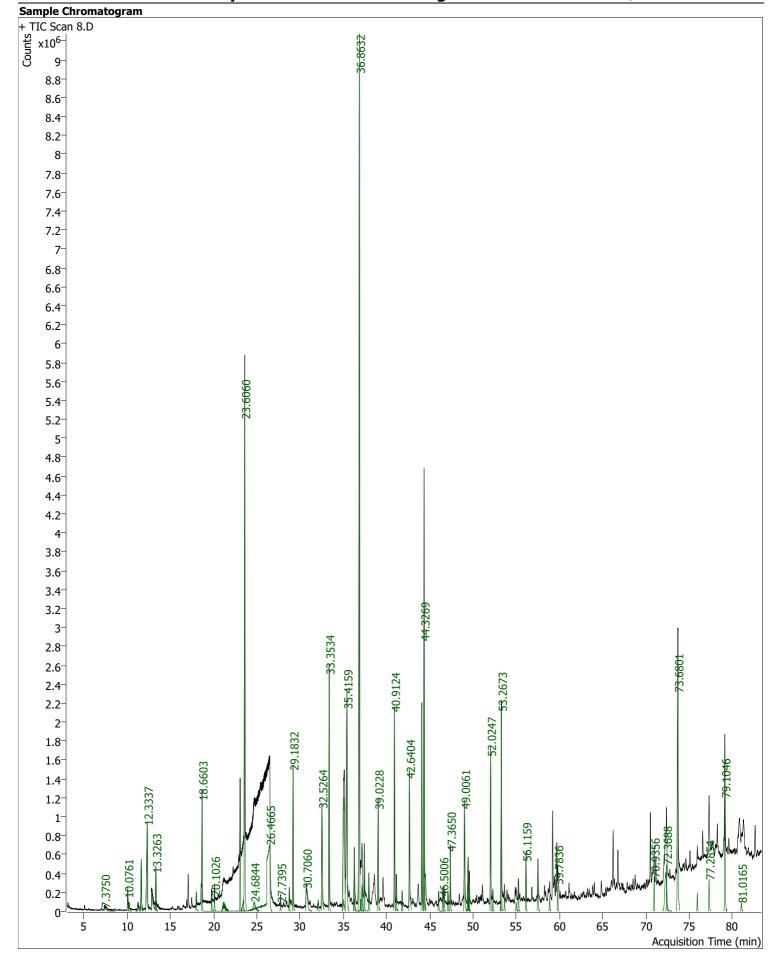
Acq. Date-Time 5/2/2024 12:12:32 AM **Instrument Name** GCMSD Dil. 1

Component R1	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
7.3750	1,3-Propanediol	504-63-2	C3H8O2	587449.6	90.7	
10.0761	2-Propanone, 1-methoxy-	5878-19-3	C4H8O2	660755.3	79.2	
10.2362	Ethanedioic acid, diethyl ester	95-92-1	C6H10O4	470373.7	76.2	
11.2401	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	509039.3	85.0	
11.6344	2-(2-methoxyethoxy)propanoic acid, O-acetyl-	1000506-61-7	C8H14O5	2473695.4	78.0	
11.6349	Ethanol, 2-(1,1-dimethylethoxy)-	7580-85-0	C6H14O2	2476129.6	78.1	
12.3337	Butyrolactone	96-48-0	C4H6O2	6456087.9	97.8	
12.8384	Methyltartronic acid	595-98-2	C4H6O5	2160242.7	96.9	
13.3201	Acetoin	513-86-0	C4H8O2	484970.7	90.9	
13.3263	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	1975182.8	80.1	
17.9958	Phenol	108-95-2	C6H6O	700432.3	95.6	
18.6603	Diisoamyl ether	544-01-4	C10H22O	4384376.5	98.0	
19.7726	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	611835.9	93.0	
20.1026	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	C6H8O2	738547.5	94.5	
21.1683	1,3,5-Trioxane	110-88-3	C3H6O3	878545.1	86.1	
21.1805	n-Propyl acetate	109-60-4	C5H10O2	1156839.0	75.3 81.2	
21.1921 23.0639	1,3,5-Trioxane	110-88-3 111-87-5	C3H6O3 C8H18O	1982775.7 3578628.8	98.2	
23.4697	1-Octanol Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	1069865.0	93.0	
23.6060	Phenol, 2-methoxy-	90-05-1	C7H8O2	23300634.5	99.1	
24.6844	Glycerol 1,2-diacetate	102-62-5	C7H12O5	1635166.6	82.4	
26.4665	Propane, 2-fluoro-2-methyl-	353-61-7	C4H9F	19869230.5	75.2	
27.7395	Sulfurous acid, isobutyl pentyl ester	1000309-13-8	C9H20O3S	399689.8	82.2	
28.7557	Naphthalene	91-20-3	C10H8	785251.3	94.7	
29.1832	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	5948493.0	99.2	
30.7060	Catechol	120-80-9	C6H6O2	3011366.3	96.4	
32.1119	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	590154.0	78.9	
32.5264	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	5945948.3	98.5	
33.3534	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	9486325.1	97.5	
35.0244	1,2-Benzenediol, 3-methyl-	488-17-5	C7H8O2	908282.5	91.9	
35.1043	Butanoic acid, anhydride	106-31-0	C8H14O3	14397735.0	82.5	
35.4159	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	15472596.7	80.1	
36.2698	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	3073015.1	82.9	
36.2717	Acetone	67-64-1	C3H6O	689384.1	79.8	
36.8632	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	44727016.7	99.2	
37.0004	Eugenol	97-53-0	C10H12O2	527898.0	79.8	
37.1553	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	2166092.2	78.9	
37.1556	3,4-Dimethoxyphenol, 2-methylpropionate	1000447-30-5	C12H16O4	1671792.7	78.8	
37.4346 37.9519	Phenol, 2-methoxy-4-propyl-	2785-87-7 634-36-6	C10H14O2 C9H12O3	2070909.7 1134466.9	94.0 90.3	
39.0228	1,2,3-Trimethoxybenzene Vanillin	121-33-5	C8H8O3	4892392.2	96.7	
40.9124	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	8266353.4	95.1	
41.1188	trans-Isoeugenol	5932-68-3	C10H12O2	1105968.8	88.8	
41.7955	Eugenol	97-53-0	C10H12O2	540676.2	88.6	
42.6404	Apocynin	498-02-2	C9H10O3	6541822.7	98.0	
44.0776	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	8203582.8	99.2	
44.3254	Ethanol, 2-phenoxy-	122-99-6	C8H10O2	8885996.3	77.4	
44.3269	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	13864490.2	94.4	
44.3392	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6700550.9	92.8	
46.0281	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	574667.8	92.2	
46.5006	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	706235.2	89.6	
46.6486	Butyrovanillone	64142-23-0	C11H14O3	717194.1	91.3	
47.0974	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	522693.2	84.9	
47.3650	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	2416772.0	96.8	
49.0061	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	5751671.5	96.9	
49.3834	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	1472988.8	91.1	
49.4331	7-Methoxy-1-naphthol	67247-13-6	C11H10O2	1294698.1	90.8	
49.4580	2,6-Dimethoxyhydroquinone	15233-65-5	C8H10O4	606239.6	81.9	
49.5612	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	1140124.2	82.7	
52.0247	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	6966394.6	98.2	
52.2956 53.1051	.beta(4-Hydroxy-3-methoxyphenyl)propionic acid 1,6-Dimethoxynaphthalene	1135-23-5 3900-49-0	C10H12O4 C12H12O2	485577.0 506378.9	91.2 80.1	
53.1951 53.2673	Syringylacetone	19037-58-2	C12H12O2 C11H14O4	8568494.0	97.4	
53.6235	3,5-Dimethoxy-4-hydroxybenzeneethanol	20824-45-7	C10H14O4	606528.3	86.8	
55.0255	3,5 5 metroxy i riyaroxyberizericedianor	2002 1 13 /	C10/11/10/	500520.5	00.0	

Library Search Results - NonTarget Hits with Details

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Component	RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
54.9781	Benzoic acid, 4-hydroxy-3,5-dimethoxy-	530-57-4	C9H10O5	502400.3	79.3	
55.2461	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5650-43-1	C11H14O4	1246281.8	92.5	
56.1159	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	2099740.4	82.6	
57.5003	5-(3-Hydroxypropyl)-2,3-dimethoxyphenol	63543-12-4	C11H16O4	2007215.0	92.7	
58.8551	Asarone	2883-98-9	C12H16O3	665825.6	78.6	
59.7836	8-Amino-6,7-dimethoxy-4-methylquinoline	1000213-07-2	C12H14N2O2	1208321.8	80.3	
70.9356	Methyl dehydroabietate	1235-74-1	C21H30O2	1447310.3	90.6	
72.2810	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6519984.3	83.1	
72.3688	Methyl dehydroabietate	1235-74-1	C21H30O2	1915049.0	75.9	
73.6801	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	13674832.1	86.2	
75.9213	5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene- 1,3-diol, trimethyl ether	22318-87-2	C18H22O4	823971.4	82.2	
77.2854	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	1616606.9	92.4	
79.1046	(E)-3,3'-Dimethoxy-4,4'-dihydroxystilbene	7329-69-3	C16H16O4	6403234.0	92.2	
81.0165	Phenol, 4,4'-methylenebis[2,6-dimethoxy-	15640-40-1	C17H20O6	468771.6	82.1	



--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 587449.6 504-63-2 7.3750 1,3-Propanediol 90.7 C3H8O2 Component RT: 7.3750 v10² 0.9 58.0 0.8 0.7^{-} 31.0 0.6 0.5 0.4 0.3 45.0 0.2 0.1 40.0 55 15 25 65 70 75 5 10 20 30 35 40 45 50 80 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts 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 5 10 15 20 25 30 35 40 45 50 65 70 75 80 Mass-to-Charge (m/z) + Scan (7.3326-8.6764 min, 227 scans) 8.D St x10² 0.9 32.0 0.8 0.7 58.0 0.6 0.5 0.4^{-} 44.0 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: 7.3750 **EIC Peaks** Counts Counts x10⁴ x10⁴ 57.0 Component 58.0 58.0 3 0.8 57.0 31.0 2.5 0.7 31.0 43.0 0.6 2

8

Acquisition Time (min)

8.2 8.4 8.6

45.0

45.0

43.0

8.5

Acquisition Time (min)

1.5

0.5

1-

7.5

0.5

 0.4°

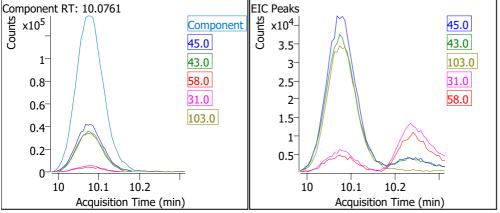
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0.2

0.1

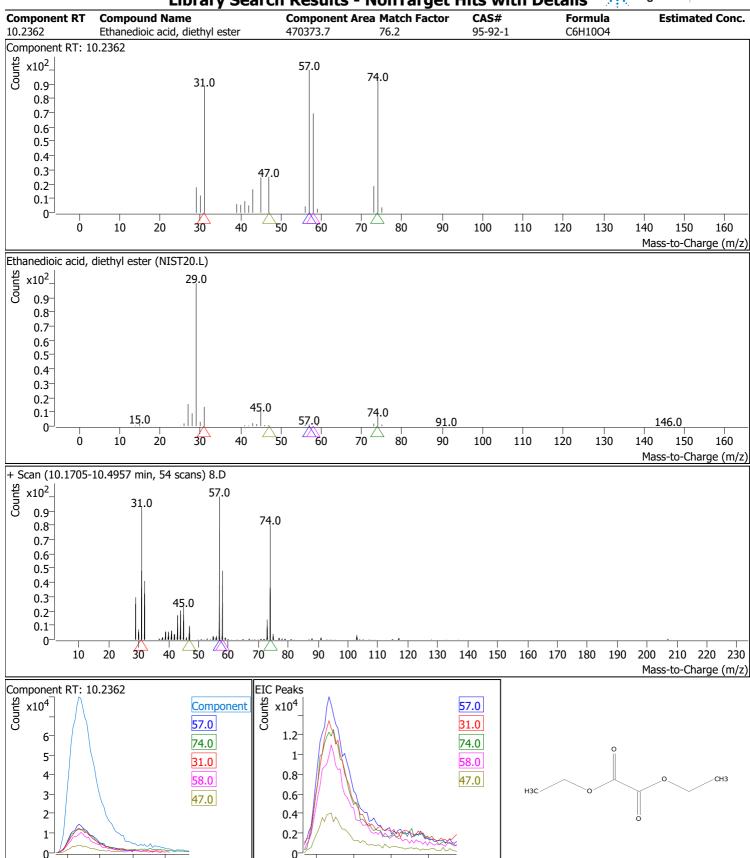
7.4 7.6 7.8

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5878-19-3 10.0761 2-Propanone, 1-methoxy-660755.3 C4H8O2 Component RT: 10.0761 v10² 0.9 45.0 0.8 0.7^{-} 0.6 43.0 0.5 0.4 0.3 0.2 58.0 0.1 31.0 74.0 89.0 0 75 85 5 10 15 20 25 30 35 40 50 55 60 65 70 90 95 Mass-to-Charge (m/z) 2-Propanone, 1-methoxy- (NIST20.L) Counts x10²_ 0.9 45.0 0.8 43.0 0.7 0.6 0.5 58.0 0.4 0.3 0.2 29.0 0.1 15.0 27.0 31.0 88.0 39.0 53.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (9.9804-10.3115 min, 56 scans) 8.D st x10² 0.9 0.8 103.0 0.7 0.6 0.5 57.0 0.4^{-} 31.0 0.3 74.0 0.2 117.1 88.0 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: 10.0761 **EIC Peaks** x10⁴_ 45.0 Component



Library Search Results - NonTarget Hits with Details





10.2

10.3

10.4

Acquisition Time (min)

10.5

10.2 10.3 10.4 10.5

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 623-39-2 11.2401 1,2-Propanediol, 3-methoxy-509039.3 85.0 C4H10O3 Component RT: 11.2401 v10² 0.9 45.0 0.8 0.7^{-} 0.6 0.5 43.0 75.0 0.4 0.3 61.0 31.0 0.2 33.0 88.0 0.1 10 15 20 25 30 55 60 75 80 85 100 105 110 115 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Counts x10²_ 0.9 45.0 0.8 0.7 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 15.0 0.2 33.0 18.0 0.1 88.0 63.0 103.0 71.0 10 15 20 25 30 35 40 50 55 60 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (11.1817-11.4769 min, 49 scans) 8.D St x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4^{-} 75.0 31.0 0.3 0.2 61.0 0.1 88.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.2401 **EIC Peaks** Counts x10⁴ Counts x10⁴ 45.0 Component 45.0 43.0 1.6 43.0 75.0 1.4



11.1 11.2 11.3 11.4

Acquisition Time (min)

75.0

61.0

31.0

11.4

3

2

1

11.2

Acquisition Time (min)

1.2

1

0.8

0.6

0.4

0.2

CH3

ОН

31.0

61.0

··· 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-1000506-61-7 11.6344 2473695.4 78.0 C8H14O5 Component RT: 11.6344 x10². 103.0 43.0 0.9 87.0 8.0 0.7 57.0 0.6 31.0 0.5 0.4 0.3 0.2^{-} 117.0 0.1 0-30 0 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) 2-(2-methoxyethoxy)propanoic acid, O-acetyl- (NIST20.L) $x10^{2}$ 43.0 0.9 0.8 59.0 0.7 0.6 0.5 0.4 103.0 0.3 0.2 29.0 0.1 15.0 87.0 73.0 117.0 130.0 147.0 0 30 40 90 130 0 10 20 50 60 70 80 100 110 120 140 150 160 Mass-to-Charge (m/z) + Scan (11.5145-11.8575 min, 58 scans) 8.D x10². 0.9 103.0 0.8 0.7 87.0 0.6 31.0 0.5 57.0 0.4 0.3 0.2 0.1 117.0 96.0 0 30 40 90 200 210 220 10 20 50 60 70 80 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) Component RT: 11.6344 **EIC Peaks** Counts Counts x10⁴ x10⁵ 103.0 Component 103.0 43.0 4 6 43.0 87.0 3.5 5 87.0 3 57.0

11.7

Acquisition Time (min)

11.8

31.0

нзс

4

3

2

11.6

57.0

31.0

2.5

1.5

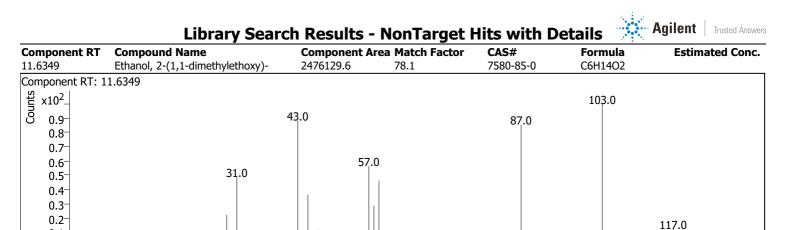
2

1⁻ 0.5⁻

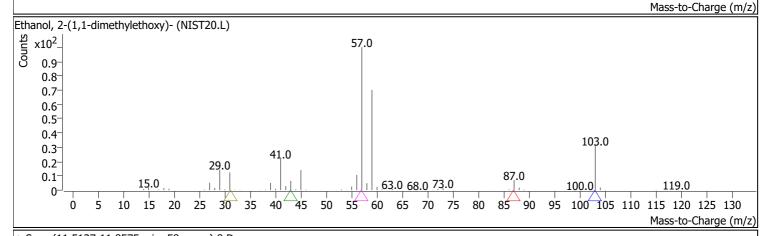
11.7

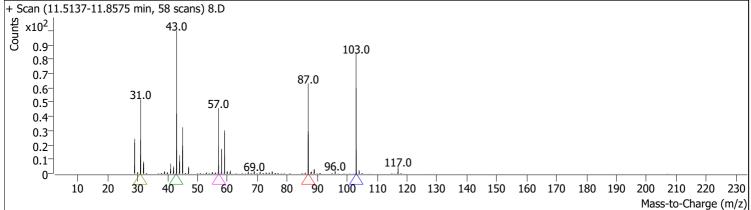
Acquisition Time (min)

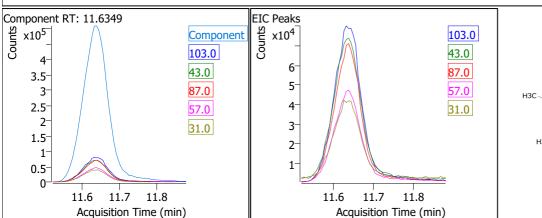
11.8



80 85







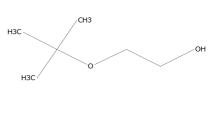
40[∠]

50 55 60 65 70 75

25 30 35

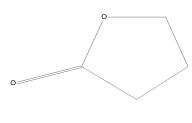
15

0.1



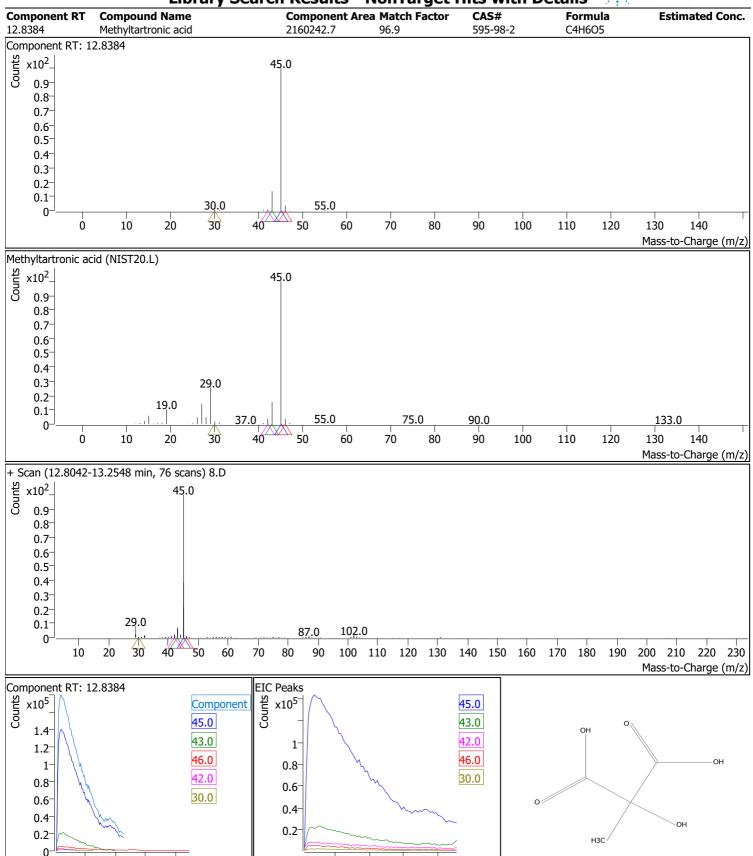
95 100 105 110 115 120 125 130

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 96-48-0 12.3337 Butyrolactone 6456087.9 97.8 C4H6O2 Component RT: 12.3337 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 25 40 55 75 20 30 35 45 50 60 65 70 80 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) Counts x10²_ 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 (12.1454-12.5116 min, 62 scans) 8.D St x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 86.0 0.3 29.0 56.0 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 12.3337 Counts Counts x10⁵-42.0 Component 42.0 2.25 41.0 41.0 86.0 6 1.75



Library Search Results - NonTarget Hits with Details





13

13.1

Acquisition Time (min)

13.2

12.9

13.2 13.4 13.6

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13.4

Acquisition Time (min)

47.0

88.0

39.0

13.5

3

2-

13.3

0.6

 0.5^{-}

 0.4^{-}

0.3⁻ 0.2⁻ 0.1⁻

13.3

13.4

Acquisition Time (min)

88.0

39.0

13.5

нзс

ОН

-CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 13.3263 Propane, 1,1-diethoxy-1975182.8 80.1 C7H16O2 Component RT: 13.3263 v10² 0.9 103.0 0.8 43.0 87.0 0.7 0.6 57.0 31.0 0.5 0.4 0.3 0.2 0.1 0 40² 30 70 130 10 20 50 60 90 100 110 120 140 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 78.0 131.0 130 10 20 30 40 50 60 70 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (13.2251-13.5105 min, 49 scans) 8.D St x10² 0.9 45.0 0.8 103.0 0.7 0.6 0.5 87.0 0.4^{-} 57.0 29.0 0.3 0.2 0.1 117.0 69.0 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: 13.3263 **EIC Peaks** Counts Counts x10⁴ 103.0 Component 103.0 43.0 6 3 43.0 87.0 5 Н3С < 2.5 87.0 57.0

31.0



57.0

31.0

3

2-

13.3

13.4

Page 13 of 81

Acquisition Time (min)

13.5

2

1.5

0.5

13.3

13.4

Acquisition Time (min)

13.5

--- 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 17.9958 Phenol 700432.3 95.6 C6H6O Component RT: 17.9958 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 55.0 63.0 50.0 95 25 20 30 35 40 45 50 55 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) Phenol (NIST20.L) S 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 95 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 Mass-to-Charge (m/z) + Scan (17.9236-18.2495 min, 55 scans) 8.D St x10² 0.9 94.0 0.8 0.7 0.6 0.5 61.0 0.4^{-} 43.0 65.0 0.3 0.2 32.0 117.0 0.1 103.0 75.0 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: 17.9958 **EIC Peaks** Counts Counts x10⁴ 94.0 Component 94.0 66.0 4.5 66.0 65.0 1 39.0 65.0 3.5 0.8 3

18.1

Acquisition Time (min)

18.2

95.0

39.0

95.0

2.5

1.5⁻

2-

18

0.6

0.4

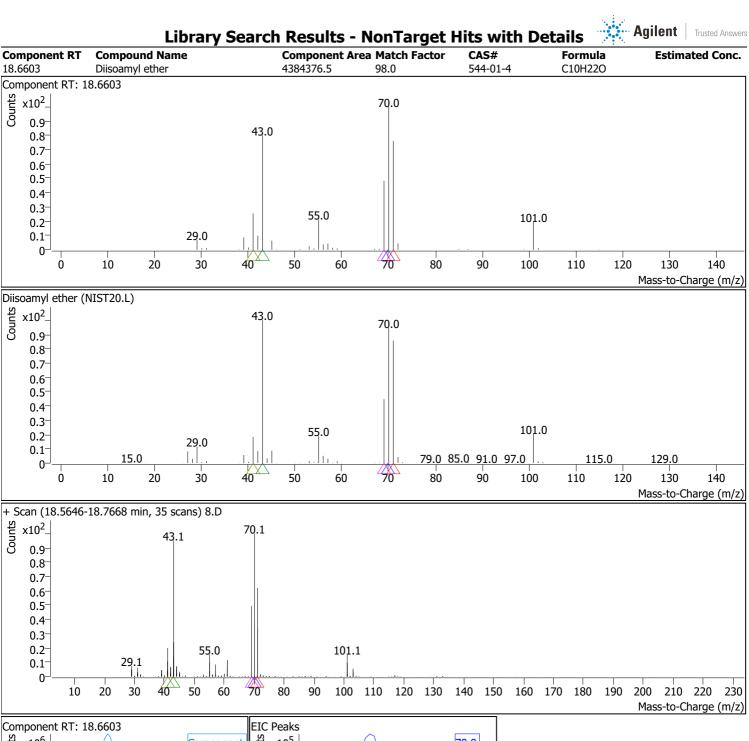
0.2

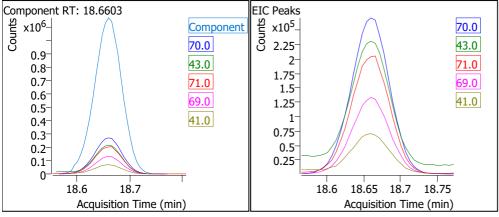
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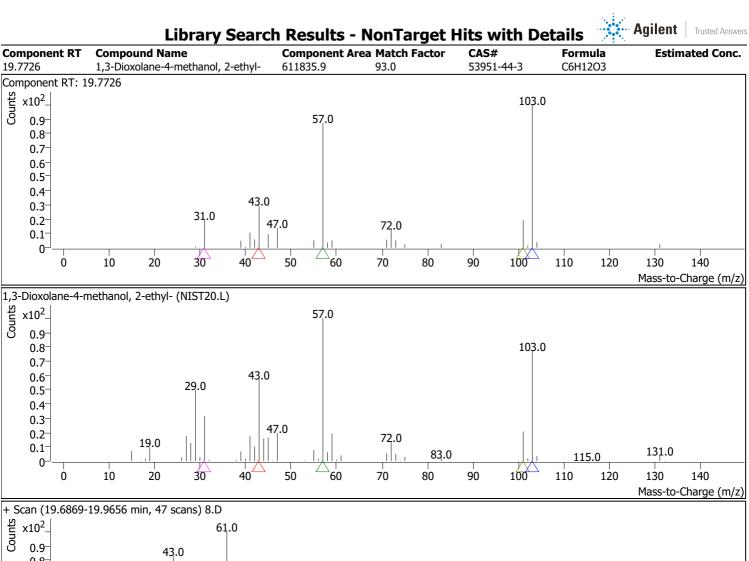
18.1

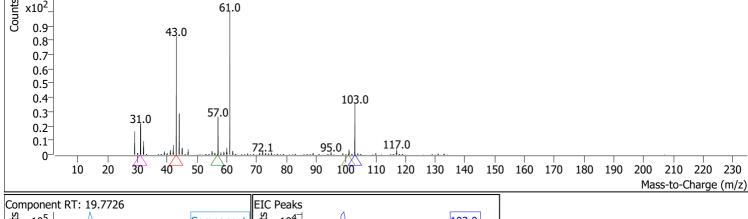
Acquisition Time (min)

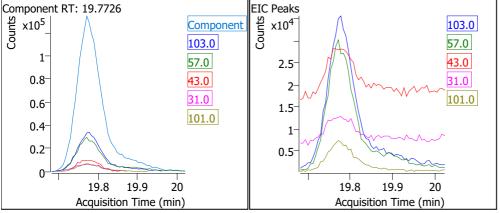
18.2











--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 80-71-7 20.1026 2-Cyclopenten-1-one, 2-hydroxy-3-738547.5 94.5 C6H8O2 methyl-Component RT: 20.1026 x10². 112.0 0.9 8.0 0.7 0.6 0.5 69.1 55.0 0.4 41.1 83.0 0.3 39.0 0.2^{-} 99.0 0.1 0-70 55 30 35 40 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 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (20.0255-20.2414 min, 37 scans) 8.D x10². 61.0 0.9 0.8 0.7 0.6 0.5 112.0 0.4 0.3 31.0 55.0 0.2 69.0 83.0 0.1 117.0 103.0 0 70 190 200 210 220 230 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 20.1026 **EIC Peaks** Counts Counts $x10^{4}$ x10⁵ 112.0 Component 112.0 55.0 3 1.2 69.1 69.1 2.5 1 55.0 41.1 2 8.0 41.1 83.0 нзс

20.1

20.2

Acquisition Time (min)

1.5

0.5

1

83.0

0.6

0.4

0.2

20.1

20.2

Acquisition Time (min)

ОН

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 110-88-3 21.1683 1,3,5-Trioxane 878545.1 86.1 C3H6O3 Component RT: 21.1683 v10² 0.9 89.0 0.8 0.7 0.6 0.5 31.0 0.4 61.0 0.3 0.2 42.0 0.1 56.0 29.0 55 90 75 10 15 20 25 30 35 40 45 50 60 65 70 80 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 56.0 200 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.9234-21.7695 min, 143 scans) 8.D st x10² 0.9 0.8 0.7 43.0 0.6 0.5 0.4^{-} 0.3 31.0 0.2 89.0 0.1 90 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 21.1683 **EIC Peaks** Counts Counts x10⁴ x10⁵ Component 61.0 89.0 31.0 8.0 3.5 31.0 89.0 0.7 3 42.0 61.0 0.6 2.5 0.5 42.0 90.0 2 0.4 90.0

0.3

0.2 0.1 0-

21

21.2

21.4

Acquisition Time (min)

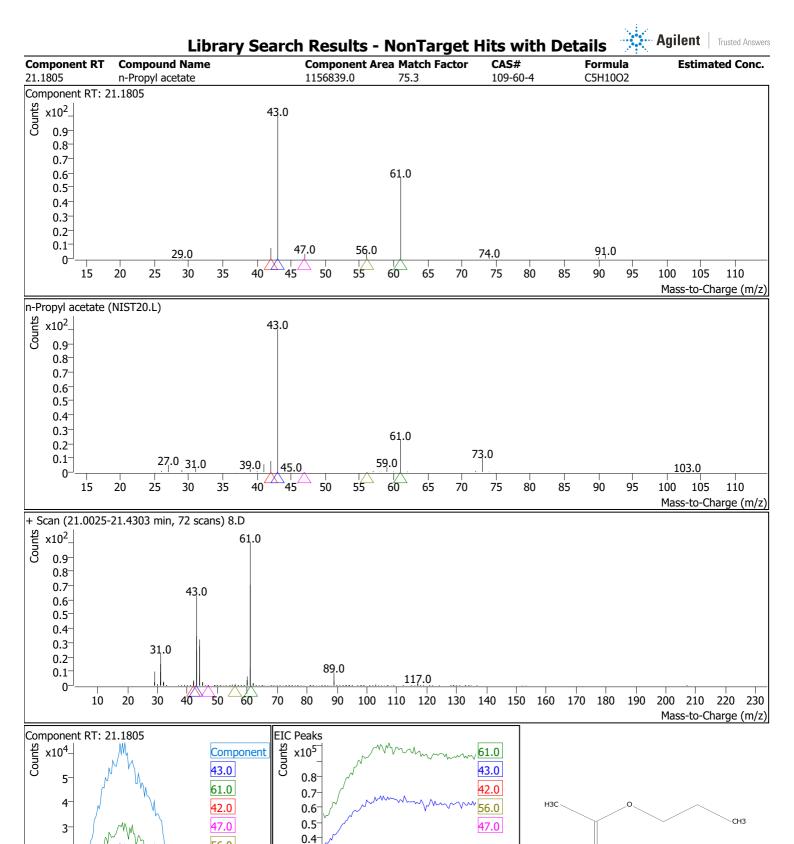
21.6

1.5

1

21

21.2 21.4 21.6





21.2

21.4

Acquisition Time (min)

56.0

0.3⁻

0.1

21

2

1

21.2

21.4

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 21.1921 1,3,5-Trioxane 1982775.7 81.2 110-88-3 C3H6O3 Component RT: 21.1921 v10² 0.9 61.0 0.8 0.7 43.0 89.0 0.6 0.5 0.4 0.3 31.0 0.2 0.1 47.0 56.0 55 690 10 15 20 25 30 35 50 60 65 70 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 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.9234-21.7695 min, 143 scans) 8.D st x10² 0.9 0.8 0.7 43.0 0.6 0.5 0.4^{-} 0.3 31.0 0.2 0.1 89.0 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: 21.1921 **EIC Peaks** Counts Counts x10⁴ x10⁵ Component 61.0 43.0 7 0.8 43.0 31.0 0.7 6 89.0 89.0 0.6 5 0.5 31.0 42.0 4 0.4 42.0 3

21.2

21.4

Acquisition Time (min)

21.6

0.3

0.2

2

21.2 21.4 21.6

--- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0639 1-Octanol 3578628.8 98.2 111-87-5 C8H18O Component RT: 23.0639 v10² 0.9 56.0 41.0 69.0 0.8 0.7 84.0 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 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 (22.9812-23.1690 min, 32 scans) 8.D st x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4^{-} 31.0 0.3 55.1 0.2^{-} 70.1 84.1 0.1 103.0 117.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 23.0639 EIC Peaks Counts x10⁵⁻ Counts x10⁵-56.0 Component 56.0 55.0 0.8 6 55.0 41.0 0.7 5 41.0 70.0 0.6

23.1

23.2

Acquisition Time (min)

4

3

2

1

23

23.1

23.2

Acquisition Time (min)

69.0

70.0

0.5⁻ 0.4⁻

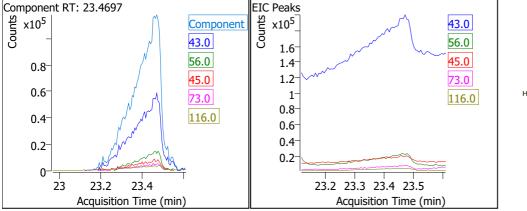
0.3

0.2

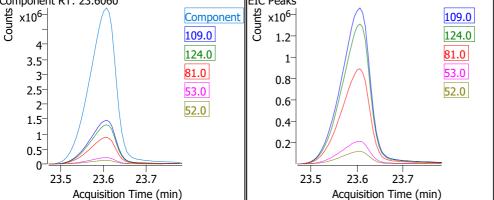
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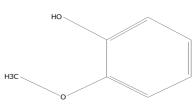
23

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1069865.0 23.4697 Pentanoic acid, 4-oxo-93.0 123-76-2 C5H8O3 Component RT: 23.4697 v10² 0.9 43.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 56.0 0.2 45.0 73.0 116.0 0.1 101.0 31.0 100 105 110 115 120 15 20 25 30 35 40 55 60 70 85 90 Mass-to-Charge (m/z) Pentanoic acid, 4-oxo- (NIST20.L) st x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 56.0 0.3 0.2 29.0 0.1 101.0 116.0 | 31.0 39.0 53.0 100 105 110 115 120 125 15 20 25 35 40 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (23.2620-23.5534 min, 49 scans) 8.D st x10² 0.9 0.8 61.0 0.7^{-} 0.6 0.5 0.4^{-} 109.0 0.3 124.0 31.0 0.2 81.0 0.1 56.0 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: 23.4697 **EIC Peaks** Counts Counts x10⁵ Component 43.0 43.0 56.0 1.6



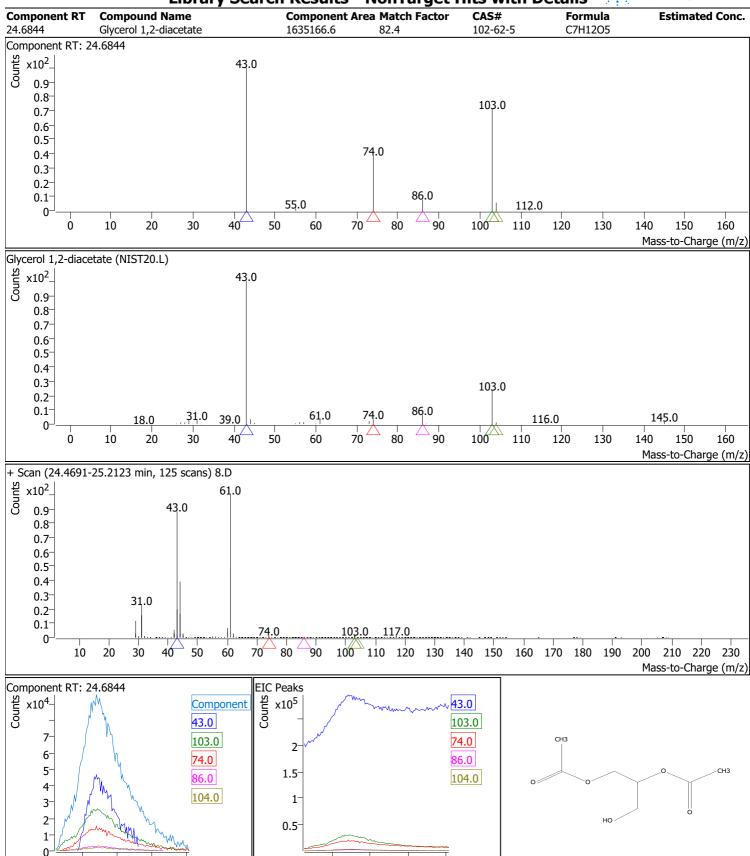
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6060 Phenol, 2-methoxy-23300634.5 99.1 C7H8O2 Component RT: 23.6060 v10² 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 53.0 0.1 39.0 63.0 110 50 80 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 95.0 15.0 110 50 10 20 30 40 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4701-23.7852 min, 54 scans) 8.D st x10² 0.9 109.0 0.8 0.7 124.0 43.0 61.0 0.6 81.0 0.5 0.4^{-} 0.3 0.2 31.0 53.0 0.1 39.0 77.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.6060 Counts Counts x10⁶ 109.0 Component 109.0 124.0 1.2 4 124.0 81.0 1 3.5











24.8

25

Acquisition Time (min)

24.6

24.8

Acquisition Time (min)

24.6

25

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 26.4665 Propane, 2-fluoro-2-methyl-19869230.5 353-61-7 C4H9F Component RT: 26.4665 v10² 0.9 61.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 30.0 45.0 56.0 45 30 55 60 70 75 10 15 20 25 35 40 50 80 Mass-to-Charge (m/z) Propane, 2-fluoro-2-methyl- (NIST20.L) st x10² 0.9 61.0 0.8 0.7 0.6 0.5 0.4 0.3 41.0 0.2 59.0 28.0 0.1 39.0 33.0 47.0 15.0 51.0 60 15 45 10 20 25 30 35 40 50 55 65 70 75 80 Mass-to-Charge (m/z) + Scan (23.9755-26.6512 min, 451 scans) 8.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 0.1 0-20 40 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 Mass-to-Charge (m/z) EIC Peaks Component RT: 26.4665 Counts Counts x10⁵ 61.0 Component CH3 61.0 60.0 4.5 4 5 60.0 62.0 3.5 62.0 45.0 3 30.0 30.0

20 21 22 23 24 25 26

Acquisition Time (min)

2.5

1.5

0.5

45.0

2

3

2

1

20

22

24

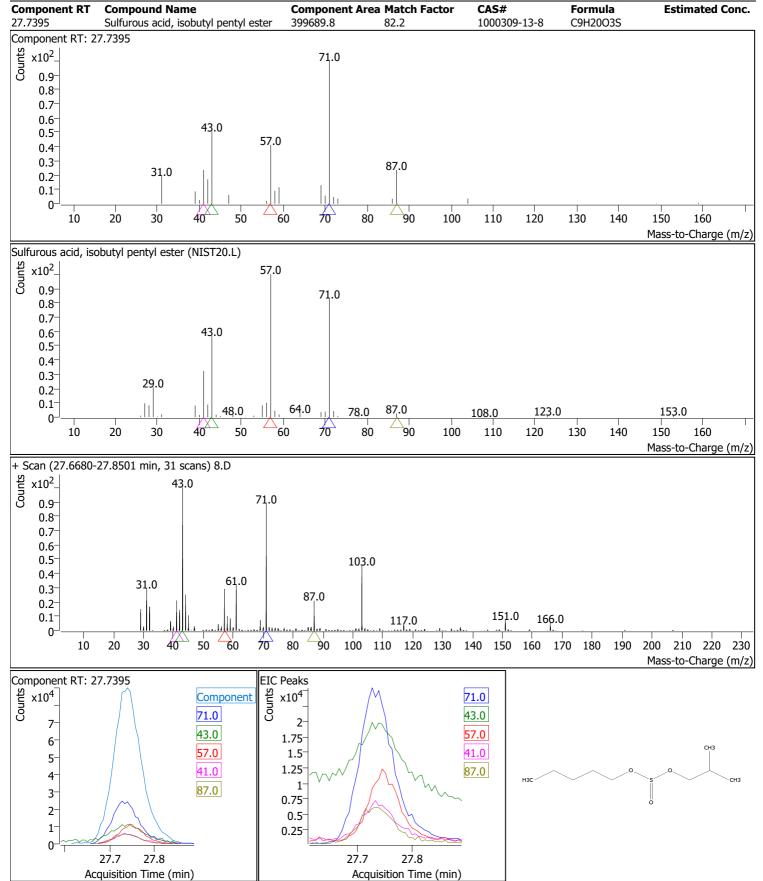
Acquisition Time (min)

26

нзс

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.** 91-20-3 28.7557 Naphthalene 785251.3 C10H8 Component RT: 28.7557 y x10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 77.0 64.0 122.0 130 45 55 75 100 105 110 115 120 Mass-to-Charge (m/z) Naphthalene (NIST20.L) x10²_ 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 51.0 63.0 75.0 87.0 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 135 140 Mass-to-Charge (m/z) + Scan (28.6491-28.9345 min, 49 scans) 8.D St x10²_ 0.9 128.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 103.0 43.0 32.0 57.0 0.1 77.0 138.0 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 28.7557 Counts st x10⁵-1.6x10⁴-128.0 Component 128.0 127.0 1.6 8 7 1.4 127.0 129.0 1.2 6 129.0 102.0 5 1-102.0 126.0

28.8

Acquisition Time (min)

28.9

4

3-

2

1

28.7

126.0

 0.8^{-}

0.6

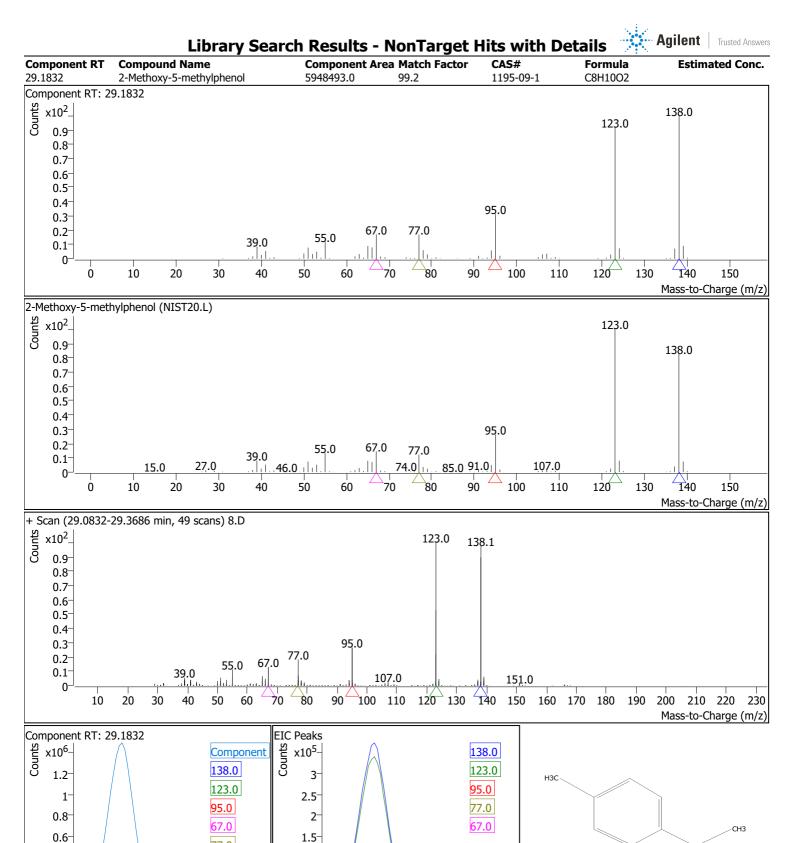
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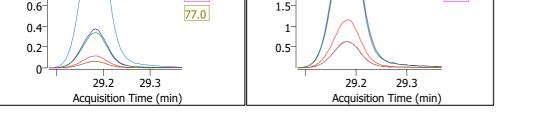
28.7

28.8

Acquisition Time (min)

28.9





--- 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 30.7060 Catechol 3011366.3 96.4 C6H6O2 Component RT: 30.7060 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 ² 95 110 115 120 125 10 15 35 50 55 75 80 85 90 100 105 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10² 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 40 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.6113-31.3642 min, 127 scans) 8.D st x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 81.0 92.0 32.0 0.1 53.0 125.0 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.7060 EIC Peaks Counts Counts x10⁵x10⁵ 110.0 Component 110.0 64.0 0.8 1.75 64.0 63.0 0.7 1.5 63.0 81.0 0.6



31

Acquisition Time (min)

31.2

92.0

0.5

 0.4^{-}

0.3

0.2

 0.1°

81.0

92.0

31.2

1.25

0.75

0.5

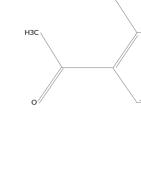
0.25

30.8

31 Acquisition Time (min)

1

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 590154.0 1450-72-2 32.1119 Ethanone, 1-(2-hydroxy-5-78.9 C9H10O2 methylphenyl)-Component RT: 32.1119 x10²_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 96.0 43.0 0.3 77.0 0.2^{-} 67.0 0.1 0-150 0 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) $x10^{2}$ 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 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 (32.0205-32.2643 min, 42 scans) 8.D st x10² 0.9 135.0 0.8 0.7 0.6 0.5 43.0 0.4 96.0 0.3 150.0 32.0 0.2 77.0 0.1 61.0 110.0 0 Ó 80 100 140 200 220 260 300 20 40 60 120 160 180 240 280 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 32.1119 Counts Counts x10⁴– 135.0 x10⁵ Component НО 135.0 96.0 8.0 2 150.0 150.0 0.7 нзс 1.75 96.0 43.0 0.6 1.5 0.5 77.0 43.0 1.25



32.1

Acquisition Time (min)

32.2

1

0.75

0.5

0.25

32

77.0

0.4

0.3

0.2

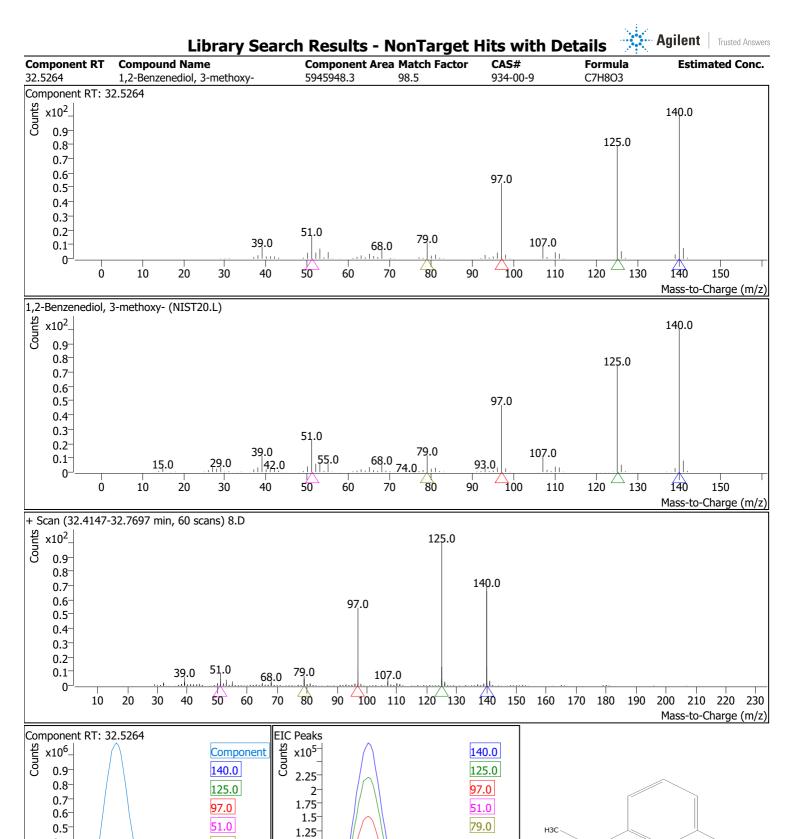
0.1

32

32.1

Acquisition Time (min)

32.2





32.6

Acquisition Time (min)

32.7

0.4

0.3

0.2

0.1

32.5

32.6

Acquisition Time (min)

32.7

79.0

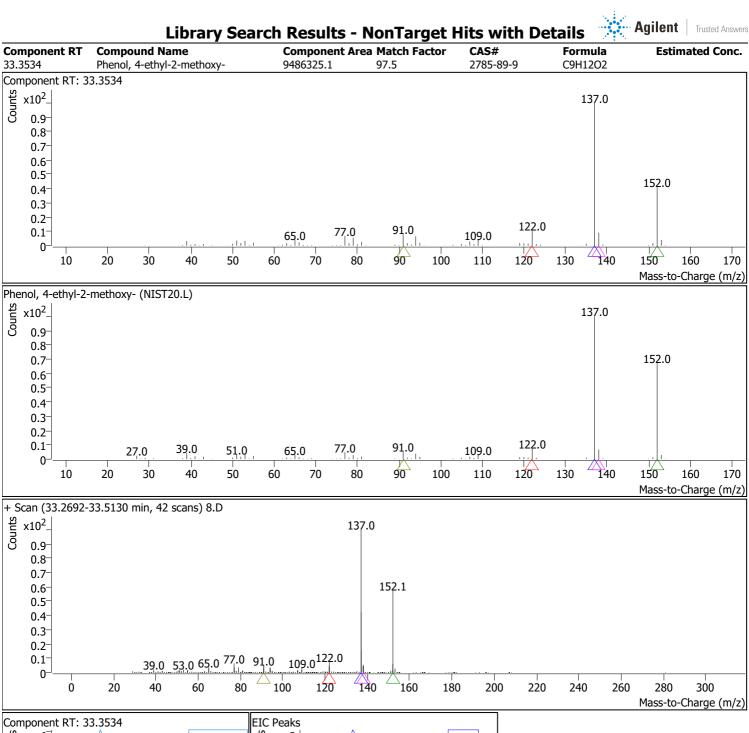
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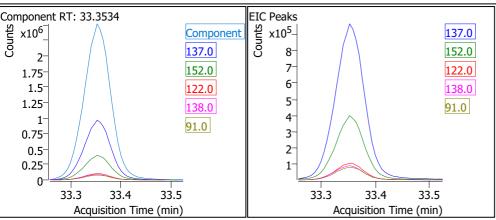
0.5

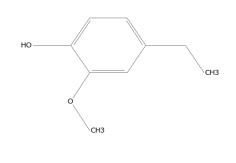
32.5

0.25

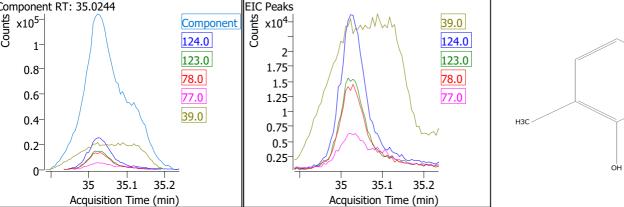
ОН



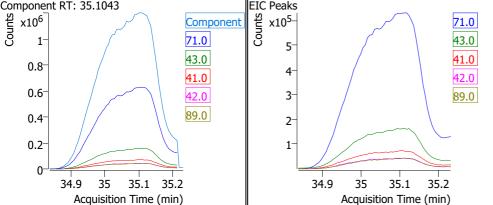


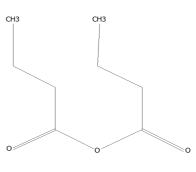


- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 488-17-5 35.0244 1,2-Benzenediol, 3-methyl-908282.5 91.9 C7H8O2 Component RT: 35.0244 v10² 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 39.0 0.2 51.0 106.0 0.1 40 100 105 110 115 120 125 130 135 35 50 55 65 70 80 85 15 Mass-to-Charge (m/z) 1,2-Benzenediol, 3-methyl- (NIST20.L) Counts x10²_ 0.9 124.0 0.8 0.7 0.6 78.0 0.5 0.4 0.3 0.2 39.0 51.0 106.0 95.0 0.1 62.0 27.0 47.0 81.0 18.0 40 10 15 20 25 30 35 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (34.9287-35.2420 min, 52 scans) 8.D st x10² 0.9 71.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 43.1 0.2 0.1 57.0 31.0 89.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 35.0244 EIC Peaks Counts x10⁵ Counts x10⁴ 39.0 Component 124.0 124.0 1 2 123.0 123.0 1.75 0.8



-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 106-31-0 35.1043 Butanoic acid, anhydride 14397735.0 82.5 C8H14O3 Component RT: 35.1043 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 89.0 0.1 57.0 90 25 85 10 15 20 30 35 40 50 55 60 65 70 75 80 95 Mass-to-Charge (m/z) Butanoic acid, anhydride (NIST20.L) st x10²_ 0.9-71.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 27.0 41.0 0.1 55.0 29.0 15.0 60.0 85.0 89.0 90 5 10 15 20 25 35 40 45 50 55 60 65 70 75 80 95 Mass-to-Charge (m/z) + Scan (34.8389-35.2135 min, 64 scans) 8.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 57.0 31.0 89.0 -20 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.1043 Counts Counts x10⁶ x10⁵ 71.0 Component CH3 CH3 71.0 43.0 5 43.0 41.0 0.8





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 35.4159 2-Furanmethanol, tetrahydro-15472596.7 80.1 97-99-4 C5H10O2 Component RT: 35.4159 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 57.0 89.0 0.1 31.0 10 25 30 35 55 60 65 85 90 100 105 110 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 67.0 102.0 10 15 20 25 35 40 45 50 55 60 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (35.2135-35.6298 min, 71 scans) 8.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 43.1 0.2 0.1 31.0 57.0 114.0 131.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 35.4159 **EIC Peaks** Counts x10⁶-Counts x10⁶ 71.0 Component 71.0 43.0 0.8 1.6 43.0 41.1 1.4 0.7 41.1 57.0



42.0

0.6 0.5

 0.4^{-}

0.3

0.2

0.1

35.3

35.4

35.5

Acquisition Time (min)

35.6

57.0

42.0

1.2

0.8

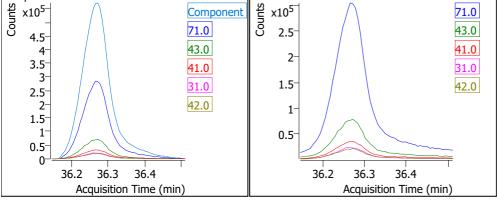
0.6

0.4

0.2

35.3 35.4 35.5

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.2698 2-Furanmethanol, tetrahydro-3073015.1 82.9 97-99-4 C5H10O2 Component RT: 36.2698 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 57.0 45.0 10 15 25 30 35 55 60 65 90 100 105 110 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 53.0,57.0 61.0 15.0 67.0 102.0 10 15 20 25 35 40 45 50 55 65 70 75 80 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (36.1654-36.5150 min, 58 scans) 8.D St x10²_ 0.9 71.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 57.0 131.1 10 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 36.2698 **EIC Peaks** Counts Counts x10⁵ 71.0 Component 71.0 43.0 2.5 4.5 43.0 41.0 2



--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.2717 Acetone 689384.1 67-64-1 C3H6O Component RT: 36.2717 y x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 42.0 0.2 39.0 58.0 0.1 47.0 60.0 24 26 28 30 32 36 38 52 58 Mass-to-Charge (m/z) Acetone (NIST20.L) St x10²_0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 58.0 15.0 0.2 0.1 14.0 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 46 48 50 52 54 56 60 62 Mass-to-Charge (m/z) + Scan (36.1519-36.4919 min, 58 scans) 8.D st x10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 43.1 0.1 57.0 131.1 10 20 40 50 60 70 08 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 36.2717 **EIC Peaks** Counts Counts x10⁴ 43.0 Component 43.0 42.0 1 42.0 39.0 5 0.8 58.0 58.0 4 39.0 75.0

36.3

36.4

Acquisition Time (min)

3-

2

36.2

75.0

0.6

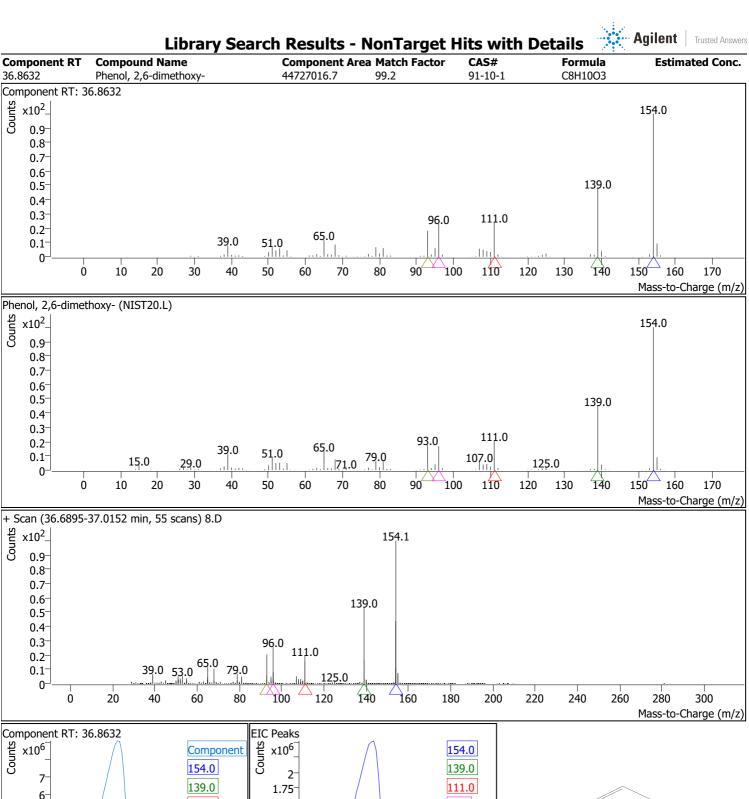
0.4

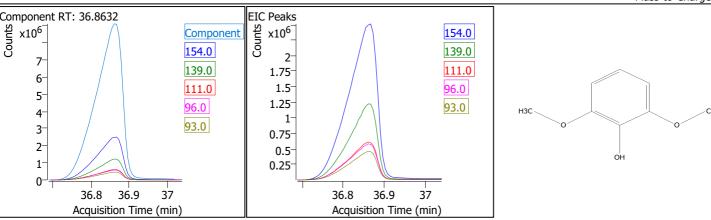
0.2

36.2

36.3

36.4





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 37.0004 Eugenol 527898.0 79.8 97-53-0 C10H12O2 Component RT: 37.0004 y x10² 0.9 164.0 0.8 0.7^{-} 0.6 91.0 0.5 0.4 149.0 103.0 131.0 0.3 77.0 29.0 55.0 0.2 0.1 90 150 170 10 20 30 50 60 70 80 100 110 120 130 140 180 Mass-to-Charge (m/z) Eugenol (NIST20.L) Counts x10²_ 0.9 164.0 0.8 0.7 0.6 0.5 0.4 149.0 0.3 131.0 0.2 77.0 103.0 91.0 55.0 121.0 0.1 39.0 65.0 27.0 115.0 74.0 ı 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 Mass-to-Charge (m/z) + Scan (36.9201-37.1698 min, 43 scans) 8.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4 154.0 0.3 61.0 0.2 29.0 139.0 117.0 71.0 91.0 0.1 164.1 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 37.0004 **EIC Peaks** Counts Counts x10⁵ x10⁴ 164.0 Component 164.0 91.0 1 1.4 91.0 131.0 0.8 1.2 149.0 103.0 1-

37.1

Acquisition Time (min)

0.6

0.4

0.2

103.0

131.0

37.1 37.2

Acquisition Time (min)

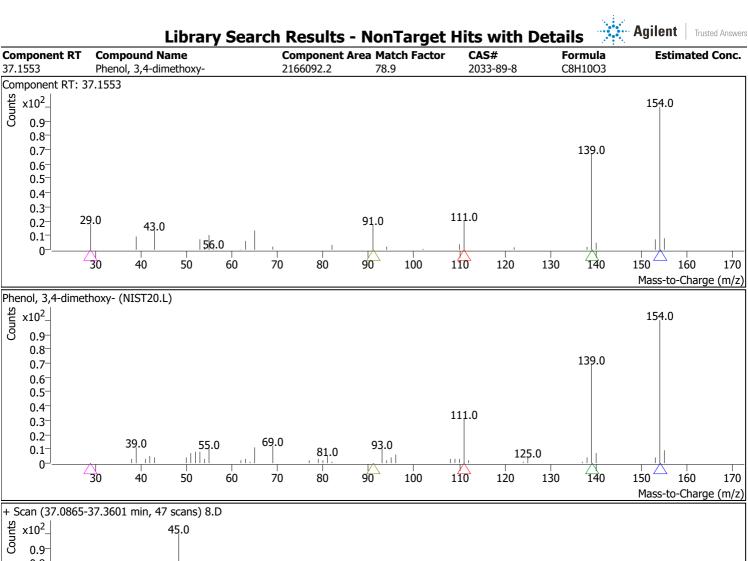
0.8

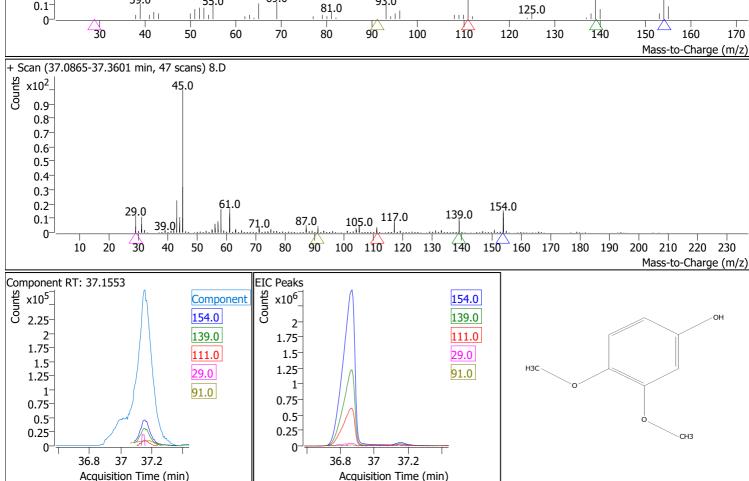
0.6

 0.2^{-}

149.0

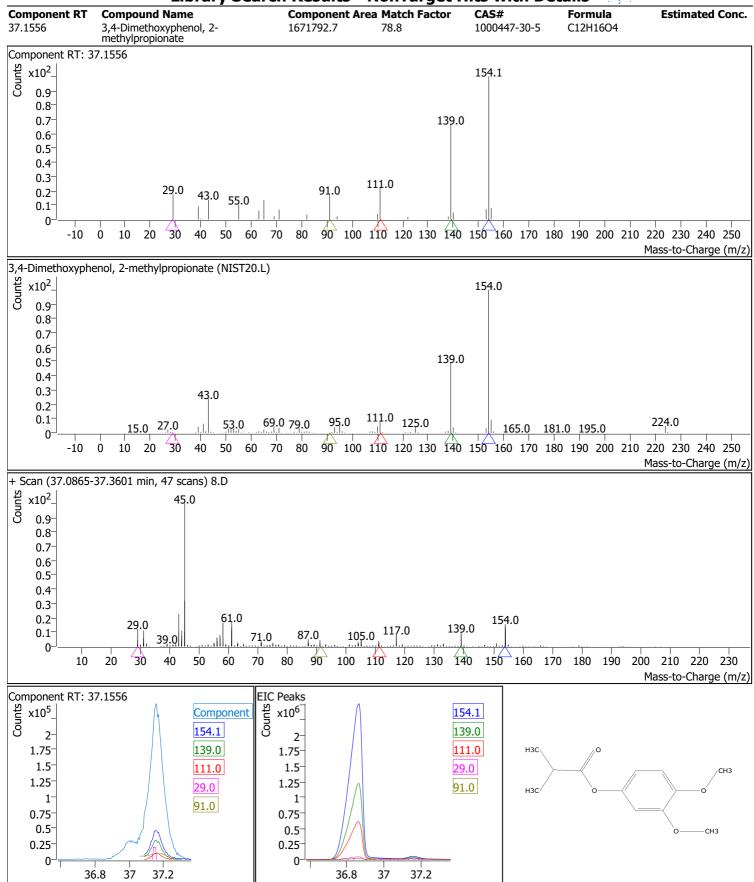
CH2





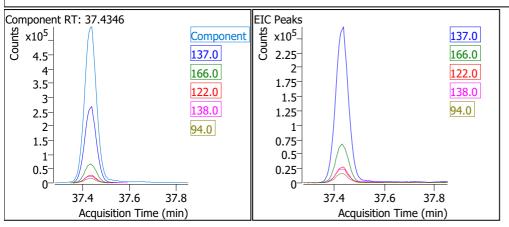
Library Search Results - NonTarget Hits with Details

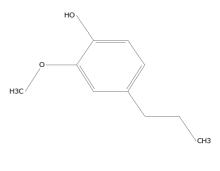




Acquisition Time (min)

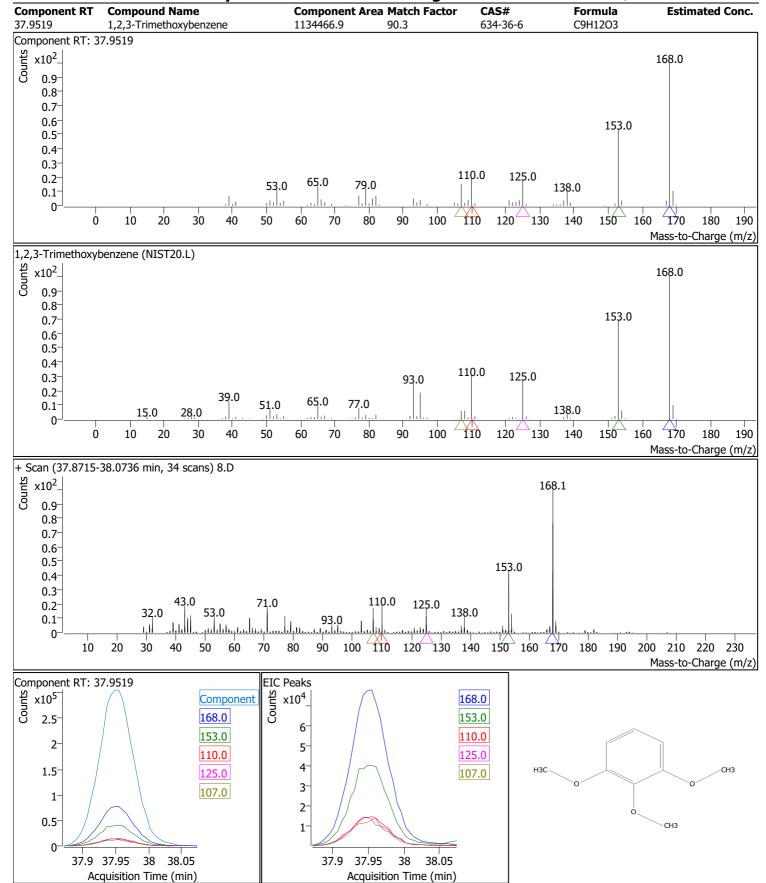
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4346 Phenol, 2-methoxy-4-propyl-2070909.7 C10H14O2 Component RT: 37.4346 v10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 77.0 29.0 65.0 105.0 160 - 170 10 20 30 40 50 60 70 80 100 110 120 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10²_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 150 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 180 Mass-to-Charge (m/z) + Scan (37.3495-37.5682 min, 37 scans) 8.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 166.1 0.2 122.0 45.0 _{57.0} 103.0 0.1 154.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 37.4346 **EIC Peaks** 137.0 Component

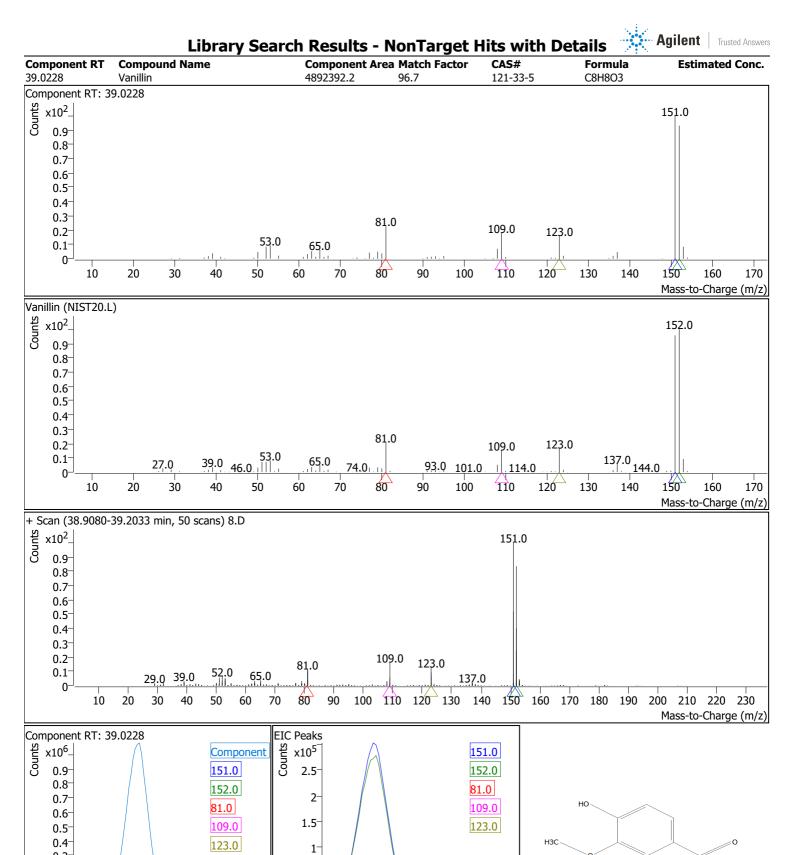














39.1

Acquisition Time (min)

0.5

0.3⁻ 0.2⁻

 0.1^{-}

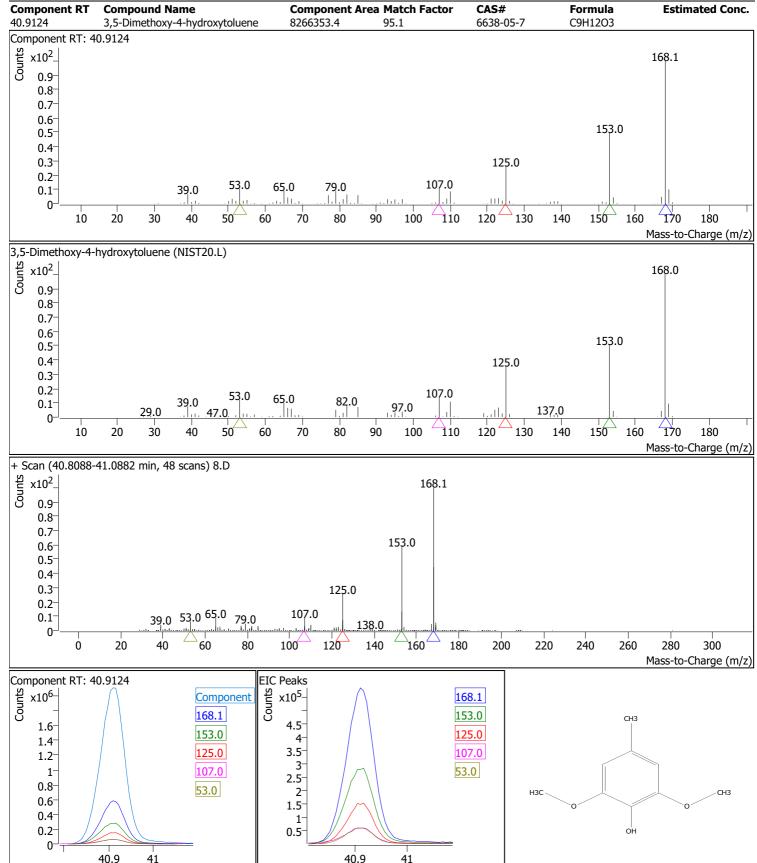
38.9

39

39.1

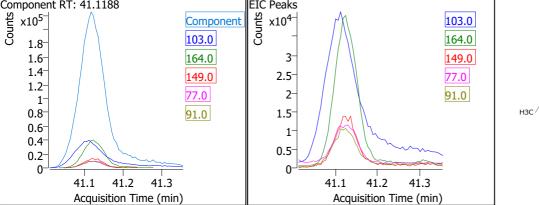
Library Search Results - NonTarget Hits with Details

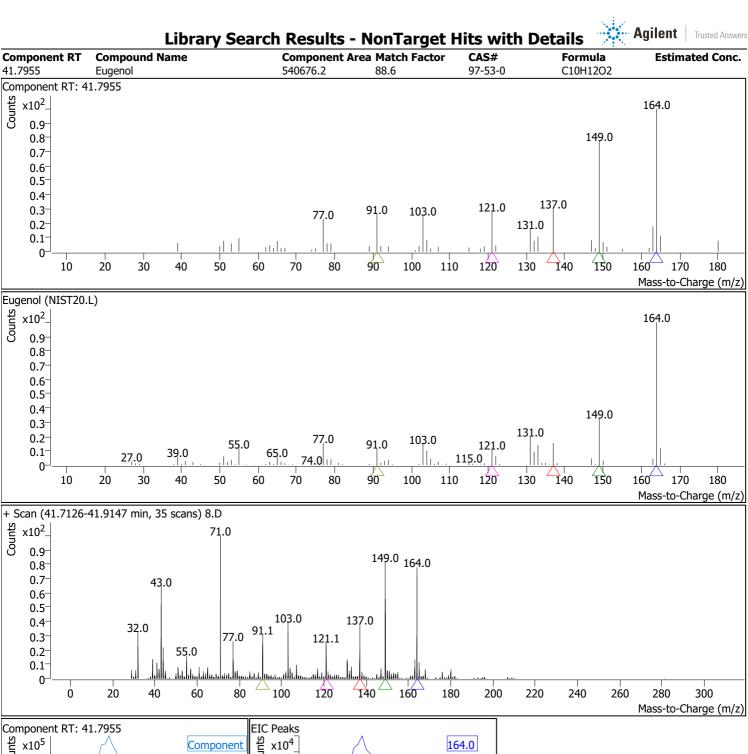


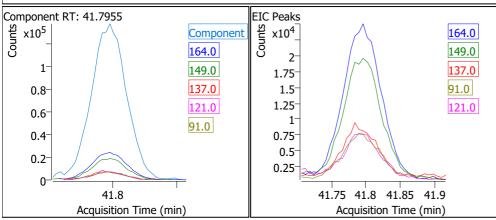


Acquisition Time (min)

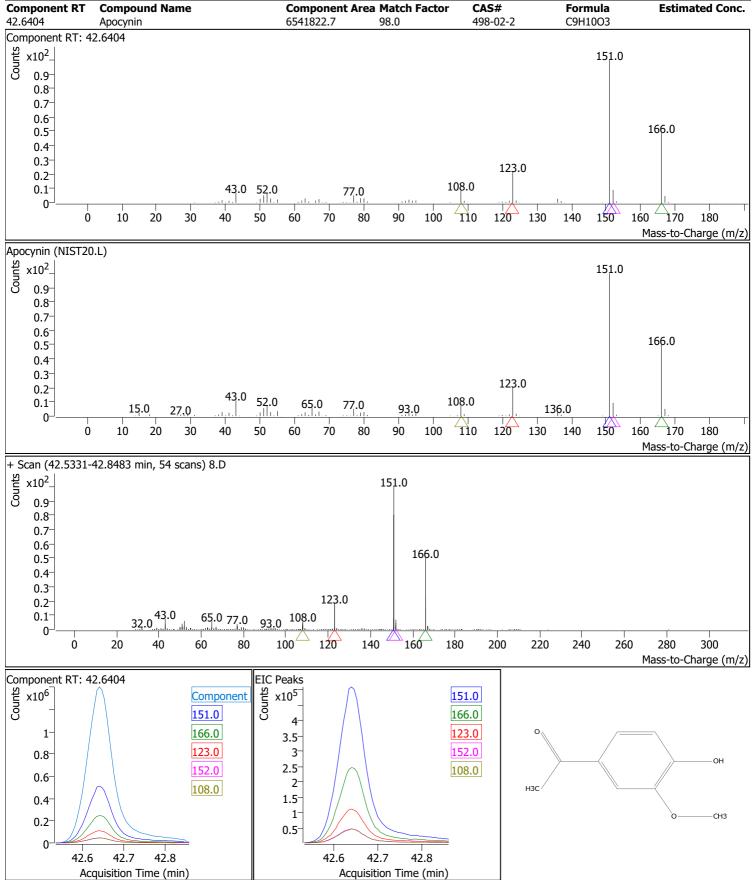
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 41.1188 trans-Isoeugenol 1105968.8 88.8 5932-68-3 C10H12O2 Component RT: 41.1188 $x10^{2}$ 103.0 164.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 149.0 0.3 77.0 91.0 131.0 0.2 41.0 121.0 0.1 10 20 30 40 50 60 70 90 100 110 120 130 140 150 170 180 Mass-to-Charge (m/z) trans-Isoeugenol (NIST20.L) Counts x10²_ 0.9 164.0 0.8 0.7 0.6 0.5 0.4 149.0 103.0 0.3 77.0 91.0 131.0 0.2 55.0 121.0 65.0 0.1 39.0 137.0 27.0 115.0 15.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 Mass-to-Charge (m/z) + Scan (41.0347-41.2785 min, 42 scans) 8.D st x10² 0.9 103.0 0.8 0.7 71.0 0.6 164.1 0.5 43.0 0.4^{-} 0.3 32.0 57.0 77.0 89.0 0.2 133.0 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: 41.1188 Counts Value 1.8 x10⁴ 103.0 Component 103.0 164.0 1.8





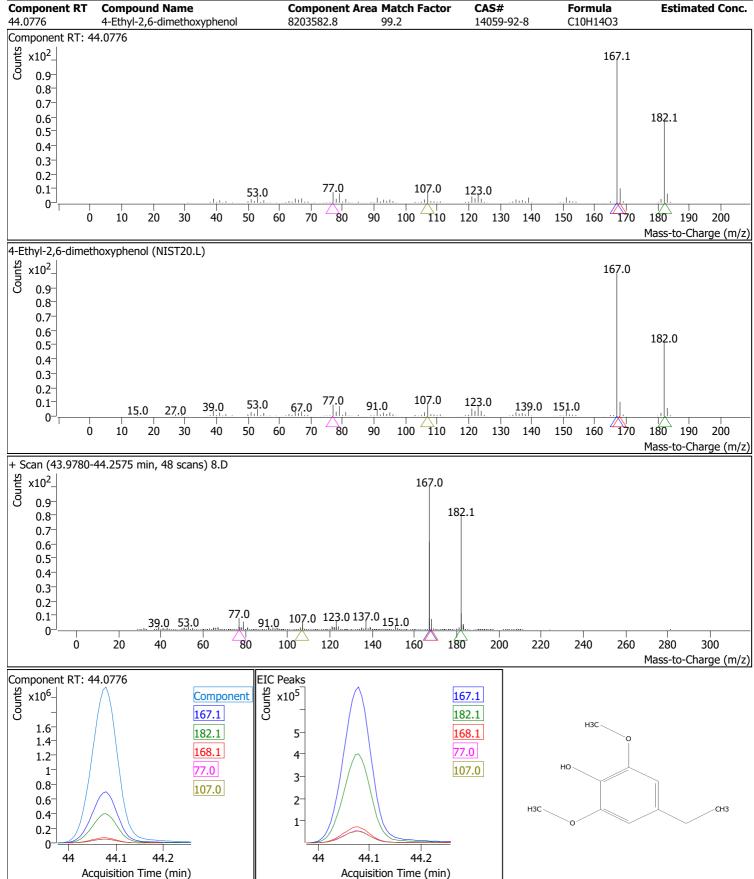




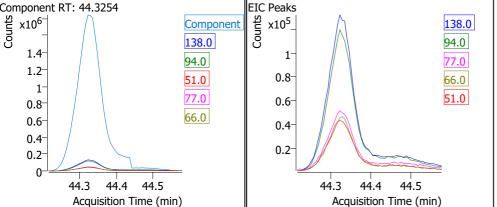


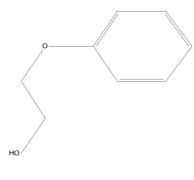
Library Search Results - NonTarget Hits with Details





-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 8885996.3 122-99-6 44.3254 Ethanol, 2-phenoxy-77.4 C8H10O2 Component RT: 44.3254 Counts $x10^{2}$ 138.0 0.9 94.0 0.8 0.7^{-} 0.6 0.5 0.4 51.0 0.3 77.0 66.0 0.2 91.0 0.1 140 50 120 10 20 30 40 90 100 110 130 150 Mass-to-Charge (m/z) Ethanol, 2-phenoxy- (NIST20.L) Counts x10²_ 0.9 94.0 0.8 0.7 0.6 0.5 138.0 0.4 77.0 0.3 0.2 66.0 51.0 0.1 39.0 74.0 108.0 119.0 140 50 120 10 20 30 40 60 70 80 90 100 110 130 150 Mass-to-Charge (m/z) + Scan (44.2218-44.5786 min, 61 scans) 8.D st x10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 180.1 122.0 0.1 171.1 20 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 44.3254 Counts Counts x10⁵ 138.0 Component 138.0 94.0 1.4 1 94.0 77.0 1.2





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-44.3269 13864490.2 94.4 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3269 x10². 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 122.0 43.0 0.1 66.0 77.0 0-120 180 20 30 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 85.0⁹1.0 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 90 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2159-44.5369 min, 55 scans) 8.D x10². 137.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 0.3 74.0 0.2 180.1 87.0 122.0 43.0 55.0_{66.0} 0.1 171.1 0 100 140 180 Ó 20 40 60 80 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 44.3269 Counts Counts x10⁶x10⁶ 137.0 Component 180.0 137.0 2.25 1 180.0 122.0 2 0.8 1.75 138.0 122.0 1.5

44.4

Acquisition Time (min)

44.5

94.0

138.0

94.0

1.25

0.75 0.5

0.25

44.3

44.4

Acquisition Time (min)

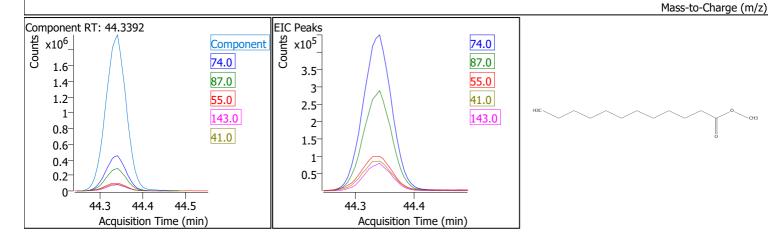
44.5

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.** 6700550.9 44.3392 Dodecanoic acid, methyl ester 92.8 111-82-0 C13H26O2 Component RT: 44.3392 Counts $x10^{2}$ 74.0 0.9 0.8 0.7^{-} 87.0 0.6 0.5 0.4 0.3 55.0 41.0 143.0 0.2 69.0 0.1 70 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts 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 (44.2456-44.4834 min, 41 scans) 8.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 180.1 122.0 0.1 43.0 55.0 66.0



100

120

140

20

171.1

180

200

220

240

260

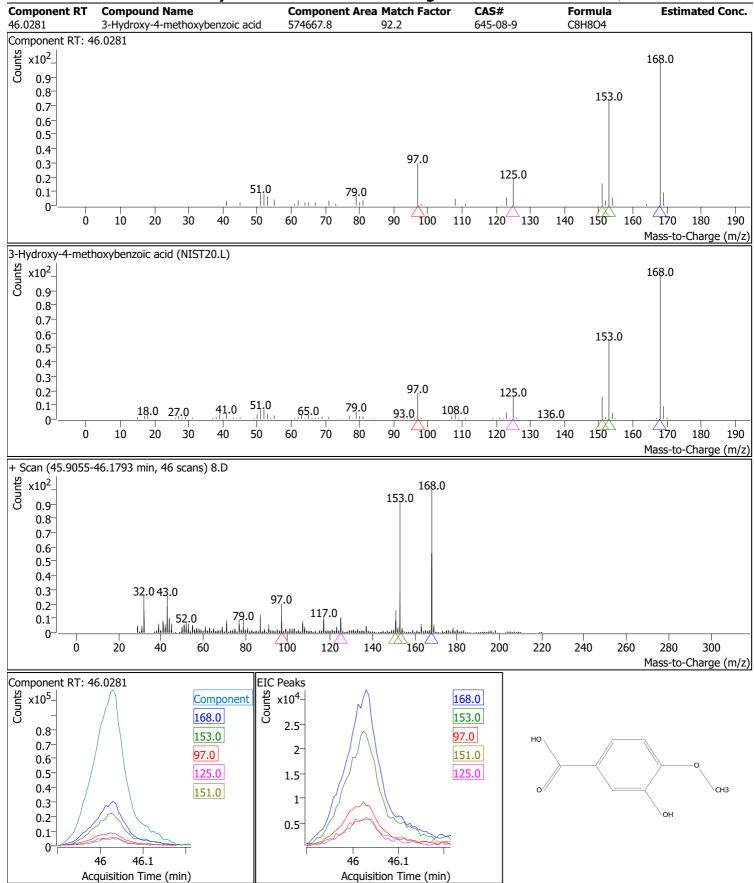
280

300

160

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.** 1-Propanone, 1-(4-hydroxy-3-1835-14-9 46.5006 706235.2 89.6 C10H12O3 methoxyphenyl)-Component RT: 46.5006 x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 123.0 108.0 0.1 52.0 65.0 77.0 0-110 150 180 10 20 30 40 50 60 70 80 90 100 120 130 140 160 170 190 200 Mass-to-Charge (m/z) 1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 0.3 180.0 123.0 0.2 108.0 77.0 93.0 0.1 52.0 65.0 29.0 39.0 136.0 164.0 0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (46.4235-46.5824 min, 27 scans) 8.D x10². 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 180.1 108.0 123.0 32.0 43.0 0.1 65.0 77.0 0 Ó 40 80 100 120 140 180 200 260 20 60 160 220 240 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 46.5006 Counts Counts x10⁴⊣ x10⁵ 151.0 Component СНЗ 180.0 151.0 6 1.2 180.0 123.0 5 1 123.0 152.0 0.8

46.4

Acquisition Time (min)

152.0

108.0

3

2

1

46.2

0.6

0.4

46.2

46.4

Acquisition Time (min)

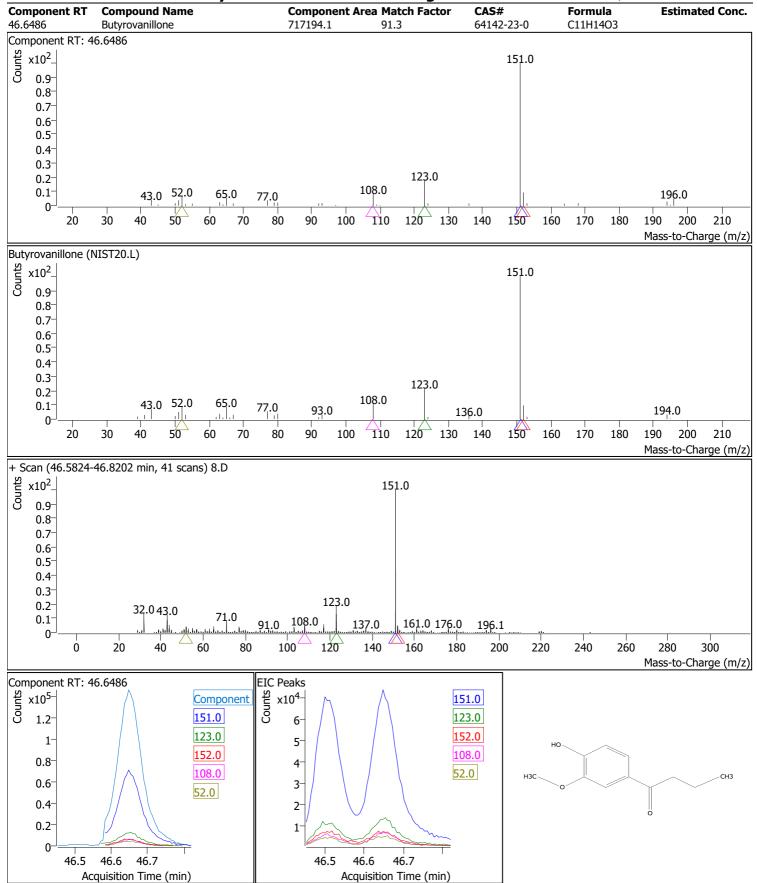
46.6

108.0

нзс







Library Search Results - NonTarget Hits with Details ··· Agilent | Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 47.0974 (E)-2,6-Dimethoxy-4-(prop-1-en-1-522693.2 84.9 C11H14O3 yl)phenol Component RT: 47.0974 x10²_ 194.0 0.9 8.0 0.7 0.6 0.5 0.4 178.0 91.0 0.3 119.0 131.0 147.0 77.0 0.2^{-} 163.0 0.1 0-180 10 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 200 210 220 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 ا 97.0 .85.0 0 150 160 170 180 90 20 50 60 70 80 100 110 120 130 140 190 200 210 220 Mass-to-Charge (m/z) + Scan (47.0319-47.1948 min, 28 scans) 8.D st x10² 194.1 0.8 0.7 0.6 0.5 0.4 32.0 43.0 0.3 178.1 0.2 51.0 65.0 77.0 151.1 131.0 107.0 220.0 0.1 0 60 180 Ó 20 40 80 100 120 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 47.0974 **EIC Peaks** Counts Counts x10⁵ x10⁴-194.0 Component 194.0 91.0 1.8 1 **Н3С** 178.0 178.0 1.6 1.4 91.0 0.8 119.0 1.2 119.0 131.0 НО 0.6 1

131.0

0.4

0.2

47.05

47.1 47.15 47.2

Acquisition Time (min)

0.8

0.6⁻ 0.4⁻

0.2

47.05

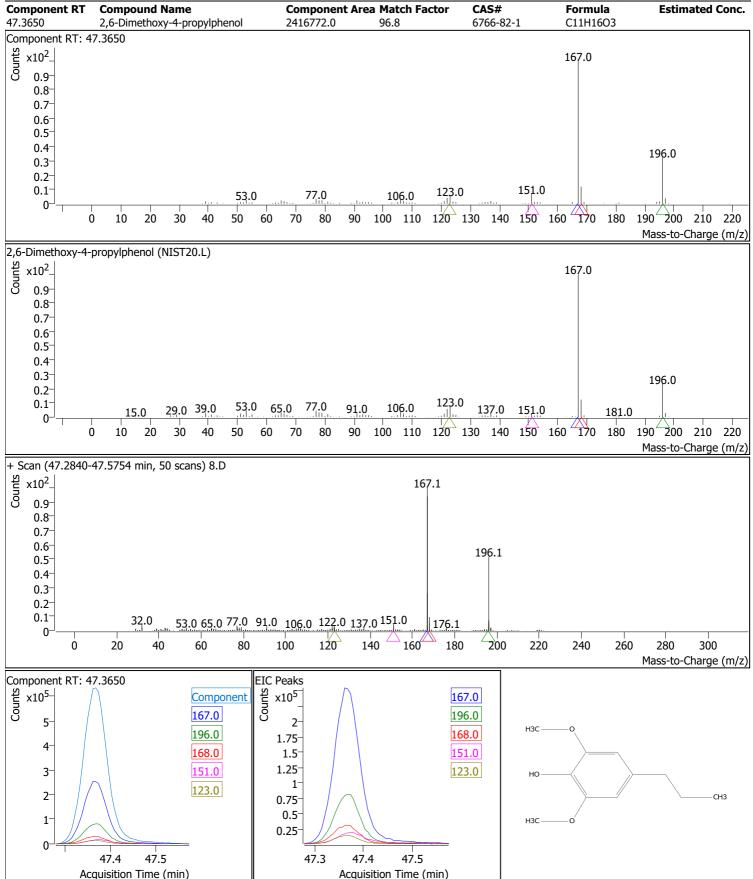
47.1

47.15

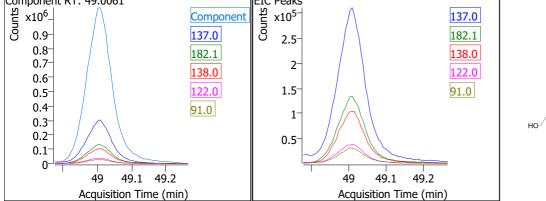
Acquisition Time (min)

НЗС

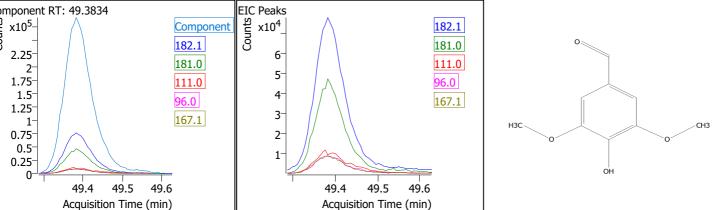
Library Search Results - NonTarget Hits with Details Agilent Trusted Answers

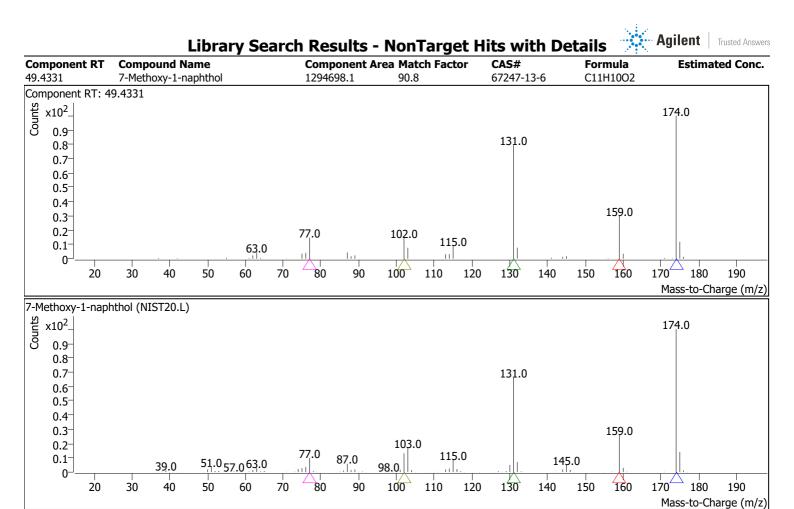


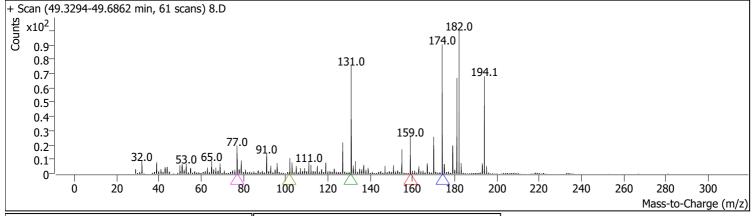
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 49.0061 Benzenepropanol, 4-hydroxy-3-5751671.5 96.9 C10H14O3 methoxy-Component RT: 49.0061 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 182.1 0.4 0.3 0.2^{-} 122.0 77.0 91.0 107.0 0.1 0-90 140 10 20 30 40 50 60 70 80 100 110 120 130 150 160 170 180 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 122.0 0.2 77.0 91.0 65.0 106.0 53.0 0.1 31.0 39.0 149.0 164.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (48.8775-49.2521 min, 64 scans) 8.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 182.1 0.4 0.3 0.2 65.0 77.0 91.0 107.0 122.0 0.1 32.043.0 149.0 164.0 0 100 120 180 200 0 20 40 60 80 140 160 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.0061 **EIC Peaks** Counts x10⁵ x10⁶_ 137.0 Component 182.1 0.9 137.0 2.5 0.8 182.1 138.0 0.7 2-122.0 138.0 0.6

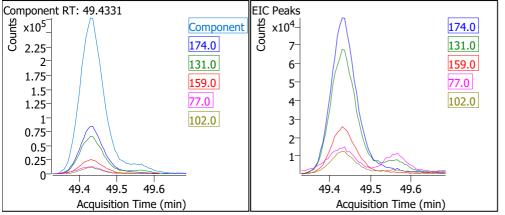


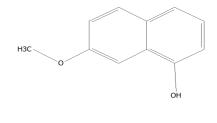
... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.3834 Benzaldehyde, 4-hydroxy-3,5-1472988.8 91.1 134-96-3 C9H10O4 dimethoxy-Component RT: 49.3834 x10²_ 182.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 111.0 96.0 167.1 139.0 0.1 175.0 0-160 170 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 190 Mass-to-Charge (m/z) Benzaldehyde, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts $x10^{2}$ 182.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 111.0 0.2 167.0 93.0 139.0 39.0 65.0 51.0 79.0 0.1 15.0 29.0 153.0 123.0 0 160 170 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 180 190 Mass-to-Charge (m/z) + Scan (49.2878-49.6325 min, 58 scans) 8.D x10². 182.0 174.0 0.9 0.8 131.0 0.7 194.1 0.6 0.5 0.4 0.3 159.0 77.0 0.2 39.0 53.0 65.0 111.0 0.1 0 180 Ó 20 40 60 80 100 120 140 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.3834 **EIC Peaks** Counts Counts x10⁴ x10⁵-182.1 Component 0 181.0 182.1 2.25 6 181.0 111.0 5 1.75 111.0 96.0





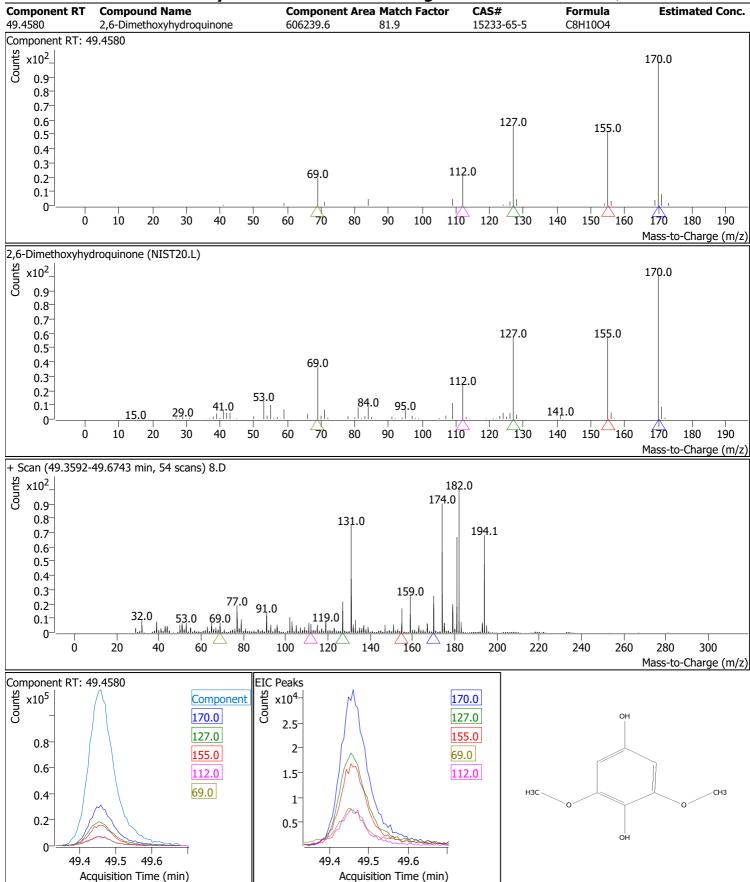












··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20675-95-0 49.5612 (E)-2,6-Dimethoxy-4-(prop-1-en-1-1140124.2 82.7 C11H14O3 yl)phenol Component RT: 49.5612 x10² 194.0 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 91.0 0.2^{-} 119.0 133.0 77.0 151.0 163.0 0.1 0-10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 200 210 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 ا 97.0 27.0 85.0 0 90 180 10 20 40 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4722-49.7277 min, 43 scans) 8.D x10². 194.1 0.9 0.8 0.7 0.6 0.5 0.4 179.0 0.3 91.0 131.0 0.2 65.0 ⁷⁷.0 32.0 44.0 103.0 155.0 0.1 0 120 180 0 20 40 60 80 100 140 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.5612 **EIC Peaks** Counts Counts x10⁴ x10⁵ 194.0 Component 179.0 194.0 2.25 **Н3С** 179.0 91.0 5 2 1.75 91.0 193.0 4 1.5 193.0 119.0 НО 1.25 3-119.0

49.6

Acquisition Time (min)

49.7

2-

1

49.5

0.75⁻

0.25

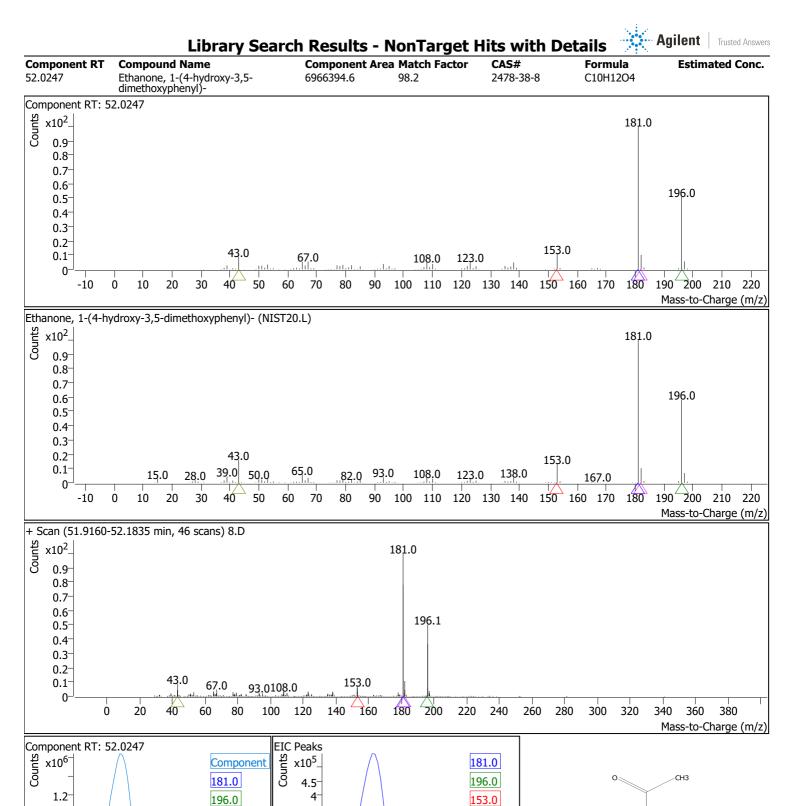
49.5

49.6

Acquisition Time (min)

49.7

НЗС



52.1

Acquisition Time (min)

182.0

43.0

52.2

3.5

2.5

0.5

3

2.5

153.0

182.0

43.0

52.2

1

0.8

0.6

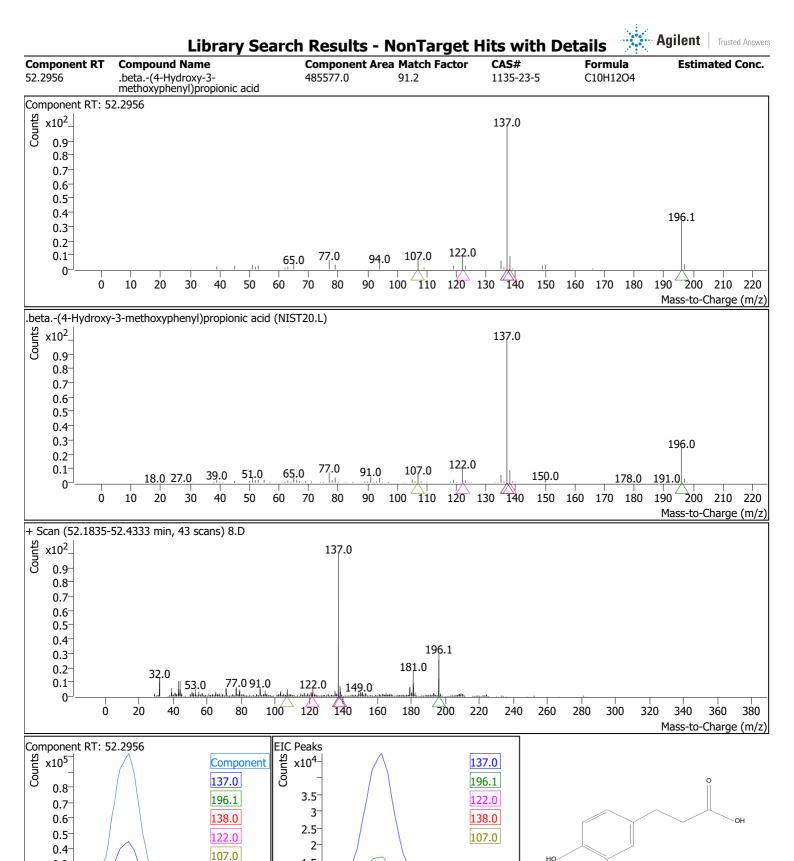
0.4

52

52.1

Acquisition Time (min)

ОН



52.3

52.4

Acquisition Time (min)

1.5

0.5

1

0.3

0.2

52.3

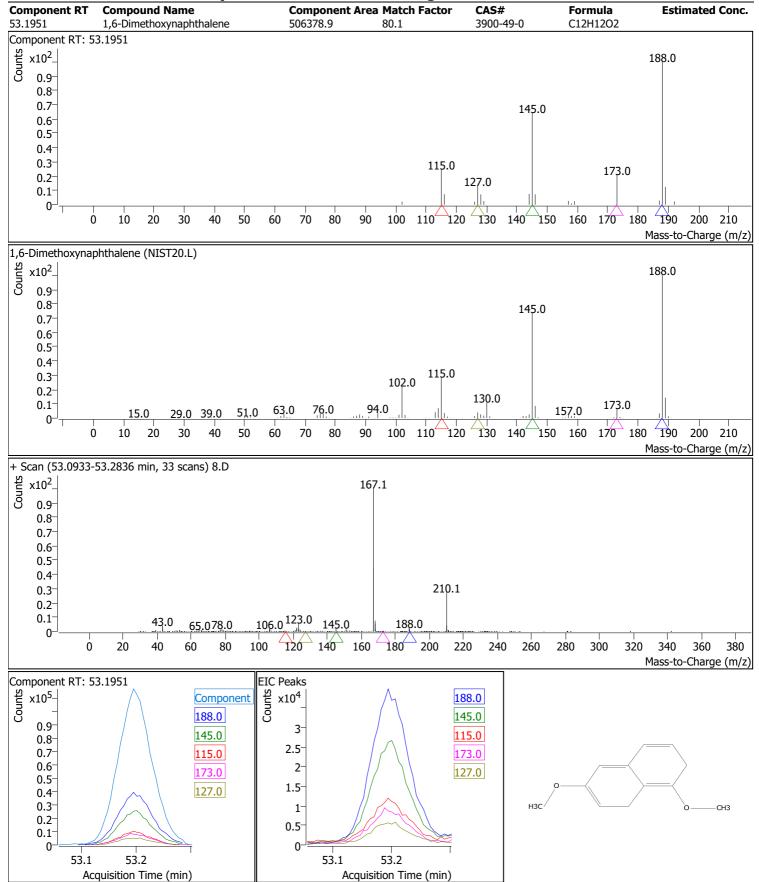
Acquisition Time (min)

52.4

СНЗ

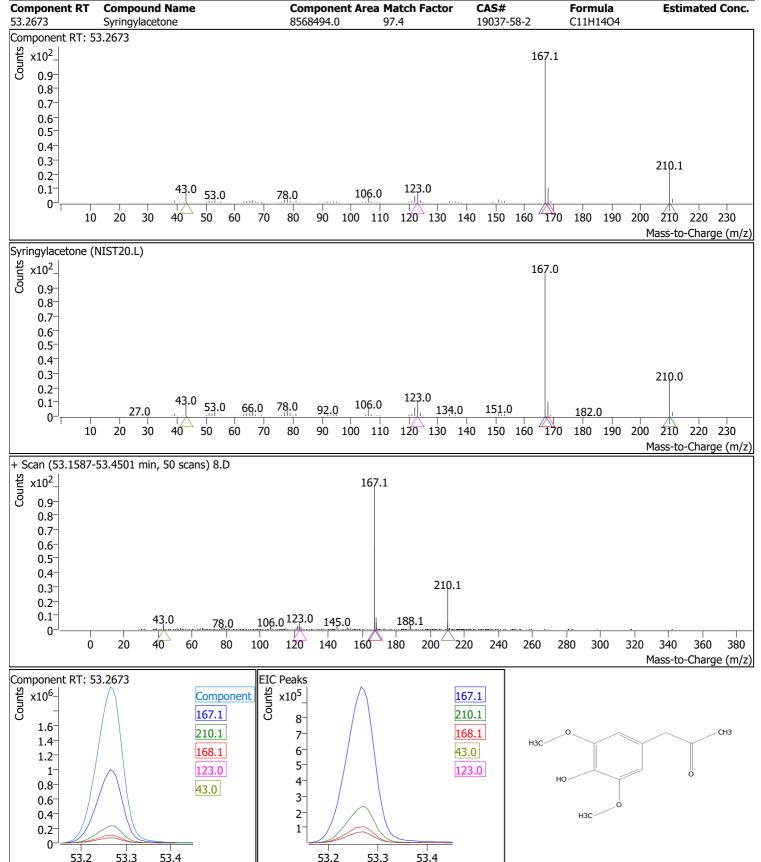




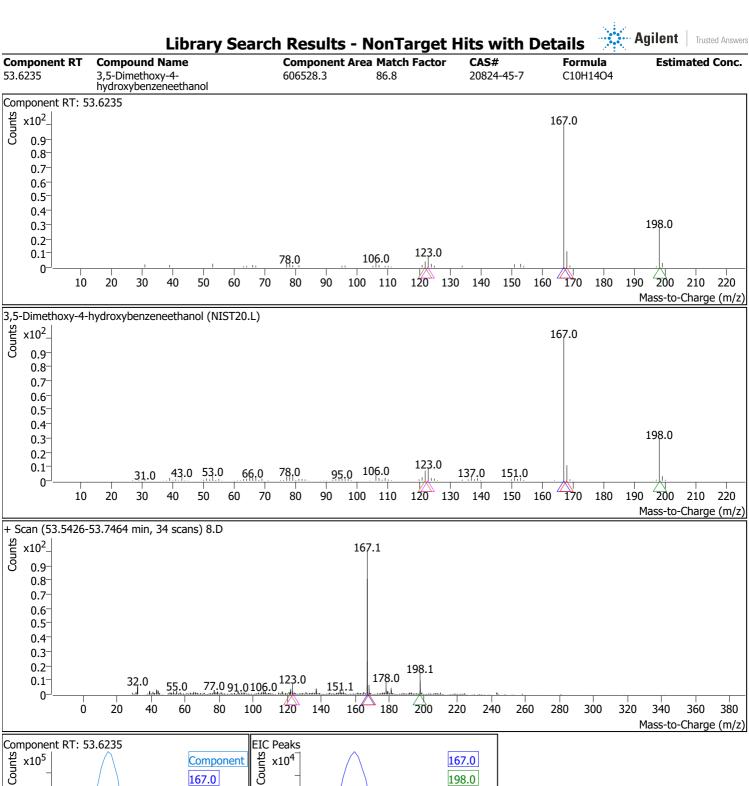


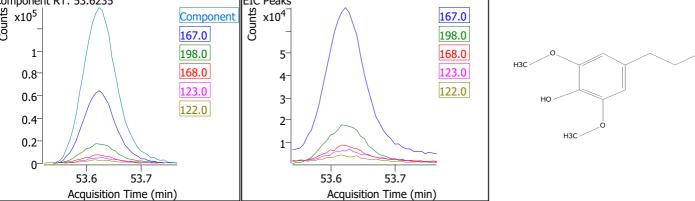






Acquisition Time (min)





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 54.9781 Benzoic acid, 4-hydroxy-3,5-502400.3 79.3 530-57-4 C9H10O5 dimethoxy-Component RT: 54.9781 x10²_ 198.0 0.9 8.0 0.7 0.6 0.5 0.4 183.0 0.3 127.0 192.0 0.2^{-} 153.0 109.0 0.1 39.0 0-180 200 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 220 Mass-to-Charge (m/z) Benzoic acid, 4-hydroxy-3,5-dimethoxy- (NIST20.L) Counts x10² 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 0 180 190 200 10 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 210 220 Mass-to-Charge (m/z) + Scan (54.8822-55.2636 min, 65 scans) 8.D x10². 181.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 198.0 0.2 135.0 153.0 210.1 32.0 0.1 65,0 0 140 200 360 20 40 60 80 100 120 160 180 220 240 260 280 300 320 340 380 Mass-to-Charge (m/z) Component RT: 54.9781 **EIC Peaks** Counts Counts x10⁴ 181.0 x10⁵ Component ОН 198.0 198.0 0.8 7 183.0 183.0 0.7 6 181.0 0.6 127.0 5

55

55.1

Acquisition Time (min)

55.2

192.0

0.5

0.4

0.3

0.2

127.0

192.0

4

3

2

54.9

55

55.1 55.2

Acquisition Time (min)

ОН

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-55.2461 1246281.8 92.5 5650-43-1 C11H14O4 Component RT: 55.2461 Counts x10²_ 181.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 210.0 0.2^{-} 153.0 0.1 67.0 108.0 123.0 138.0 224.0 0 200 210 220 230 10 20 30 50 60 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) 1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 181.0 0.9 0.8 0.7 0.6 0.5 0.4 210.0 0.3 0.2 123.0 0.1 108.0 82.0 93.0 138.0 53.0 29.0 39.0 166.0 0 120 130 140 150 160 170 180 190 200 210 220 230 10 20 30 50 60 80 90 100 110 Mass-to-Charge (m/z) + Scan (55.1045-55.4427 min, 57 scans) 8.D x10²_ 181.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 210.1 0.1 32.0 162.1 93.0 108.0123.0138.0 40 60 180 20 80 100 120 140 160 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 55.2461 **EIC Peaks** Counts Counts x10⁵ x10⁵ 181.0 Component 181.0 210.0 1.8 0.8 -CH3 210.0 182.0 1.6 0.7^{-} 1.4 182.0 0.6 153.0 H3C 1.2



67.0

0.5

0.4

0.3

 0.2^{-}

0.1

55.2

55.3

Acquisition Time (min)

55.4

153.0

67.0

1

 0.8^{-}

0.6

0.4

0.2

55.2

55.3

Acquisition Time (min)

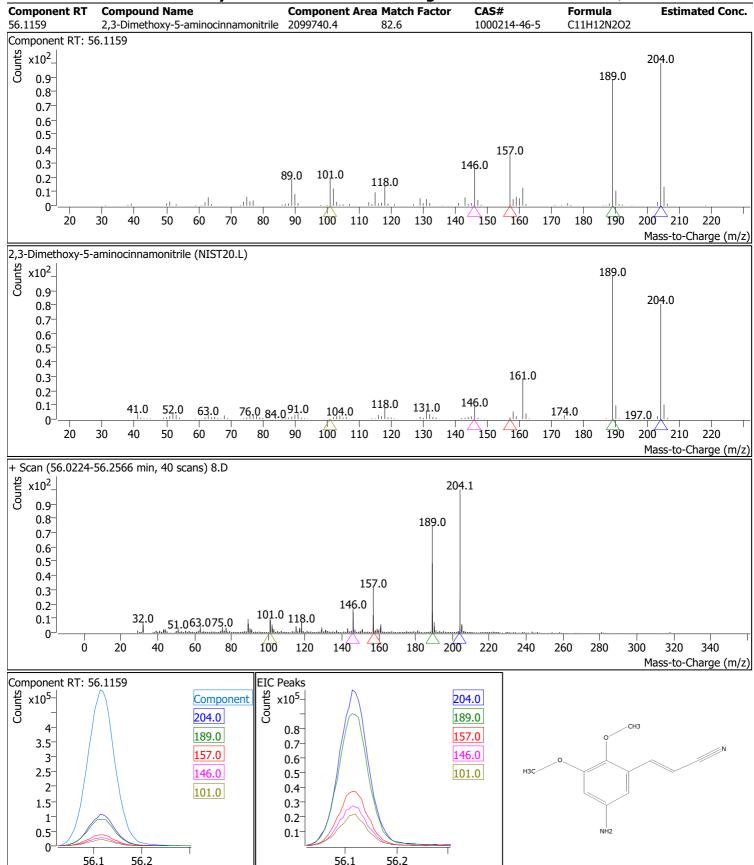
55.4

-OH

-CH3

Library Search Results - NonTarget Hits with Details





Acquisition Time (min)

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 5-(3-Hydroxypropyl)-2,3-dimethoxyphenol 57.5003 2007215.0 92.7 63543-12-4 C11H16O4 Component RT: 57.5003 x10²_ 168.0 0.9 8.0 0.7 212.0 0.6 0.5 0.4 0.3 153.0 137.0 0.2 123.0 107.0 91.0 0.1 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 31.039.0 65.0 0.1 85.0 197.0 100 110 120 130 140 150 160 170 180 190 200 10 20 30 60 70 80 90 210 220 230 240 Mass-to-Charge (m/z) + Scan (57.4042-57.7134 min, 53 scans) 8.D x10². 168.1 212.1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 153.0 77.091.0 181.0 202.0 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 57.5003 Counts Counts x10⁴x10⁵-168.0 Component 167.0 168.0 6 3.5 167.0 212.0 3 5 137.0 2.5 212.0 4

57.5

57.6

Acquisition Time (min)

153.0

153.0

137.0

3

2

2

1⁻ 0.5⁻

57.5

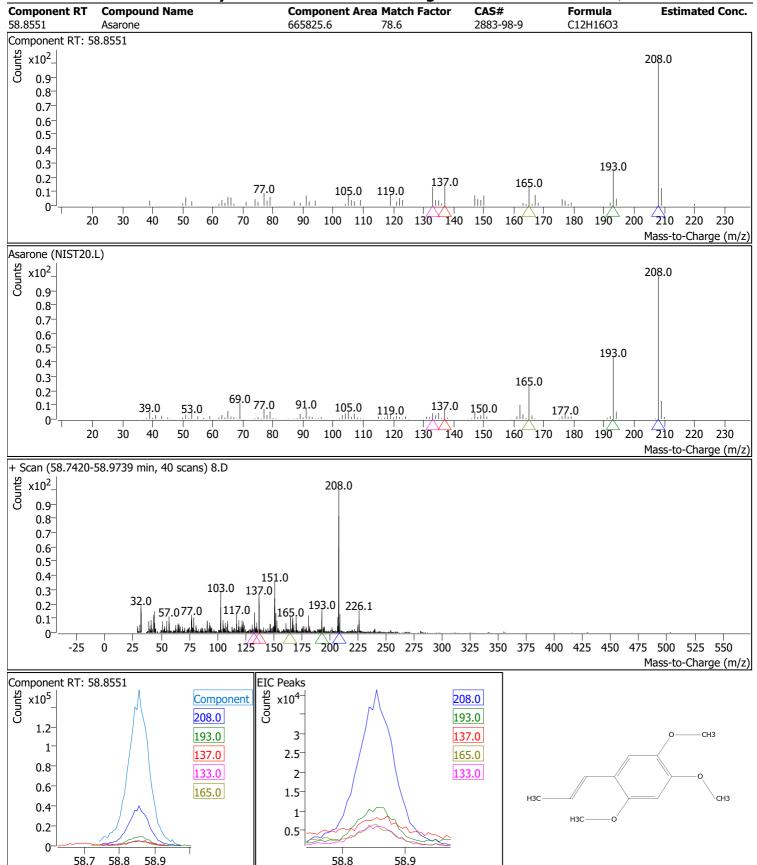
57.6

Acquisition Time (min)

1.5



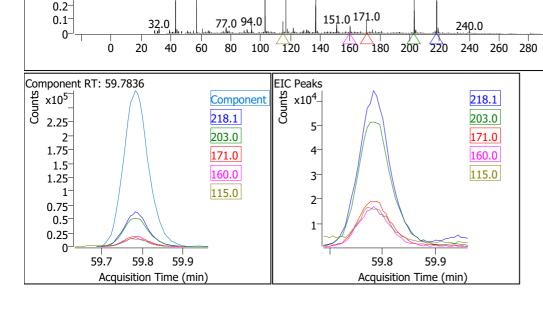




Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 59.7836 8-Amino-6,7-dimethoxy-4-1208321.8 80.3 1000213-07-2 C12H14N2O2 methylquinoline Component RT: 59.7836 x10²_ 218.1 0.9 203.0 8.0 0.7 0.6 0.5 0.4 160.0 171.0 0.3 115.0 0.2^{-} 132.0 0.1 77.0 0-200 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 230 Mass-to-Charge (m/z) 8-Amino-6,7-dimethoxy-4-methylquinoline (NIST20.L) x10². 218.0 203.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 160.0 132.0 145.0 0.2 104.0 175.0 187.0 0.1 77.0 51.0 117.0 63.0 89.0 0 200 210 220 230 240 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 Mass-to-Charge (m/z) + Scan (59.6875-59.9610 min, 47 scans) 8.D x10². 117.0 0.9 0.8 0.7 0.6 0.5 0.4

203.0

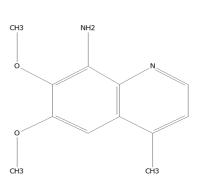


103.0

137.0

43.0

0.3



300

320

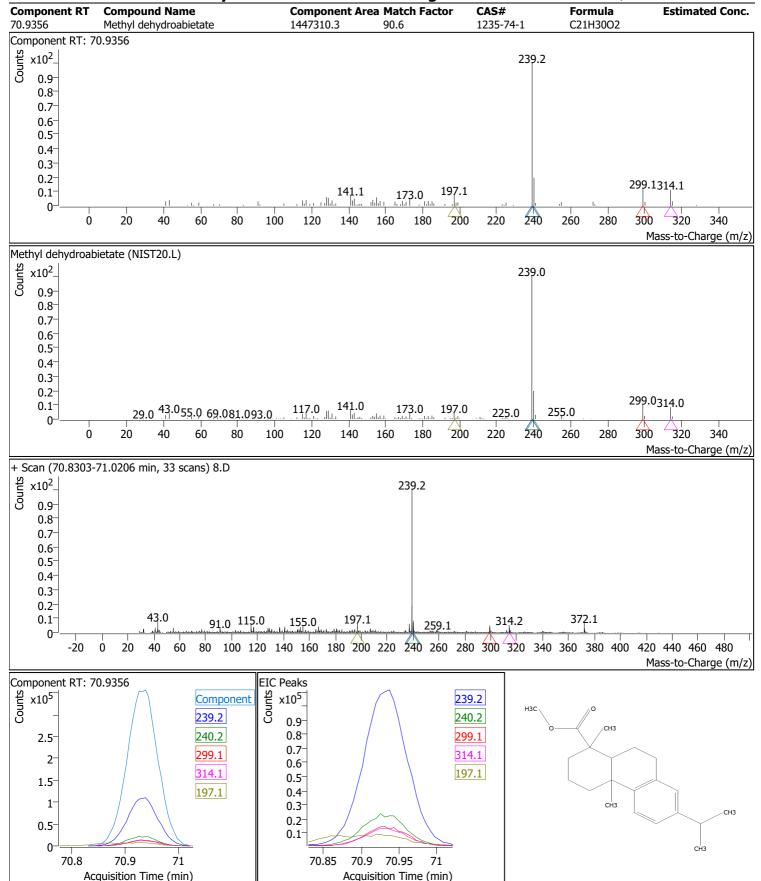
340

360 380 400 420

Mass-to-Charge (m/z)

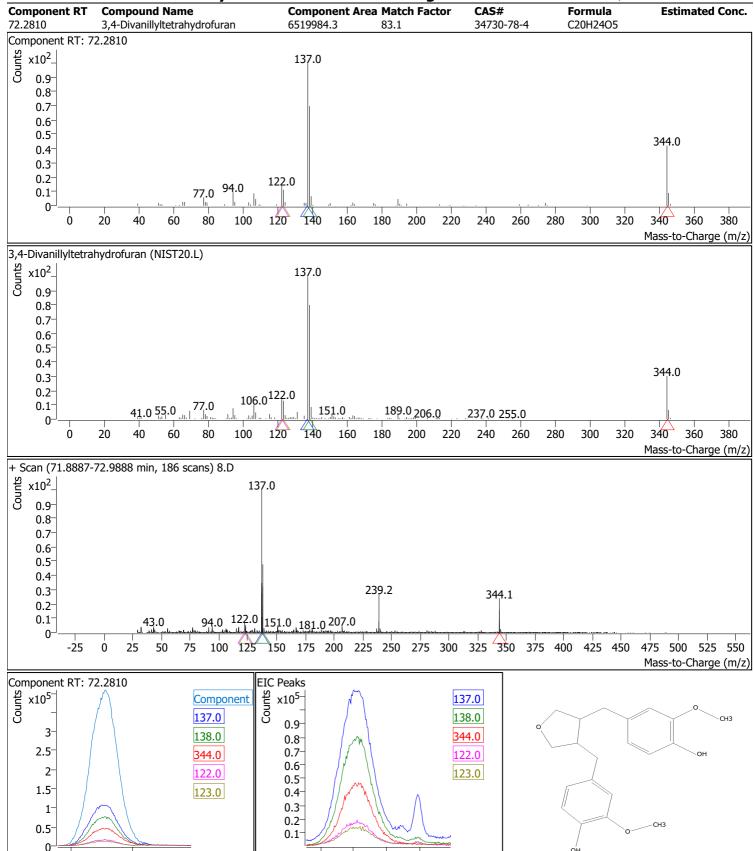












72.25 72.5 72.75

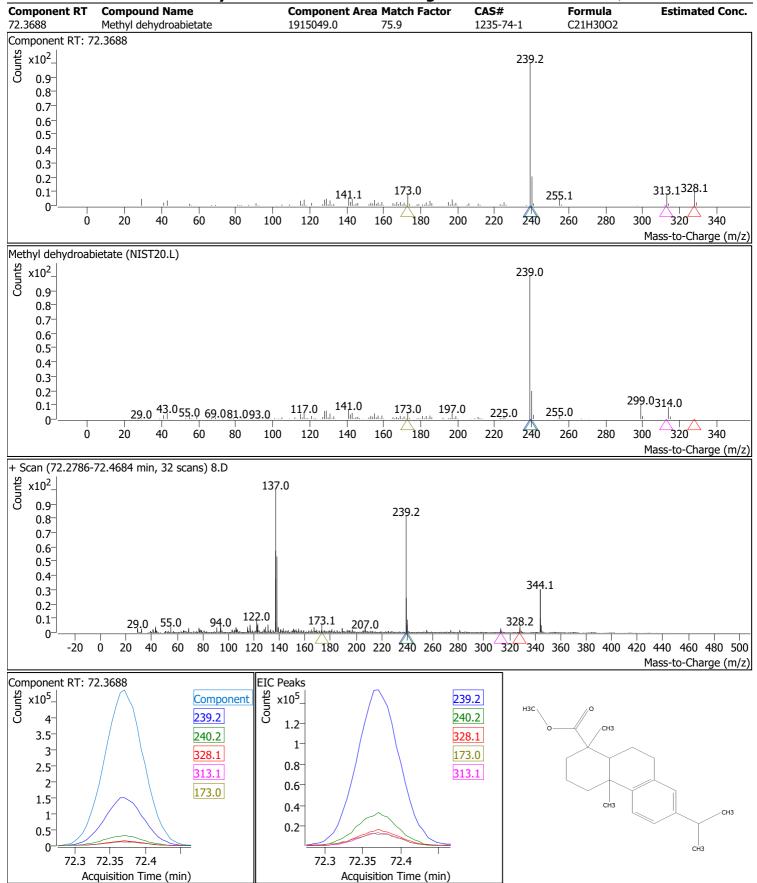
Acquisition Time (min)

72

72.5







Compound Name Component Area Match Factor CAS# **Component RT 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.)]-73.6801 13674832.1 86.2 5155-70-4 C20H28O2 Component RT: 73.6801 st x10² 0.9 239.2 285.2 0.8 0.7 0.6 0.5 197.1 0.4^{-} 300.2 0.3 141.1 0.2 0.1 300 200 220 240 280 320 0 20 40 60 80 100 120 140 160 180 260 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 0.1 183.0 225.0 255.0 240 280 300 0 20 40 60 80 100 120 140 160 180 200 220 260 320 Mass-to-Charge (m/z) + Scan (73.4942-73.8628 min, 63 scans) 8.D 돌 x10². 239.2 0.9 0.8 285.2 0.7 0.6 0.5 0.4 0.3 197.1 300.2 0.2 141.1 43.1 0.1 91.0 200 225 425 25 50 75 100 150 175 250 275 300 325 350 375 400 450 475 500 525 -25 Mass-to-Charge (m/z) Component RT: 73.6801 EIC Peaks x10⁶ x10⁵ 239.2 Component 239.2 285.2 2.5 1.8 СНЗ 285.2 197.1 1.6 2 1.4 197.1 300.2 1.2 1.5 300.2 141.1 1 141.1 0.8 1

73.7

Acquisition Time (min)

73.6

73.8

0.5

0.6⁻ 0.4⁻

0.2

73.6

73.7

Acquisition Time (min)

73.8

СНЗ

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor Component RT Compound Name** CAS# **Formula Estimated Conc.** 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether 75.9213 823971.4 82.2 22318-87-2 C18H22O4 Component RT: 75.9213 $x10^{2}$ 151.0 0.9 0.8 0.7° 0.6 0.5 0.4 0.3 0.2 302.0 0.1 108.0123.0 120 300 -20 20 40 60 100 140 160 180 200 220 240 260 280 320 340 Mass-to-Charge (m/z) 5-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]benzene-1,3-diol, trimethyl ether (NIST20.L) $x10^{2}$ 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2-302.0 15.027.039.051.0 65.077.0 91.0 107.0 0.1 165.0 181.0196.0211.0226.0241.0256.0 300 20 180 200 220 240 260 320 340 -20 40 60 80 100 120 140 160 280 Mass-to-Charge (m/z) + Scan (75.8310-76.0297 min, 34 scans) 8.D Counts x10²_ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 181.0 207.0 0.2 43.0 91.0 137.0 302.0 0.1 242.0 300 325 350 375 400 125 150 200 225 250 275 475 500 -25 25 50 75 100 175 425 450 525 550 Mass-to-Charge (m/z) Component RT: 75.9213 EIC Peaks Counts Counts x10⁵-151.0 Component 151.0 152.0 0.9 1.4 302.0 91.0 0.8 1.2 302.0 152.0 0.7 1 0.6 123.0 91.0 0.8 0.5

75.85 75.9 75.95

Acquisition Time (min)

123.0

76

0.4⁻ 0.3⁻

0.2

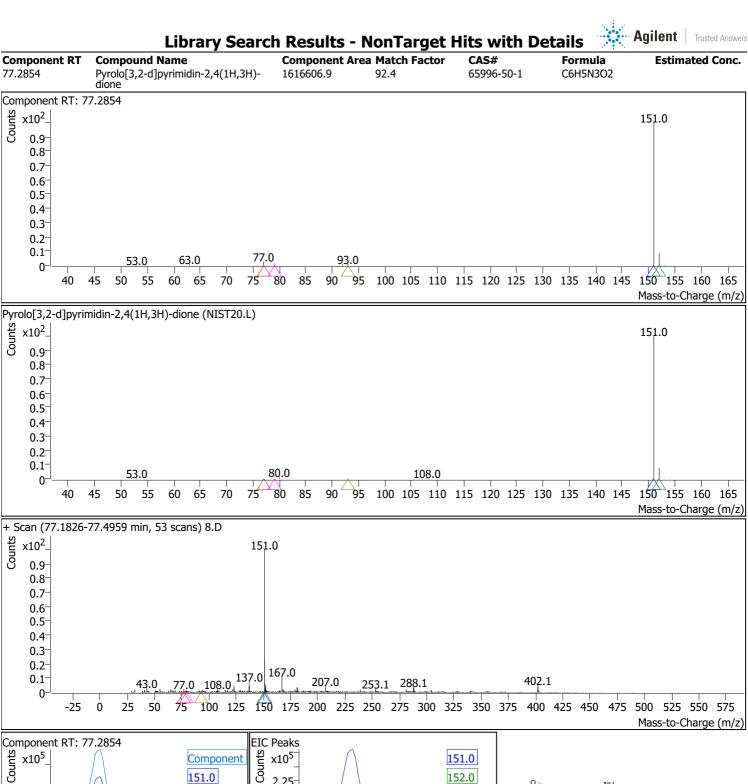
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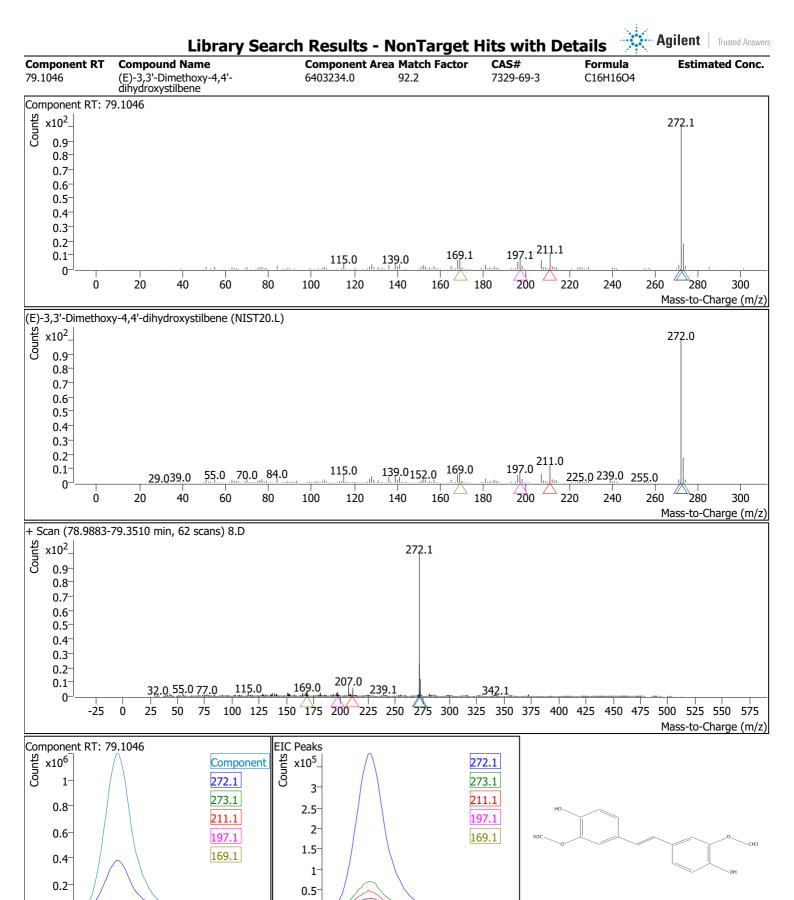
0.6

0.4

0.2

75.9





79.1

79.2

Acquisition Time (min)

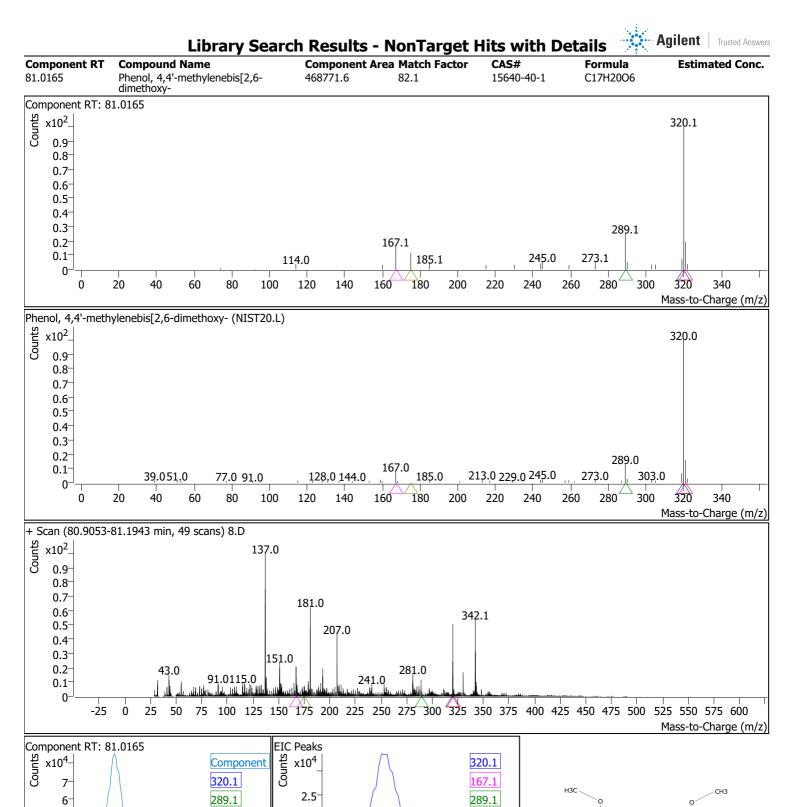
79.3

79.1

79.2

Acquisition Time (min)

79.3



81.1

Acquisition Time (min)

321.0

175.0

CH3

321.0

167.1

175.0

81.2

Acquisition Time (min)

2

1.5

1

0.5

5

4

3

2

1