Library Search Results - NonTarget Hits with Details



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Analysis File Name 250501 sample 9.uaf

Analyst Name admin Analysis Time 5/2/2024 11:47:37 AM

 File Name
 9.D
 Path Name
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 Sample Name
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 Sample Type
 Sample

 Acq. Method File
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Acq. Method File240430 scanAcq. Method PathD:\MassHunter\GCAcq. Date-Time4/30/2024 1:43:13 PMAcq. Operator

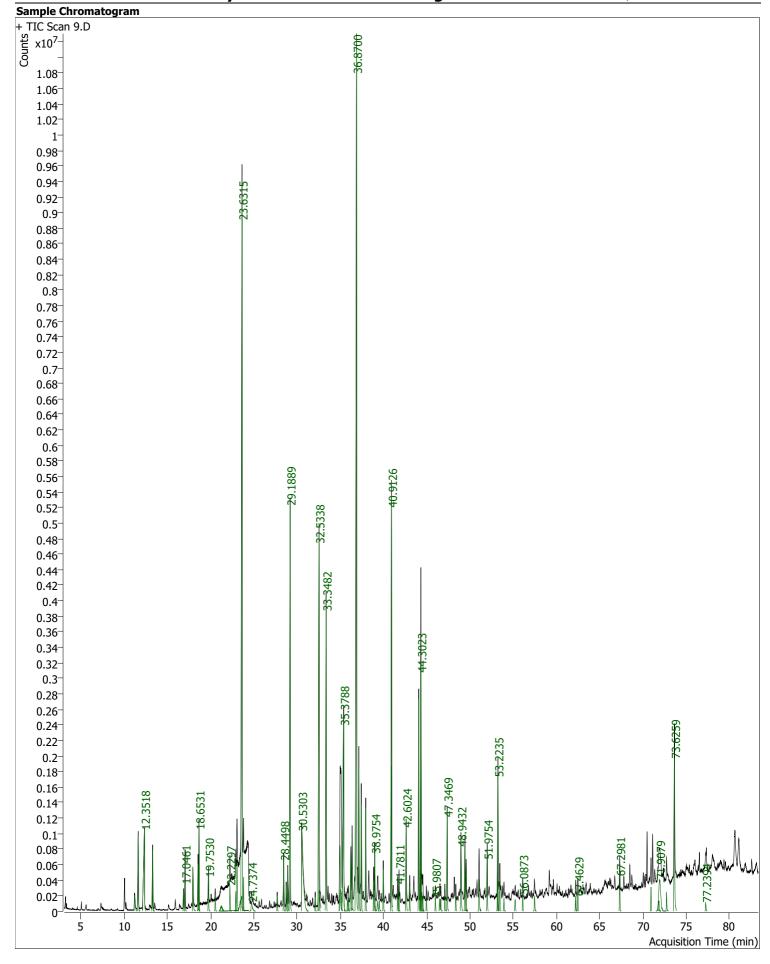
Instrument Name GCMSD Dil. 1

6		646#		_		
Component R	Г Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
11.2171	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	1244568.9	88.3	
11.6334	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	4735403.2	78.0	
12.3518	Butyrolactone	96-48-0	C4H6O2	8811086.7	98.0	
13.2988	Acetoin	513-86-0	C4H8O2	1067529.0	84.6	
13.3032	Propane, 1,1-diethoxy-	4744-08-5	C7H16O2	3725696.6	78.9	
16.8680	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	921670.6	80.4	
17.0461	Propanoic acid, 2-hydroxy-, ethyl ester	97-64-3	C5H10O3	1560453.5	76.7	
17.9480	Phenol	108-95-2	C6H6O	2484372.1	97.8	
18.5486	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2530081.2	92.5	
18.6509	Propyl pyruvate	1000431-41-8	C6H10O3	1098618.4	91.1	
18.6531	Diisoamyl ether	544-01-4	C10H22O	3959585.7	97.1	
19.7530	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	1850053.8	92.4	
20.5343	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	693632.9	91.0	
21.2222	Propanoic acid, 2-methyl-, propyl ester	644-49-5	C7H14O2	865001.8	78.7	
21.2532	1,3,5-Trioxane	110-88-3	C3H6O3	854165.2	81.7	
22.2297	Phenol, 2-methyl-	95-48-7	C7H8O	1353631.2	96.9	
22.9155	1-Propanol, 2-(2-hydroxypropoxy)-	106-62-7	C6H14O3	981370.4	76.7	
23.0521	1-Octanol	111-87-5	C8H18O	3724804.9	96.9	
23.5837	Pentanoic acid, 4-oxo-	123-76-2	C5H8O3	3488581.6	75.5	
23.6315	Phenol, 2-methoxy-	90-05-1	C7H8O2	47337003.4	98.2	
23.7974	Ethanone, 1-(2-thienyl)-	88-15-3	C6H6OS	1538025.8	94.8	
24.7374	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	1148615.3	91.3	
27.6982	Butanoic acid, 2,2-dimethylpropyl ester	23361-69-5	C9H18O2	793728.9	77.2	
28.4498	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	2466532.7	96.0	
28.7394	Naphthalene	91-20-3	C10H8	1083034.1	97.3	
28.9234	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	1847288.4	96.4	
29.1889	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	21064116.0	99.2	
30.5303	Catechol	120-80-9	C6H6O2	12751056.6	97.1	
32.0929	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	690315.9	82.9	
32.5338	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	26067273.9	98.6	
32.5636	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	1087795.9	81.6	
33.3482	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	15518067.9	97.0	
34.9598	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	5458484.5	88.1	
35.0520	2-Propanone, 1-hydroxy-	116-09-6	C3H6O2	2833781.4	86.2	
35.3788	Butanoic acid, 2-methylpropyl ester	539-90-2	C8H16O2	15404553.0	79.1	
35.3788	2,3-dihydroxypropyl isobutyrate	1010458-45-6	C7H14O4	15711811.8	78.7	
35.8212	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	772674.3	76.9	
35.9277	3-Methoxy-5-methylphenol	3209-13-0	C8H10O2	712647.7	83.1	
36.2224	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	3420119.6	79.2	
36.3575	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	4083898.2	86.6	
36.8700	2,3-Dimethoxyphenol	5150-42-5	C8H10O3	62920521.5	98.4	
37.1409	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	6947726.0	87.8	
37.4206	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	5089393.5	92.4	
37.9399	1,2,3-Trimethoxybenzene	634-36-6	C9H12O3	4871237.9	91.4	
38.8506	4-Ethylcatechol	1124-39-6	C8H10O2	1866866.3	94.8	
38.9754	Vanillin	121-33-5	C8H8O3	3144709.7	92.8	
39.2887	3-Ethoxy-4-methoxyphenol	65383-57-5	C9H12O3	795565.4	75.0	
39.4927	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	638325.6	86.7	
39.9625	4-Methoxy-2-methyl-1-(methylthio)benzene	22583-04-6	C9H12OS	2140776.4	84.4	
40.9107	2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]-	1000131-52-4	C8H11NO2	8157951.5	77.5	
40.9126	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	22508846.0	94.6	
41.6227	3-Hydroxy-4-methoxybenzoic acid	645-08-9	C8H8O4	920326.8	77.8	
41.7811	Eugenol	97-53-0	C10H12O2	1325802.7	84.7	
42.6024	Apocynin	498-02-2	C9H10O3	4597245.2	98.3	
43.0170	Benzene, 1,2,3-trimethoxy-5-methyl-	6443-69-2	C10H14O3	1123631.9	87.2	
		14059-92-8			98.8	
44.0596	4-Ethyl-2,6-dimethoxyphenol		C10H14O3	10158912.7		
44.3023	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	13134927.4	95.7 75.0	
44.3039	O-(2,6-Dimethylpyrid-3-yl)-N-phenylbenzimidate	32953-48-3	C20H18N2O	2286017.0	75.9	
44.3275	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	6793335.9	93.8 75.0	
44.4343	Homovanillyl alcohol	2380-78-1	C9H12O3	1357274.5	75.0	
44.5306	Flopropione	2295-58-1	C9H10O4	914413.6	84.3	
44.9527	3,4-Dimethoxyphenylacetone	776-99-8	C11H14O3	657847.6	82.9	
45.9807	Ethanone, 1-(2,3-dihydro-1,4-benzodioxin-6-yl)-	2879-20-1	C10H10O3	678689.8	79.1	
46.4694	1-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	1835-14-9	C10H12O3	633294.3	78.2	

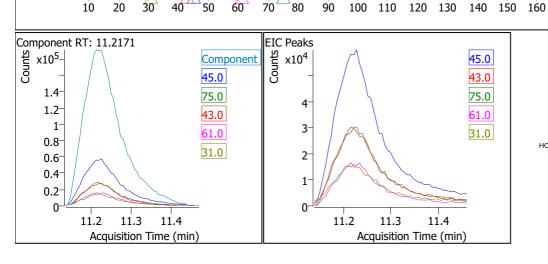
Library Search Results - NonTarget Hits with Details

Agilent	Trusted Answers
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Component	RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
46.6126	Butyrovanillone	64142-23-0	C11H14O3	668009.8	89.8	
47.0829	Phenol, 2-methoxy-4-methyl-6-[propenyl]-	201359-63-9	C11H14O2	750062.3	76.5	
47.3469	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	4507386.4	92.4	
48.3432	Benzeneacetic acid, .alpha.,4-dihydroxy-3-methoxy-, methyl ester	2911-74-2	C10H12O5	821880.8	75.1	
48.9432	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	3855643.1	89.1	
49.4088	2-Naphthalenol, 3-methoxy-	18515-11-2	C11H10O2	3370642.3	96.0	
49.5436	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	1940729.7	88.2	
51.0303	Phlorobutyrophenone	2437-62-9	C10H12O4	2039806.9	80.0	
51.9754	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	2675600.3	96.8	
53.1685	1,6-Dimethoxynaphthalene	3900-49-0	C12H12O2	1410079.5	81.8	
53.2235	Syringylacetone	19037-58-2	C11H14O4	6668429.2	96.8	
53.4358	Naphthalene, 2,3-dimethoxy-	10103-06-7	C12H12O2	1715273.0	86.8	
53.9148	1,6-Dimethoxynaphthalene	3900-49-0	C12H12O2	639469.1	81.5	
55.2104	1-Propanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	5650-43-1	C11H14O4	848213.7	79.4	
56.0873	2,3-Dimethoxy-5-aminocinnamonitrile	1000214-46-5	C11H12N2O2	872179.3	78.7	
57.4473	Dihydrosyringenin	20736-25-8	C11H16O4	986653.8	91.3	
62.2099	2,5-Dimethyl-4-(3-amino-4-methylphenyl)pyridine	71153-33-8	C14H16N2	819468.3	75.8	
62.2101	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimethyl-	119-93-7	C14H16N2	842652.2	76.4	
62.4629	.betaCarboline, 8-methoxy-1-methyl-	212332-24-6	C13H12N2O	819448.1	77.4	
67.2981	2-Isopropyl-10-methylphenanthrene	66552-97-4	C18H18	1890099.9	95.5	
70.9154	Methyl dehydroabietate	1235-74-1	C21H30O2	1241025.0	93.4	
71.8303	8-Isopropyl-1,3-dimethylphenanthrene	135886-06-5	C19H20	684404.5	85.4	
71.9079	3,4-Divanillyltetrahydrofuran	34730-78-4	C20H24O5	6831900.6	83.4	
72.7167	1-(2,4-Dihydroxyphenyl)-2-(3,4- dimethoxyphenyl)ethanone	24126-98-5	C16H16O5	1009259.2	79.1	
73.6259	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	10433003.5	94.4	
77.2394	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	541806.4	85.9	



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61.0

88.0

31.0

0.2

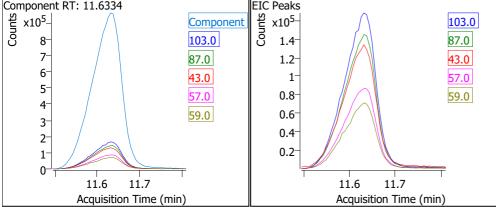
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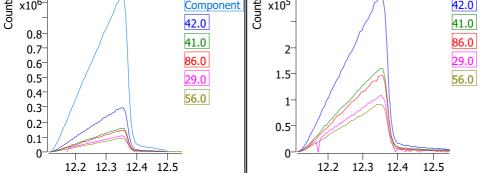
200 210 220 230 Mass-to-Charge (m/z)

170 180

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 11.6334 Propane, 1,1-diethoxy-4735403.2 78.0 C7H16O2 Component RT: 11.6334 v10² 0.9 103.0 87.0 43.0 0.8 0.7 0.6 57.0 0.5 31.0 0.4 0.3 0.2 117.0 0.1 40 70 130 10 20 30 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 78.0 131.0 130 10 20 30 40 50 60 70 80 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (11.4904-11.8041 min, 53 scans) 9.D St x10² 0.9 103.0 43.0 87.0 0.8 0.7 0.6 59.0 0.5 29.0 0.4^{-} 0.3 0.2 117.0 0.1 67.0 96.0 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: 11.6334 **EIC Peaks** x10⁵ 103.0 Component



-- 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 12.3518 Butyrolactone 8811086.7 98.0 C4H6O2 Component RT: 12.3518 v10² 0.9 42.0 0.8 0.7 0.6 86.0 0.5 0.4 29.0 56.0 0.3 39.0 0.2 0.1 0 25 40 55 20 30 35 45 50 65 70 75 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 (12.1142-12.4879 min, 63 scans) 9.D St x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 86.0 29.0 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) Component RT: 12.3518 **EIC Peaks** Counts Counts x10⁵ 42.0 Component 42.0 41.0 0.8 41.0 86.0 0.7^{-1} 2



Acquisition Time (min)



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13.3

13.4

Acquisition Time (min)

13.5

88.0

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13.3

13.4

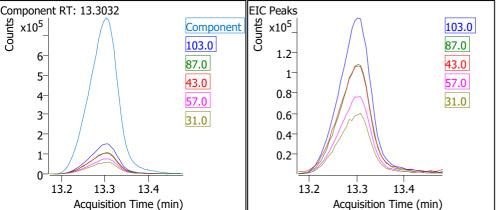
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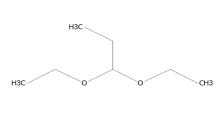
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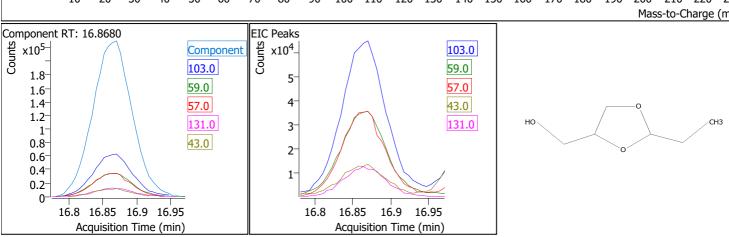
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--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4744-08-5 13.3032 Propane, 1,1-diethoxy-3725696.6 78.9 C7H16O2 Component RT: 13.3032 v10² 0.9 103.0 0.8 87.0 43.0 0.7 0.6 57.0 0.5 31.0 0.4 0.3 0.2 0.1 0 30 40 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 78.0 131.0 130 0 10 20 30 40 50 60 70 80 90 100 110 120 140 Mass-to-Charge (m/z) + Scan (13.1783-13.4750 min, 50 scans) 9.D St x10² 0.9 103.0 43.0 0.8 87.0 0.7 0.6 57.0 0.5 0.4^{-} 31.0 0.3 0.2 0.1 117.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 13.3032 x10⁵ 103.0 Component 87.0



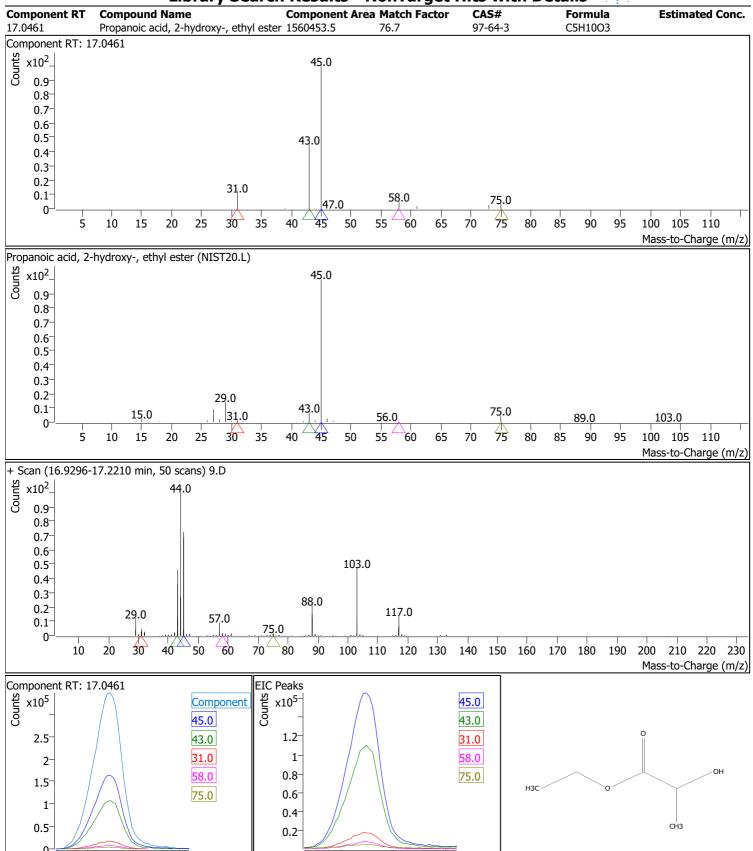


- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 16.8680 1,3-Dioxolane-4-methanol, 2-ethyl-921670.6 80.4 C6H12O3 Component RT: 16.8680 v10² 0.9 103.0 0.8 0.7 0.6 59.0 0.5 0.4 0.3 131.0 43.0 31.0 0.2 0.1 40 100 130 Ó 10 20 30 50 70 80 90 110 120 140 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 60 0 10 20 30 40 50 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (16.7821-16.9752 min, 32 scans) 9.D St x10² 0.9 103.0 0.8 0.7 0.6 0.5 57.0 0.4^{-} 0.3 0.2 29.0 0.1 117.0 68.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 16.8680 x10⁴-103.0 Component



Library Search Results - NonTarget Hits with Details





17.1

Acquisition Time (min)

17.2

17

17.1

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18

18.1

Acquisition Time (min)

18.2

95.0

2.5

1.5

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2

1

18

18.1

Acquisition Time (min)

18.2

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95.0

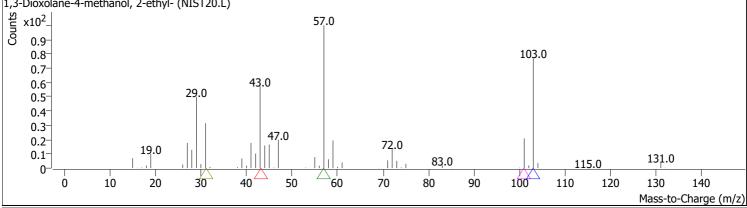
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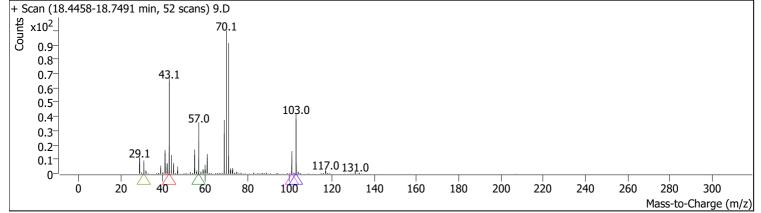
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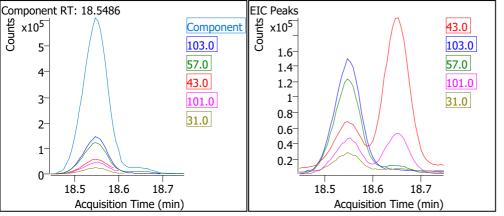
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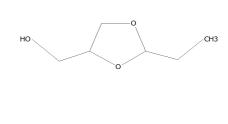
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-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 18.5486 1,3-Dioxolane-4-methanol, 2-ethyl-2530081.2 92.5 C6H12O3 Component RT: 18.5486 v10² 0.9 103.0 57.0 0.8 0.7 0.6 0.5 43.0 0.4 0.3 0.2 47.0 73.0 0.1 30 130 Ó 10 20 50 70 80 90 100 110 120 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) 57.0 103.0 0.8



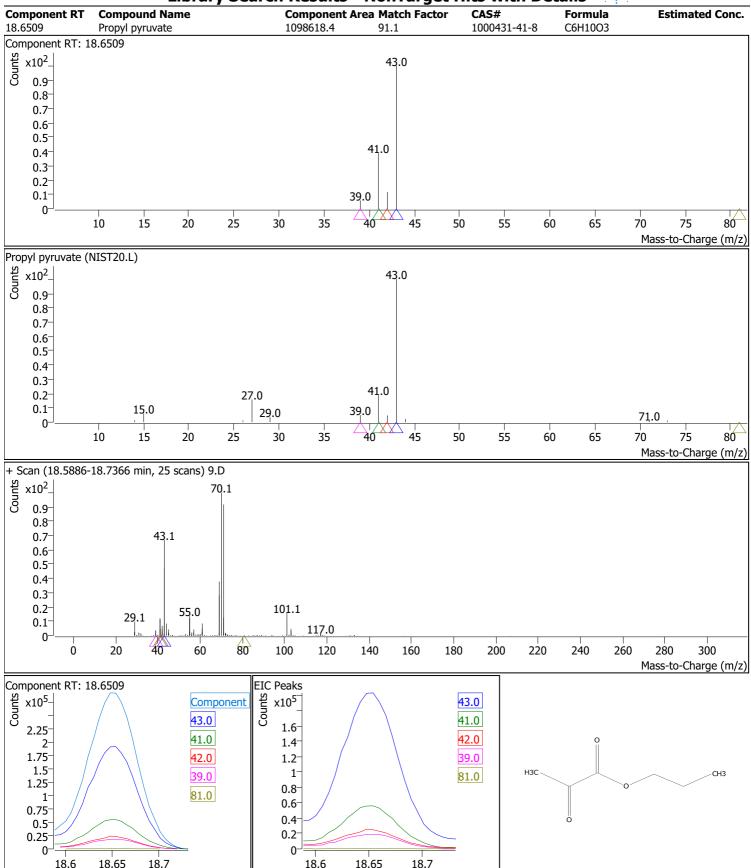












Acquisition Time (min)

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3959585.7 544-01-4 18.6531 Diisoamyl ether 97.1 C10H22O Component RT: 18.6531 v10² 0.9 70.0 0.8 43.0 0.7^{-} 0.6 0.5 0.4 0.3 55.0 101.0 0.2 0.1 29.0 70 100 130 10 20 30 40 50 60 80 90 110 120 140 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) S 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 Mass-to-Charge (m/z) + Scan (18.5529-18.7491 min, 34 scans) 9.D st x10² 0.9 0.8 43.1 0.7 0.6 0.5 0.4 0.3 103.0 57.0 0.2 29.1 0.1 117.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 18.6531 Counts Counts x10⁵ 70.0 Component 70.0 43.0 2 0.8 71.0 71.0 1.75 0.7^{-1}



18.7

Acquisition Time (min)

43.0

69.0

41.0

0.6

0.5

 0.4^{-}

0.3

0.2-

0.1

18.6

18.7

Acquisition Time (min)

1.5

1.25

0.75

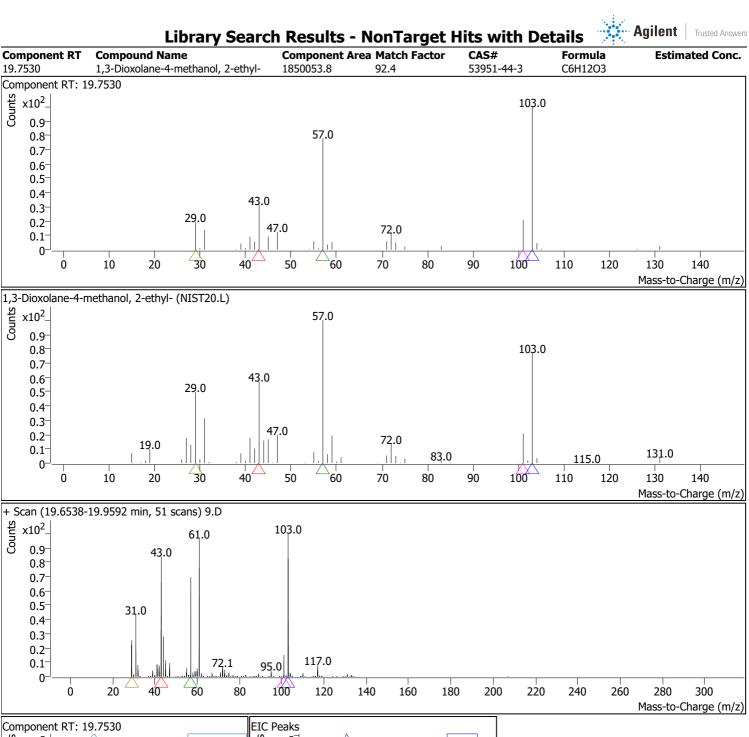
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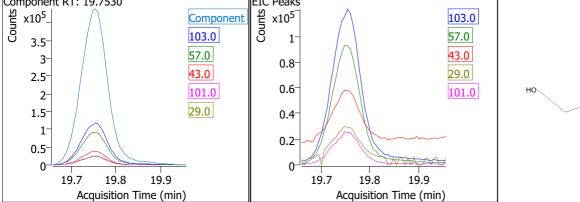
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18.6

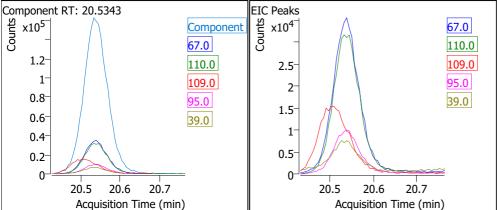
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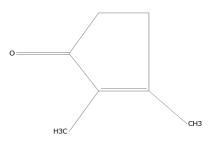
69.0

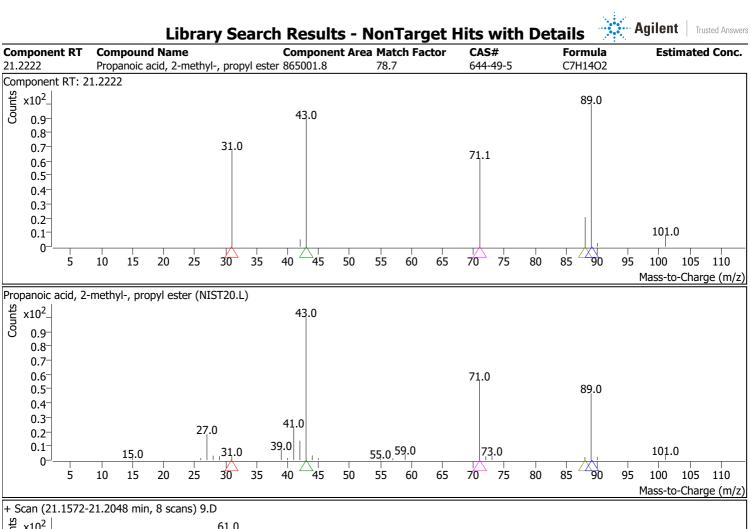


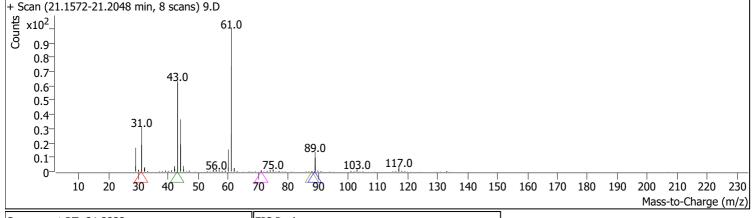


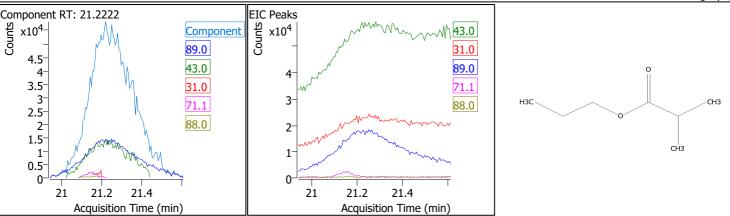
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.5343 2-Cyclopenten-1-one, 2,3-dimethyl-693632.9 91.0 1121-05-7 C7H10O Component RT: 20.5343 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 0.3 39.0 0.2 53.0 81.0 124.0 0.1 29.0 40 105 110 115 120 125 10 25 30 35 50 55 65 80 85 90 95 100 75 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 110.0 67.0 0.8 0.7 0.6 0.5 0.4 82.0 95.0 0.3 54.0 39.0 0.2 27.0 0.1 51.0 65.0 79.0 99.0 91.0 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (20.4423-20.6459 min, 35 scans) 9.D st x10² 0.9 61.0 0.8 43.0 0.7^{-} 0.6 0.5 0.4^{-} 110.1 0.3 67.0 31.0 0.2 0.1 95.0 53.0 81.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.5343 Counts Counts x10⁴ 67.0 Component 67.0 110.0 1.2 110.0 109.0 2.5











-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** Component Area Match Factor CAS# **Component RT Compound Name Formula Estimated Conc.** 854165.2 110-88-3 21.2532 1,3,5-Trioxane 81.7 C3H6O3 Component RT: 21.2532 v10² 0.9 61.0 89.0 43.0 0.8 0.7 0.6 0.5 0.4 31.0 0.3 0.2 0.1 56.0 0 55 __90 25 75 80 10 15 20 30 35 40 50 60 65 70 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 0.4 29.0 0.3 0.2 0.1 44.0 14.0 56.0 90 10 15 20 25 30 35 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (20.9432-21.6091 min, 113 scans) 9.D st x10² 0.9 0.8 0.7 0.6 43.0 0.5 0.4 0.3 0.2 31.0 0.1 117.0 60 20 40 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 21.2532 **EIC Peaks** Counts Counts $x10^{4}$ Component 61.0 61.0 43.0 8 4.5 89.0 7 31.0 6 3.5 43.0 89.0 3 5 31.0 42.0 2.5 4 42.0 2

21.2

21.4

Acquisition Time (min)

3

2

21

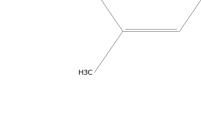
1.5

21

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.** 95-48-7 22.2297 Phenol, 2-methyl-1353631.2 96.9 C7H8O Component RT: 22.2297 v10² 0.9 108.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 90.0 0.2 39.0 51.0 0.1 90 10 15 35 50 55 65 75 95 100 105 Mass-to-Charge (m/z) Phenol, 2-methyl- (NIST20.L) Counts x10²_ 0.9 108.0 0.8 0.7 0.6 0.5 0.4 0.3 79.0 90.0 0.2 0.1 86.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (22.1467-22.4475 min, 51 scans) 9.D Sounds x10² 0.9 0.8 0.7 0.6 0.5 43.0 0.4^{-} 0.3 0.2 31.0 108.1 0.1 117.0 80 Ó 20 40 60 100 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 22.2297 Counts Counts x10⁴ 108.0 Component 108.0 107.0 2.5 107.0 77.0 6 79.0 2 77.0 5 НО



22.3

Acquisition Time (min)

22.4

90.0

79.0

90.0

1.5

1-

22.2

22.3

Acquisition Time (min)

22.4

0.5

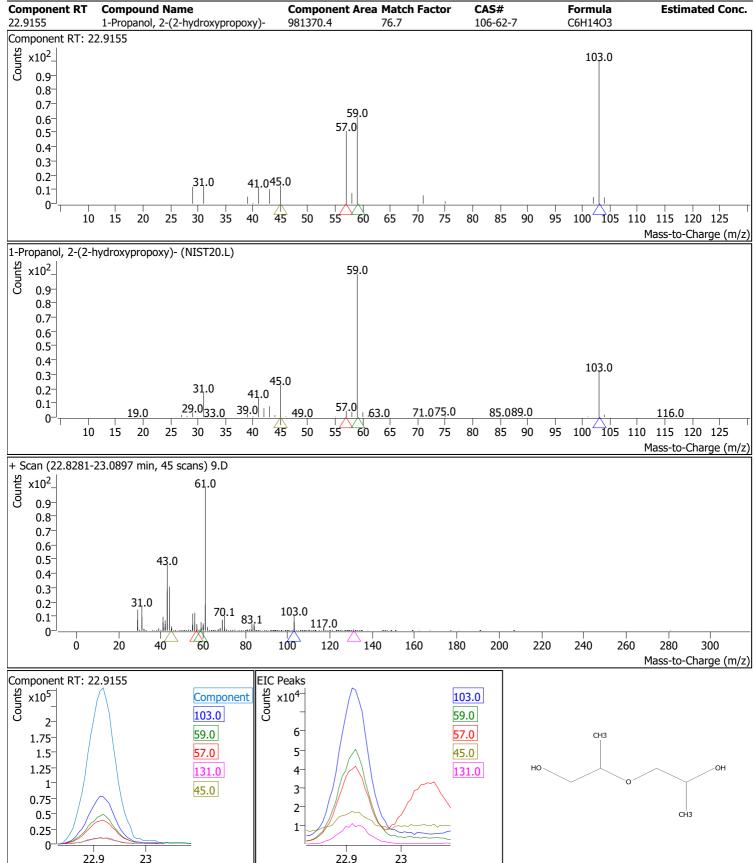
4

3-

2-







Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0521 1-Octanol 3724804.9 96.9 111-87-5 C8H18O Component RT: 23.0521 v10² 0.9 56.0 70.0 0.8 41.0 0.7^{-} 84.0 29.0 0.6 0.5 0.4 0.3 0.2 0.1 70 100 105 110 115 120 125 130 135 140 65 75 80 85 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 70 95 100 105 110 115 120 125 130 135 140 55 20 25 30 35 40 45 50 60 65 75 80 85 90 Mass-to-Charge (m/z) + Scan (22.9232-23.1670 min, 42 scans) 9.D st x10² 0.9 0.8 0.7 0.6 0.5 43.0 0.4^{-} 0.3 31.0 0.2 70.1 103.0 117.0 84.1 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.0521 Counts Counts x10⁴ 56.0 Component 56.0 55.0 5 55.0 6 41.0 5 41.0 69.0

70.0

70.0

69.0

3

2

1

22.9

23

23.1 23.2

Acquisition Time (min)

4

3-

2

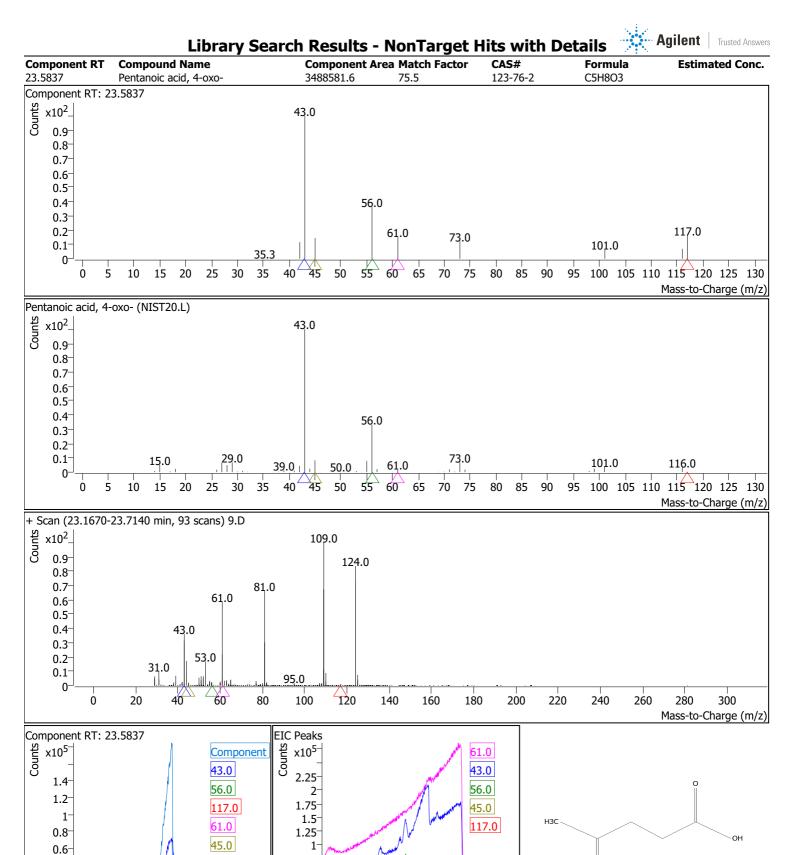
1

22.9

23

23.1

Acquisition Time (min)





23

Acquisition Time (min)

24

0.75

0.25

0.5

0.4

0.2

0

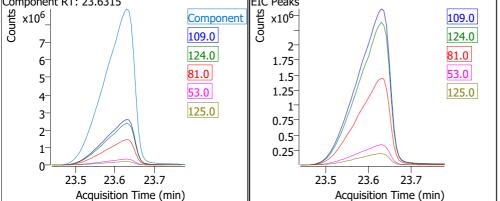
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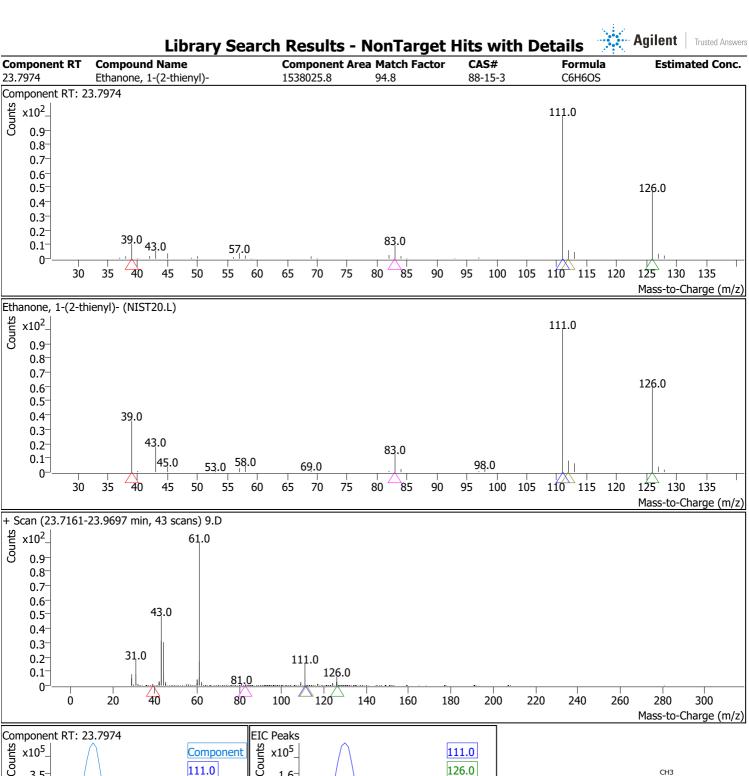
23

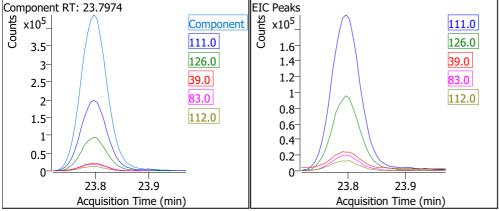
Acquisition Time (min)

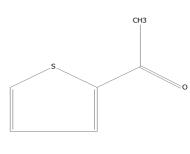
24

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6315 Phenol, 2-methoxy-47337003.4 98.2 C7H8O2 Component RT: 23.6315 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 65.0 39.0 80 110 10 20 30 40 50 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 81.0 0.7 0.6 0.5 0.4 0.3 53.0 0.2 39.0 63.0 0.1 27.0 77.0 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4405-23.7794 min, 58 scans) 9.D st x10² 0.9 109.0 124.0 0.8 81.0 0.7 0.6 0.5 61.0 0.4^{-} 43.0 0.3 53.0 0.2 31.0 0.1 95.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 23.6315 EIC Peaks Counts Counts x10⁶ 109.0 Component 109.0 124.0 7 2 124.0 81.0 6 1.75



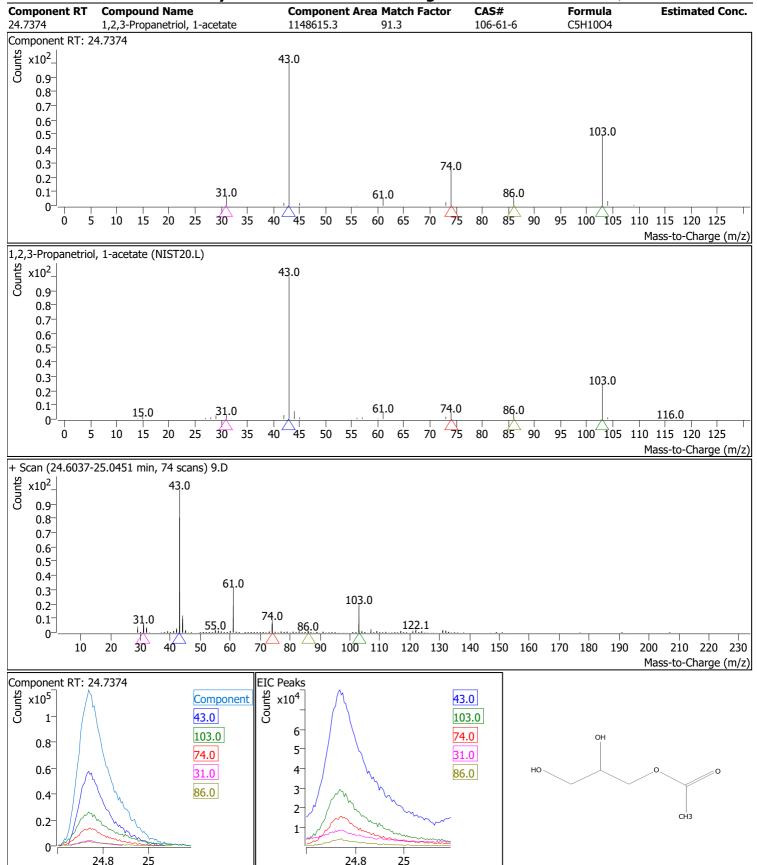






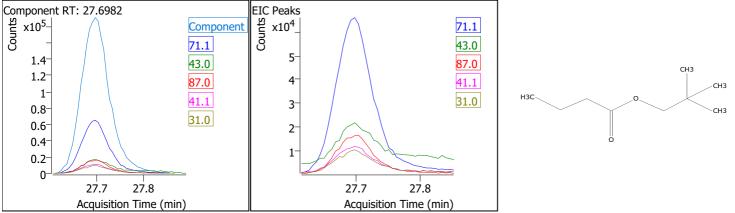




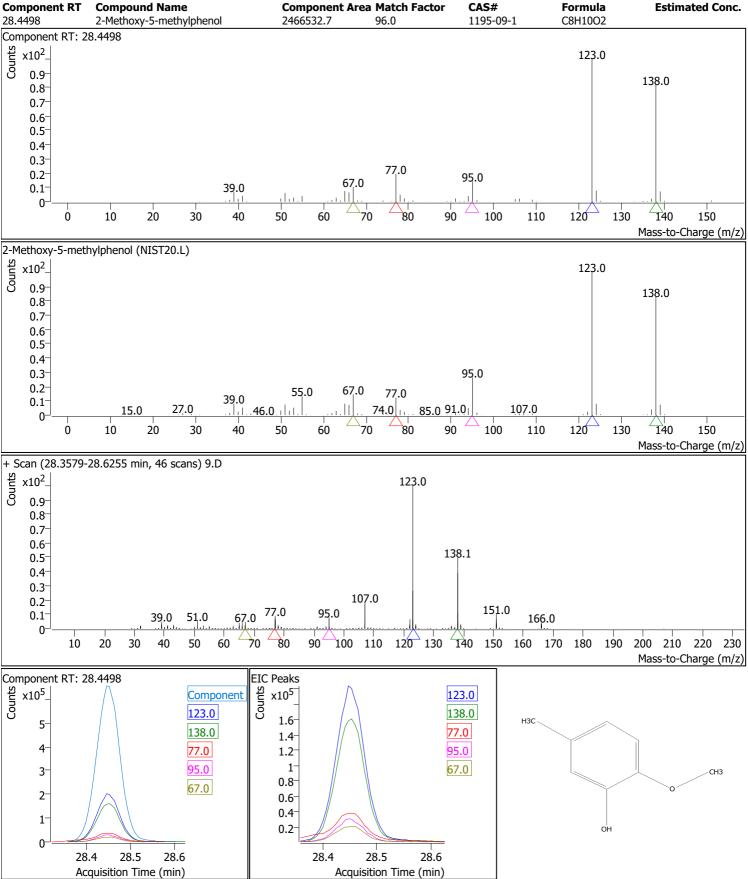


Acquisition Time (min)

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 27.6982 Butanoic acid, 2,2-dimethylpropyl 793728.9 23361-69-5 C9H18O2 Component RT: 27.6982 x10²_ 71.1 0.9 8.0 0.7 0.6 0.5 0.4 43.0 0.3 87.0 0.2^{-} 31.0 57.0 103.0 0.1 0-30 70 10 20 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 30 10 20 40 50 60 70 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (27.6213-27.8287 min, 35 scans) 9.D x10². 71.0 0.9 0.8 0.7 0.6 43.0 0.5 0.4 0.3 151.0 0.2 87.0 166.0 31.0 57.0 136.0 103.0 0.1 121.0 30 90 190 200 210 220 230 10 20 40 50 60 70 80 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) Component RT: 27.6982 **EIC Peaks**







--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Naphthalene 91-20-3 28.7394 1083034.1 C10H8 Component RT: 28.7394 v10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 51.0 77.0 64.0 45 50 55 65 70 75 85 100 105 110 115 120 135 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 (28.6501-28.9466 min, 50 scans) 9.D st x10² 0.9 128.0 0.8 0.7^{-} 138.1 123.0 0.6 0.5 0.4^{-} 0.3 0.2 95.0 151.0 67.0 77.0 166.0 103.0 43.0 51.0 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 190 200 210 220 230 170 180 Mass-to-Charge (m/z) Component RT: 28.7394 **EIC Peaks** Counts st x10⁵ x10⁵-128.0 Component 128.0 127.0 2.25 1.2 127.0 129.0 1 1.75 129.0 102.0 0.8 1.5 102.0 126.0 1.25

28.8

Acquisition Time (min)

28.9

0.6

0.4

0.2

28.7

126.0

1⁻ 0.75⁻

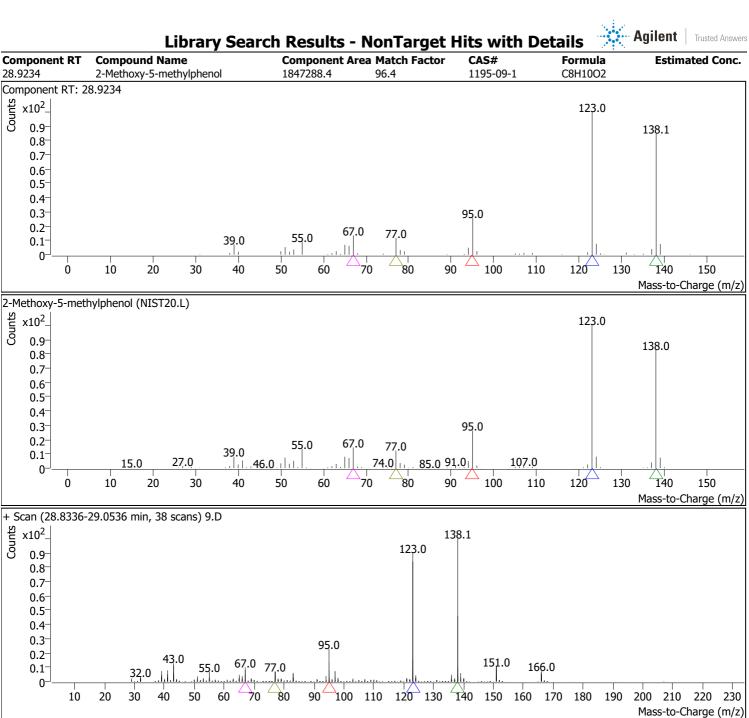
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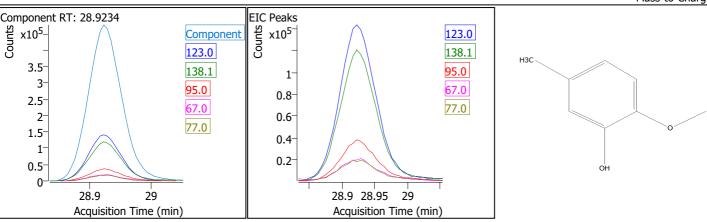
28.7

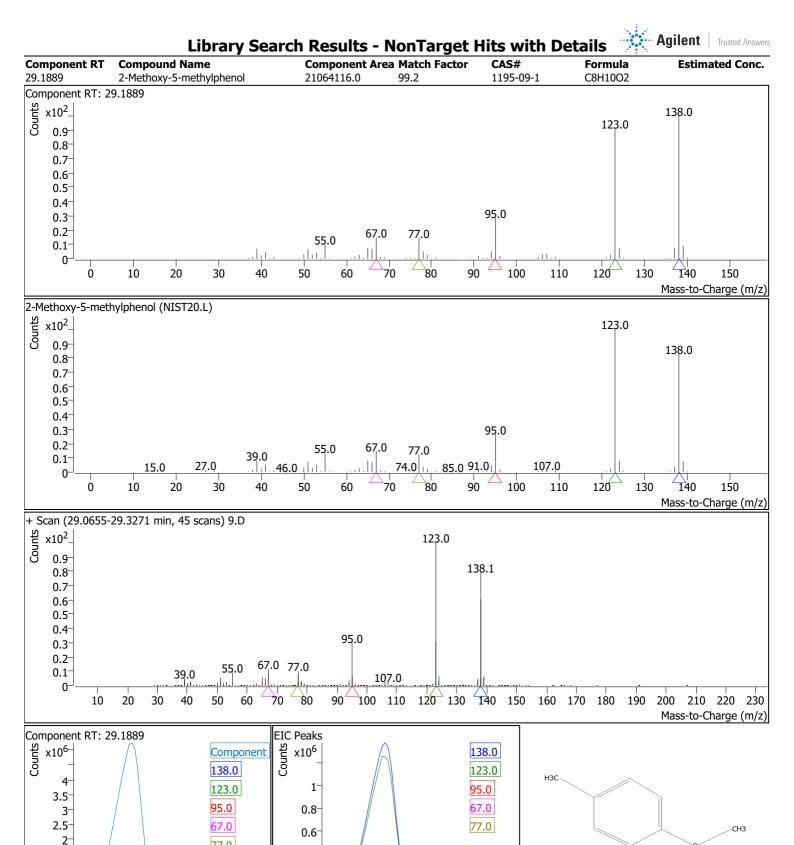
28.8

Acquisition Time (min)

28.9







29.2

Acquisition Time (min)

29.3

77.0

0.4

0.2

29.1

1.5

0.5

1-

29.1

29.2

Acquisition Time (min)

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 30.5303 120-80-9 Catechol 12751056.6 97.1 C6H6O2 Component RT: 30.5303 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 45 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 (30.4925-31.3414 min, 143 scans) 9.D st x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 64.0 0.2 81.092.0 0.1 39.0 53.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.5303 **EIC Peaks** x10⁵ Counts 110.0 Component 110.0 64.0 3.5 0.8 64.0 63.0 0.7 3-63.0 81.0 0.6 2.5

92.0

0.5

 0.4^{-}

0.3-

0.2

0.1

30.6 30.8

31

Acquisition Time (min)

31.2

81.0

92.0

2-

1

30.6

30.8

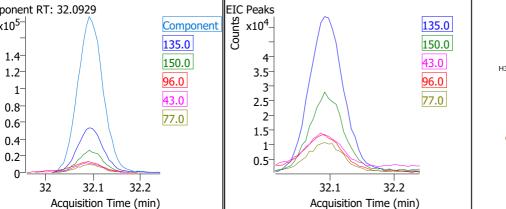
31

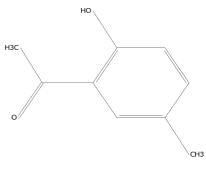
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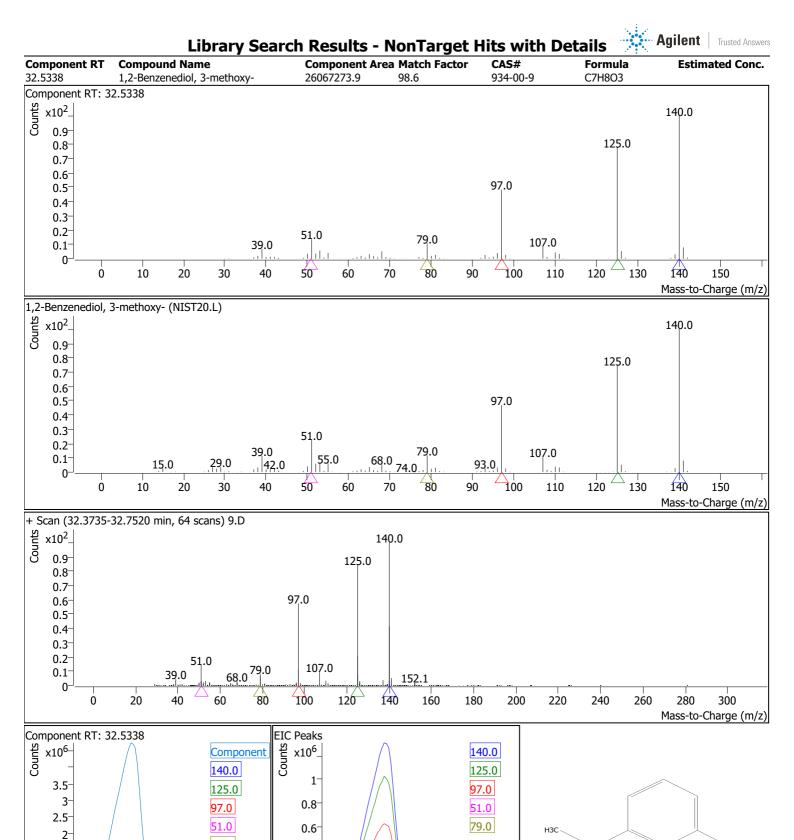
31.2

1.5

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 82.9 1450-72-2 32.0929 Ethanone, 1-(2-hydroxy-5-690315.9 C9H10O2 methylphenyl)-Component RT: 32.0929 x10²_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 0.3 96.0 43.0 77.0 0.2^{-} 67.0 0.1 121.0 0-150 20 30 50 60 70 80 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 150.0 0.6 0.5 0.4 0.3 77.0 107.0 0.2 51.0 0.1 63.0 85.0 91.0 131.0 98.0 121.0 0 130 20 30 50 60 70 80 90 100 110 120 140 150 160 170 Mass-to-Charge (m/z) + Scan (32.0116-32.2407 min, 39 scans) 9.D x10². 135.0 0.9 0.8 0.7 0.6 0.5 0.4 150.0 0.3 43.0 0.2 32.0 165.0 180.0 67.0 0.1 53.0 110.0 121.0 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 10 20 30 40 50 60 70 Mass-to-Charge (m/z) Component RT: 32.0929 **EIC Peaks** Counts Counts x10⁴x10⁵ 135.0 Component НО 135.0 150.0 1.4 4 150.0 43.0 **Н3С** 1.2 3.5 96.0 96.0 3









79.0

0.4

0.2

32.4

32.5

32.6

Acquisition Time (min)

32.7

1.5

0.5

1

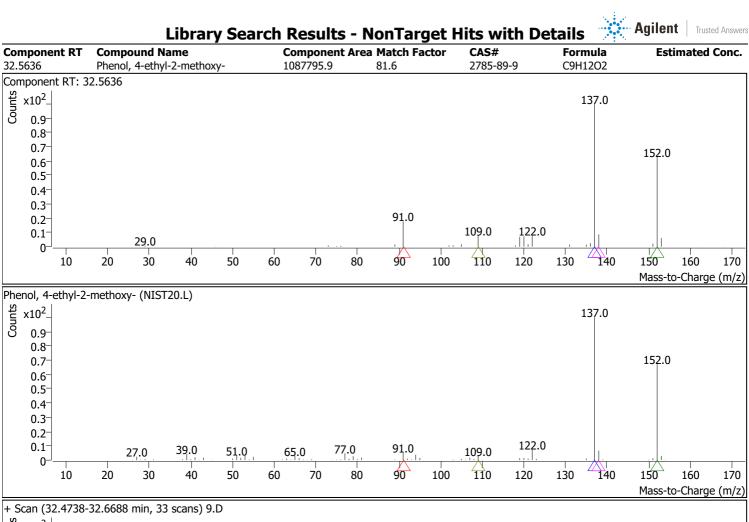
32.5

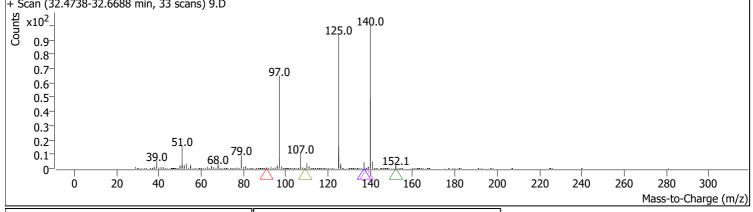
32.6

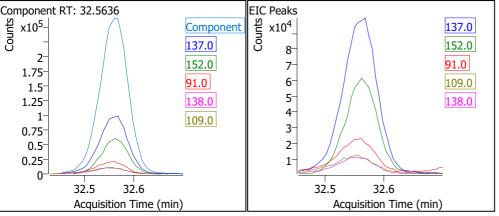
Acquisition Time (min)

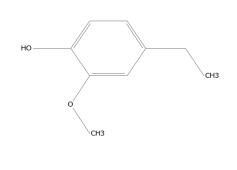
32.7

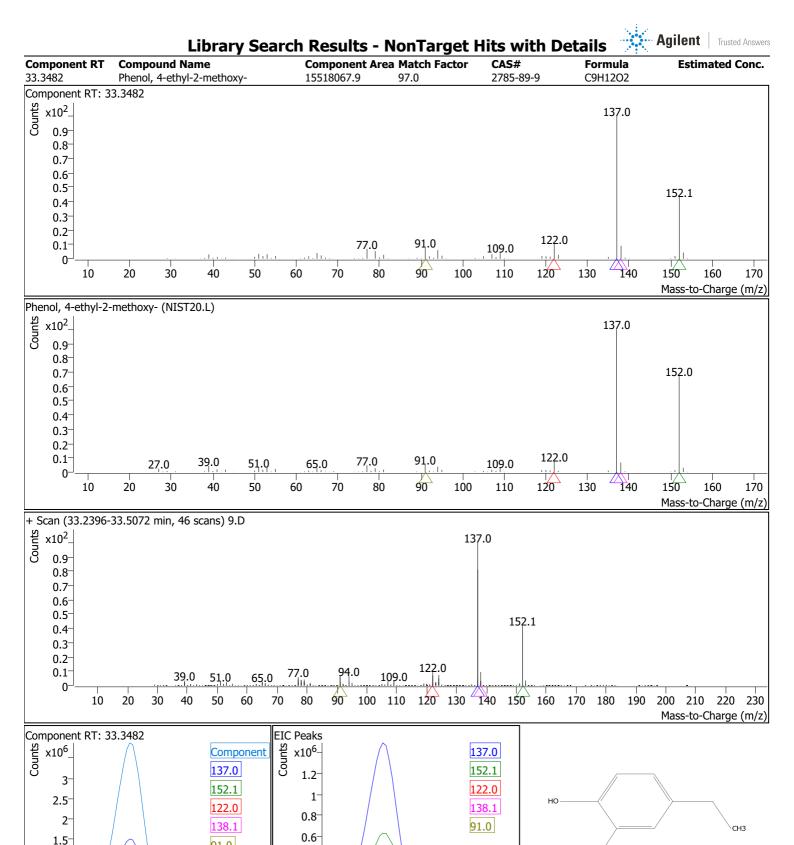
ОН











33.4

Acquisition Time (min)

91.0

1 0.5

0

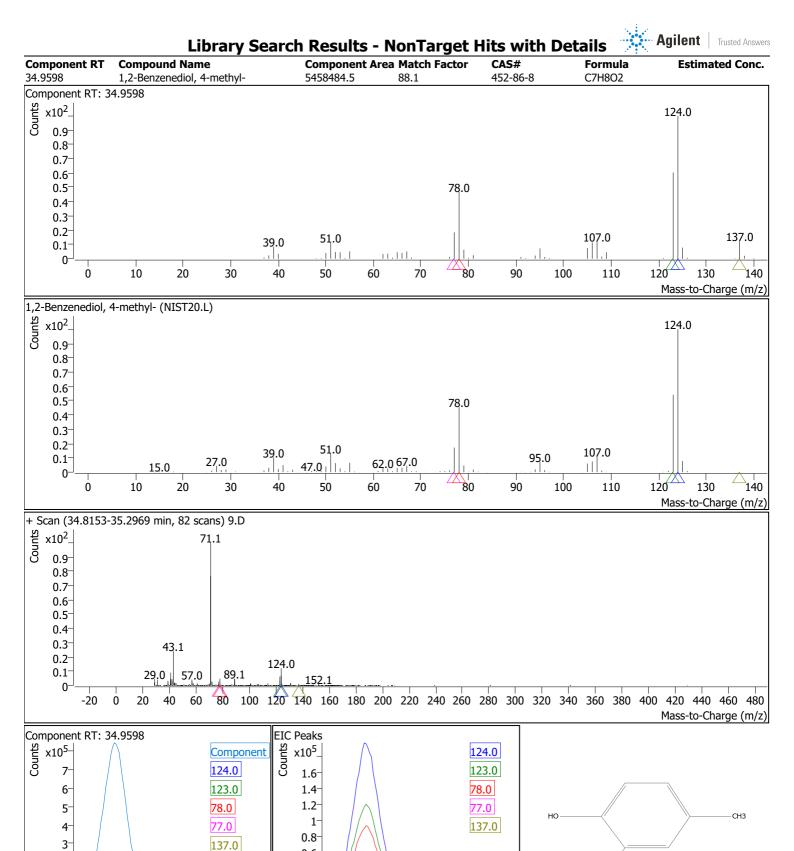
33.3

33.4

Acquisition Time (min)

0.4

0.2



35

35.1 35.2

Acquisition Time (min)

0.6

0.4

0.2

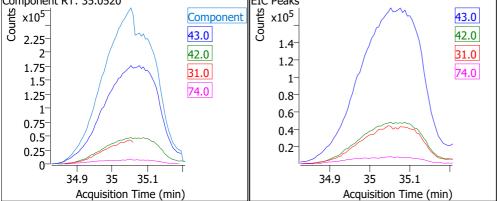
2

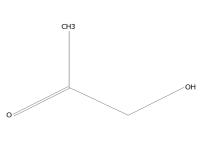
1

35

35.2

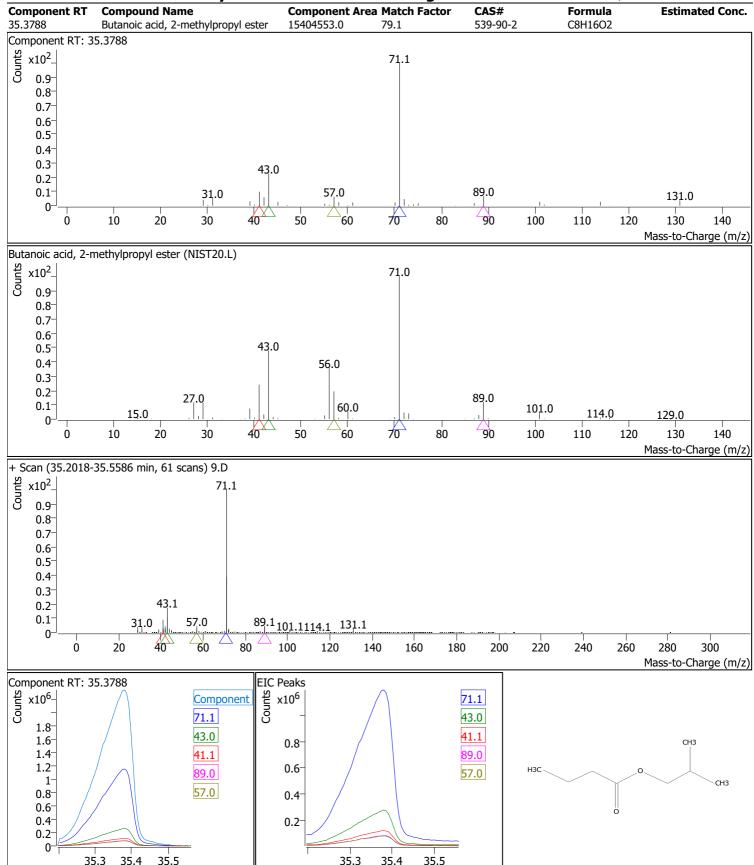
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 116-09-6 35.0520 2-Propanone, 1-hydroxy-2833781.4 86.2 C3H6O2 Component RT: 35.0520 y x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 31.0 0.3 0.2 0.1 74.0 0 $\frac{4}{5}$ 25 30 35 40 55 65 70 10 15 20 50 80 Mass-to-Charge (m/z) 2-Propanone, 1-hydroxy- (NIST20.L) Counts x10²_ 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 0.2 15.0 29.0 74.0 0.1 27.0 45.0 0-45 10 15 20 25 30 35 40 50 55 60 65 70 75 80 Mass-to-Charge (m/z) + Scan (34.8392-35.2077 min, 62 scans) 9.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 43.1 0.2 124.0 0.1 29.0 89.1 57.0 -20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.0520 st x10⁵ Counts x10⁵ 43.0 Component 43.0 42.0 2.25 1.4 СНЗ 2 42.0 31.0 1.2





Library Search Results - NonTarget Hits with Details

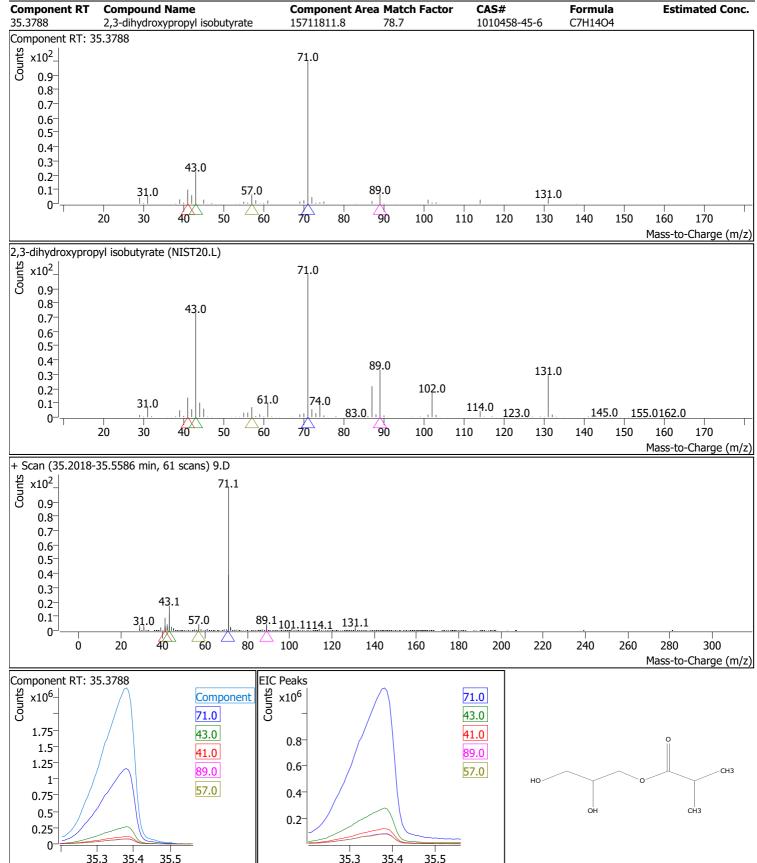




Acquisition Time (min)

Library Search Results - NonTarget Hits with Details

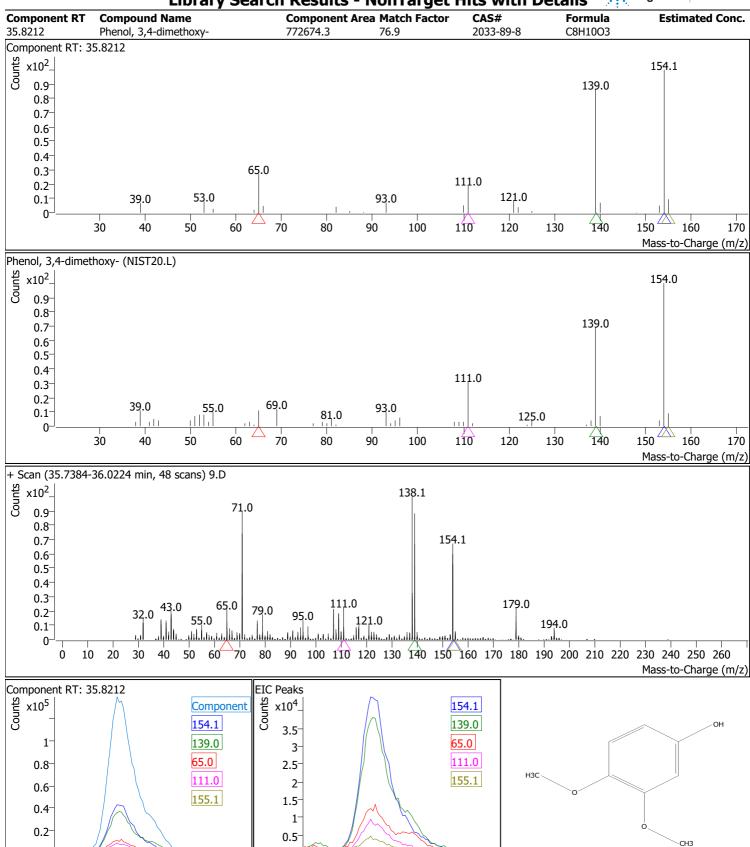




Acquisition Time (min)







35.7

35.8

35.9

Acquisition Time (min)

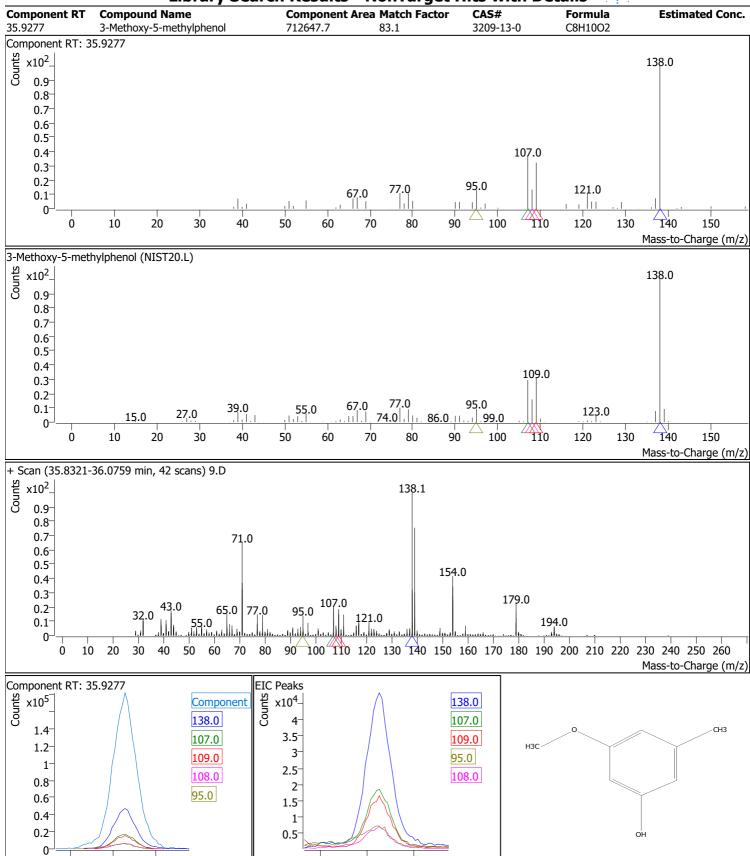
35.8

35.7

35.9







35.9

36

Acquisition Time (min)

35.8

35.8

35.9

36

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.2224 2-Furanmethanol, tetrahydro-3420119.6 C5H10O2 Component RT: 36.2224 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 45.0 31.0 0.1 57.0 10 25 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 (36.0818-36.4029 min, 55 scans) 9.D st x10² 0.9 0.8 0.7 0.6 139.0 154.0 0.5 0.4^{-} 0.3 43.1 0.2 0.1 31.0 111.0 53.0 93.0 131.0 179.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 36.2224 Counts Counts x10⁵ x10⁵ 71.0 Component 71.0 43.0 5 43.0 41.0 2.5 41.0 131.0



36.2

36.3

Acquisition Time (min)

31.0

2-

1-

1.5

0.5

31.0

131.0

3

2

1

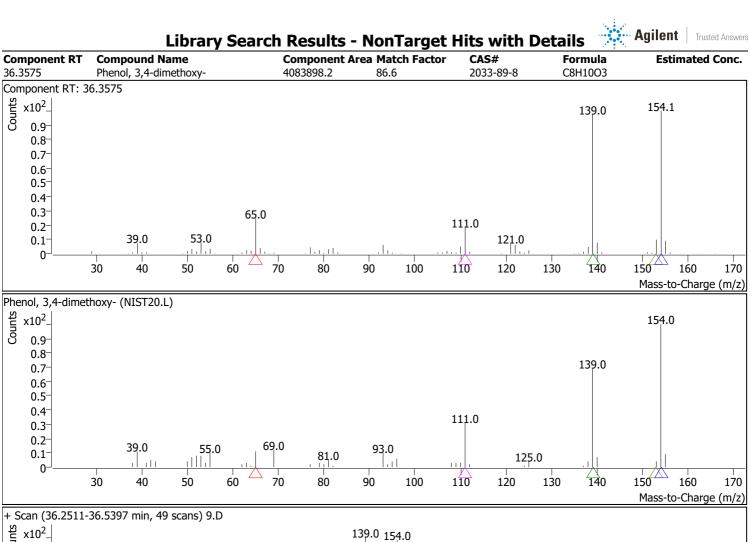
36.1

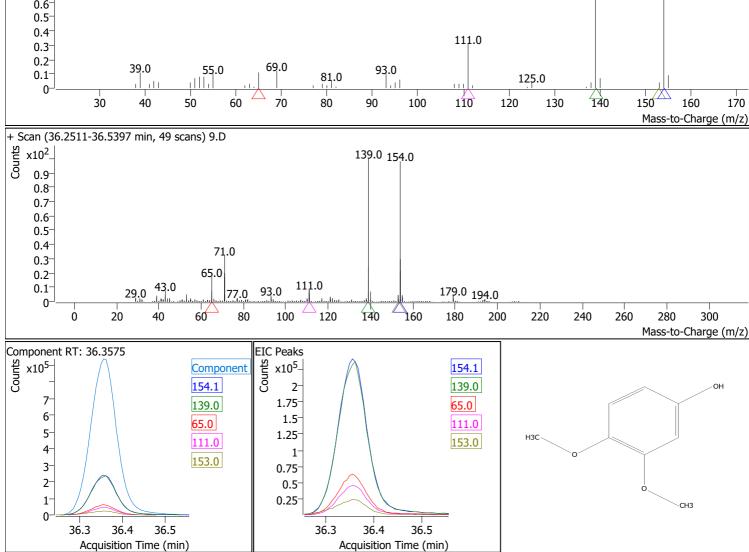
36.2

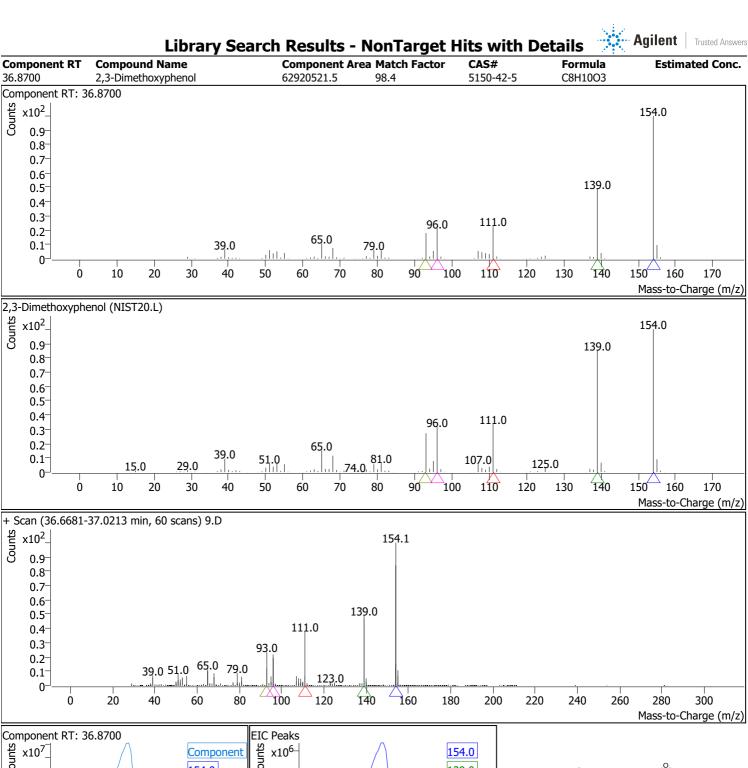
36.3

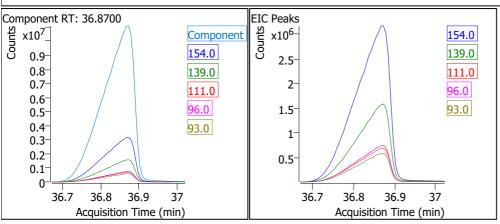
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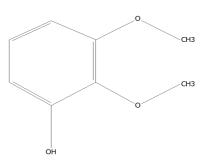
36.4

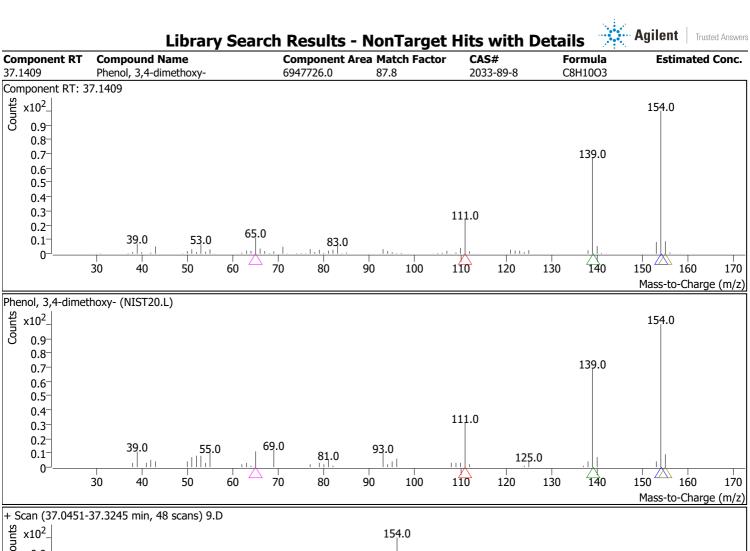


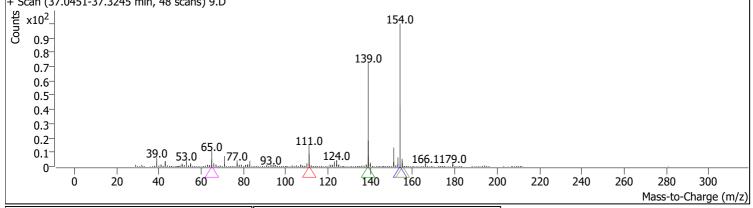


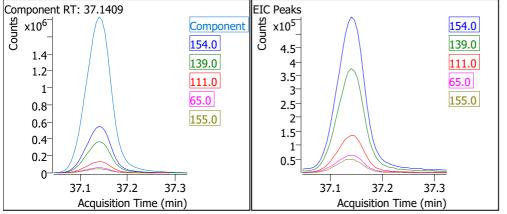


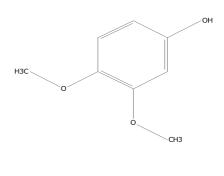




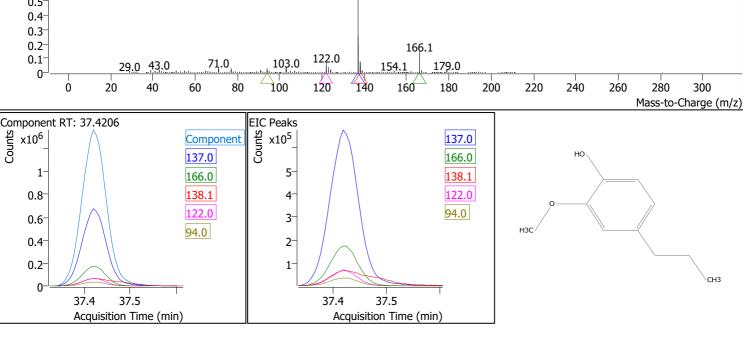






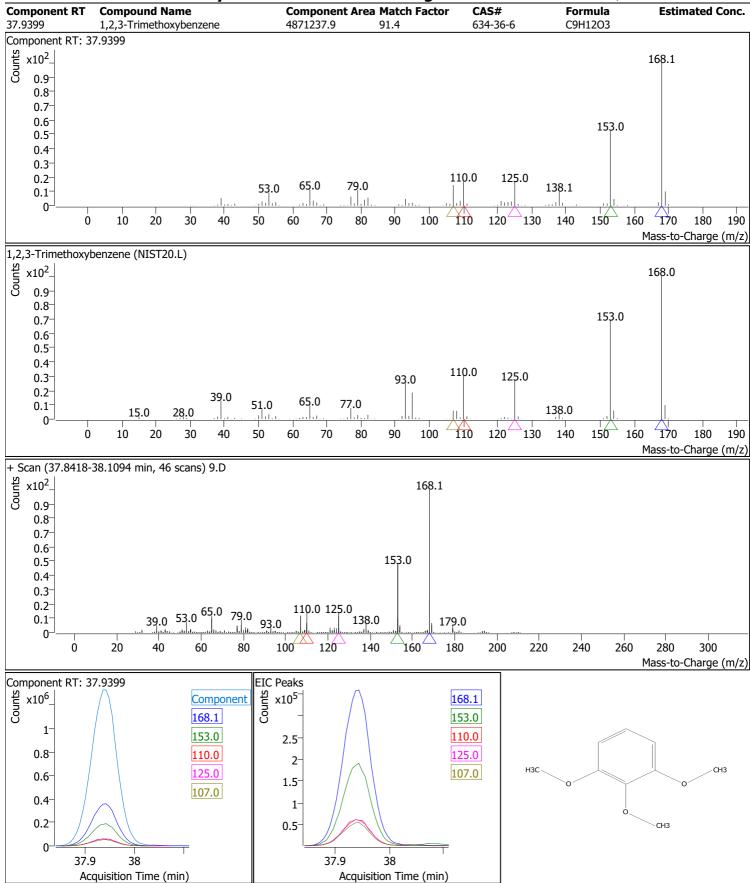


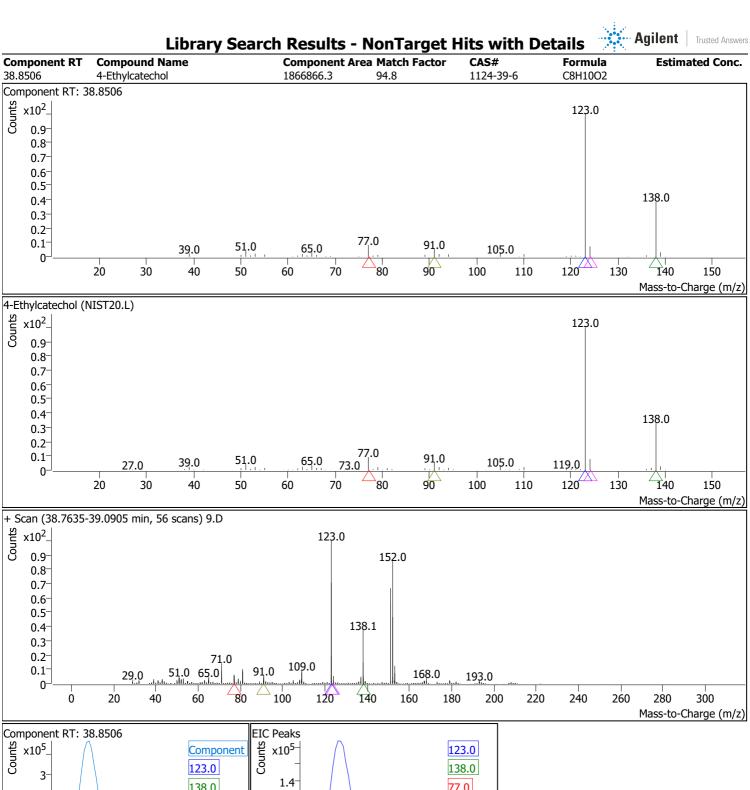
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4206 Phenol, 2-methoxy-4-propyl-5089393.5 92.4 C10H14O2 Component RT: 37.4206 v10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 94.0 77.0 65.0 105.0 160 - 170 10 20 30 40 50 60 70 80 90 100 110 120 130 180 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 **1**40 160 170 150 0 10 20 30 40 50 60 70 80 90 100 110 120 130 180 Mass-to-Charge (m/z) + Scan (37.3312-37.6089 min, 46 scans) 9.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4

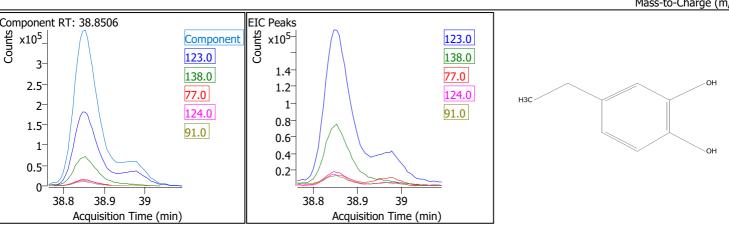


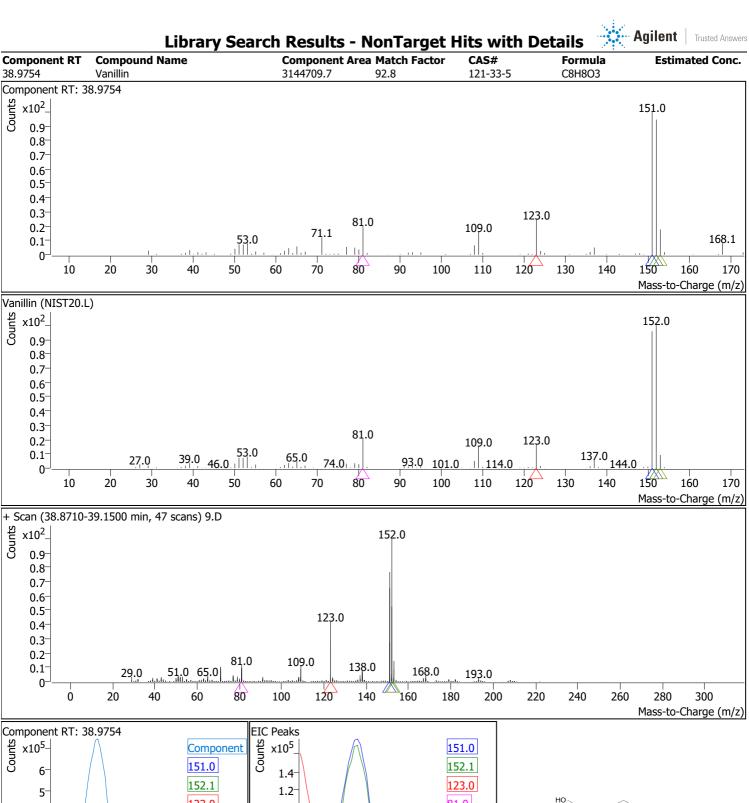


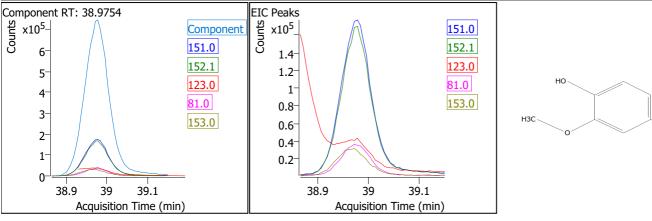


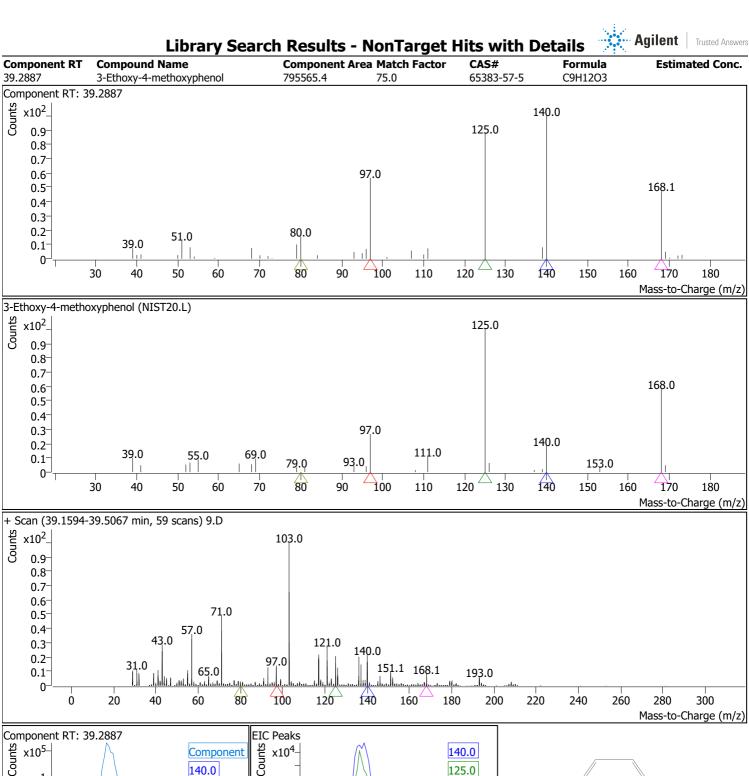


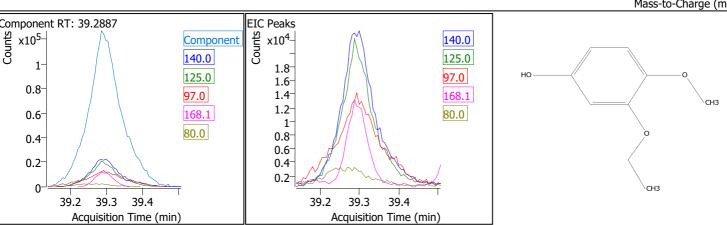






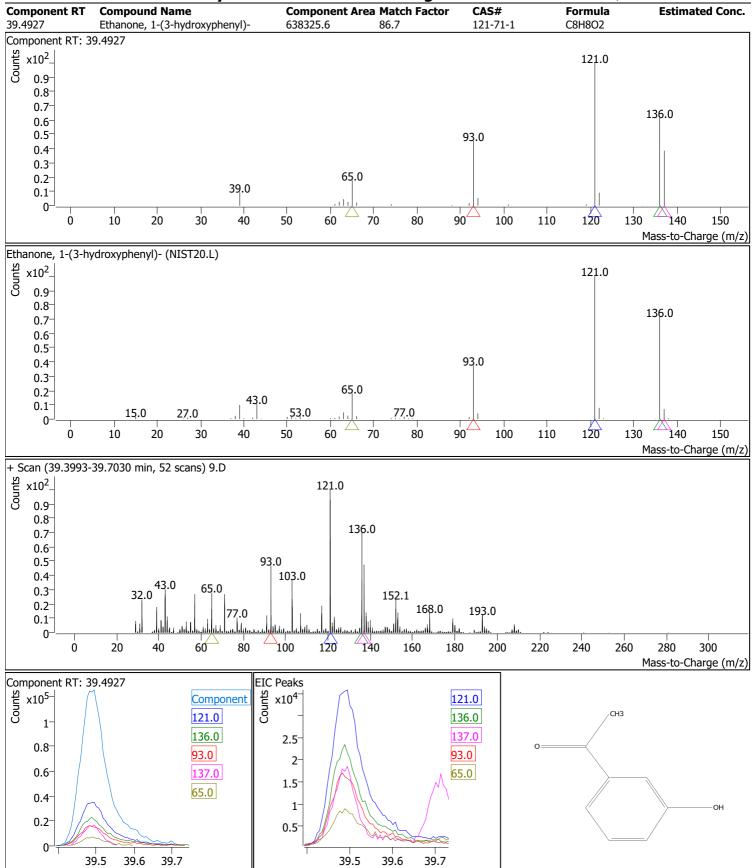






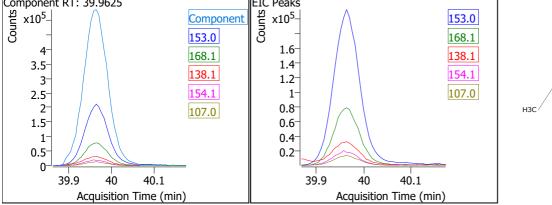






Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 39.9625 4-Methoxy-2-methyl-1-2140776.4 84.4 22583-04-6 C9H12OS (methylthio)benzene Component RT: 39.9625 x10². 153.0 0.9 8.0 0.7 0.6 0.5 168.1 0.4 0.3 0.2^{-} 138.1 0.1 107.0 77.0 0-110 140 150 0 10 20 30 40 50 60 70 80 90 100 120 130 160 180 190 Mass-to-Charge (m/z) 4-Methoxy-2-methyl-1-(methylthio)benzene (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 153.0 0.6 0.5 0.4 0.3 138.0 0.2 109.0 45.0 0.1 77.0 84.0 91.0 65.0 125.0 28.0 0 110 0 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 180 190 Mass-to-Charge (m/z) + Scan (39.8813-40.1727 min, 50 scans) 9.D st x10² 0.9 153.0 0.8 0.7 0.6 0.5 0.4 168.1 0.3 0.2 138.0 0.1 53.0 65.0 77.0 91.0 107.0 180.1 0 Ó 40 80 100 120 140 20 60 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 39.9625 **EIC Peaks** Counts Counts x10⁵x10⁵-153.0 Component 153.0 168.1 1.6 4 168.1 138.1 1.4 3.5 138.1 154.1 1.2 3



--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1000131-52-4 40.9107 2-Cyclohexen-3-ol-1-one, 2-[1-8157951.5 77.5 C8H11NO2 iminoethyl]-Component RT: 40.9107 x10²_ 153.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 0.1 0-70 30 80 90 100 120 130 140 150 160 170 Mass-to-Charge (m/z) 2-Cyclohexen-3-ol-1-one, 2-[1-iminoethyl]- (NIST20.L) $x10^{2}$ 153.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 69.0 83.0 97.0 125.0 112.0 138.0 0 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (40.7970-41.0051 min, 36 scans) 9.D st x10² 0.9 168.1 0.8 0.7 0.6 0.5 153.0 0.4 0.3 125.0 0.2 107.0 39.0 53.0 65.0 77.0 0.1 97.0 138.0 0 Ó 20 40 60 80 100 160 200 220 260 120 140 180 240 280 300 Mass-to-Charge (m/z) Component RT: 40.9107 EIC Peaks Counts Counts x10⁶ x10⁵ 153.0 Component 153.0 107.0 1.4 6 154.1 53.0 1.2 5 107.0 110.0 1 4 110.0 154.1

40.9

41

Acquisition Time (min)

3-

2

53.0

0.8

0.6

0.4 0.2

40.8

40.9

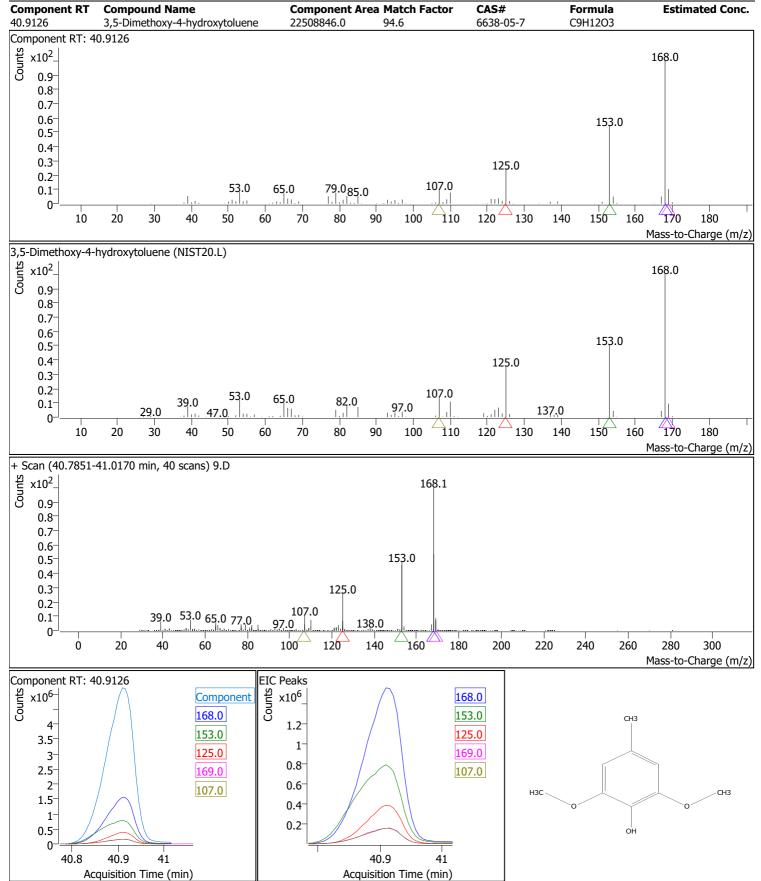
41

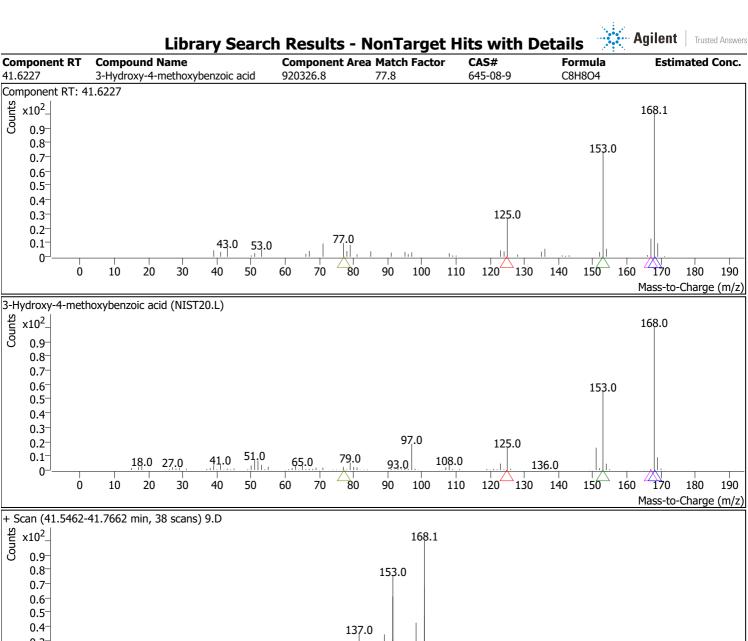
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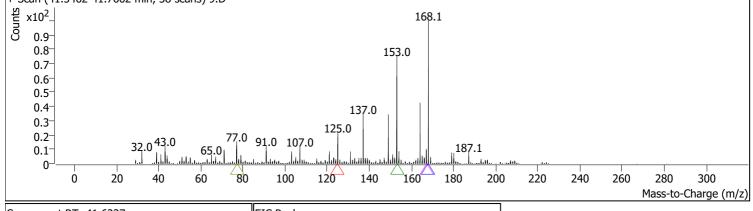
CH3

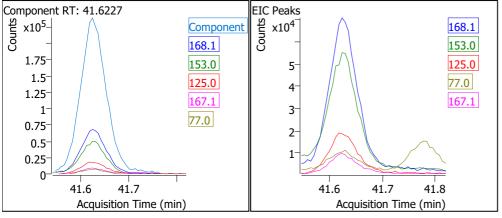


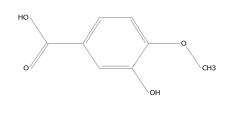


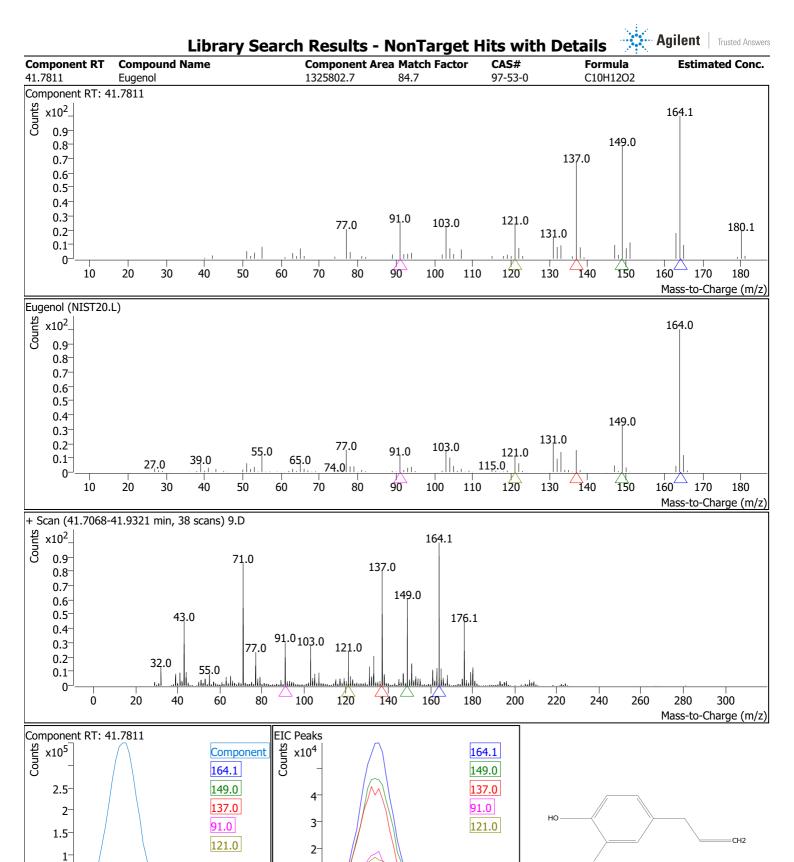














41.8

Acquisition Time (min)

41.9

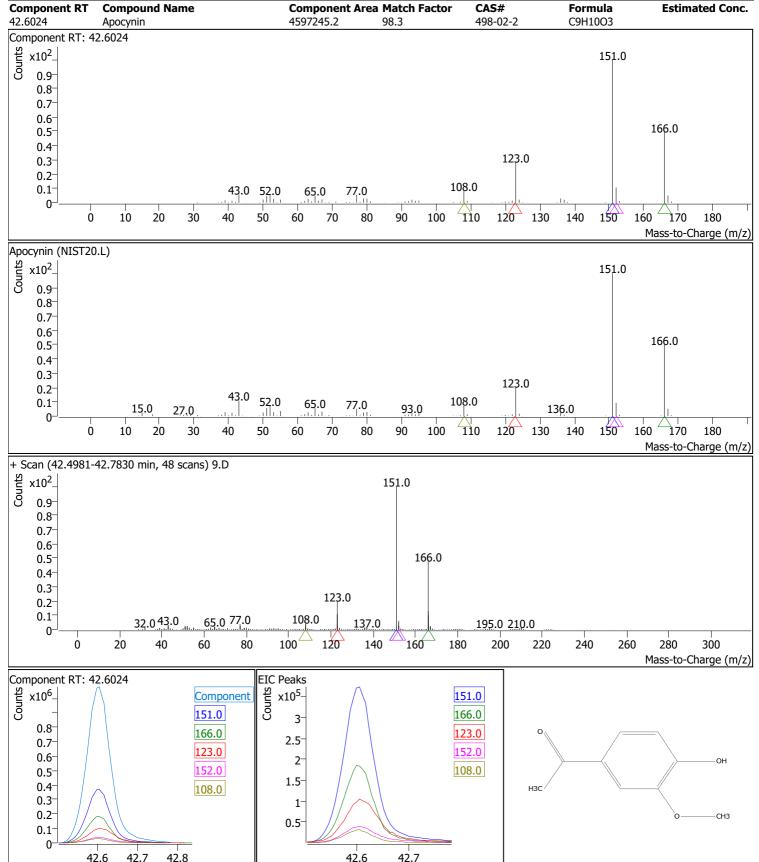
0.5

41.8

Acquisition Time (min)

41.9

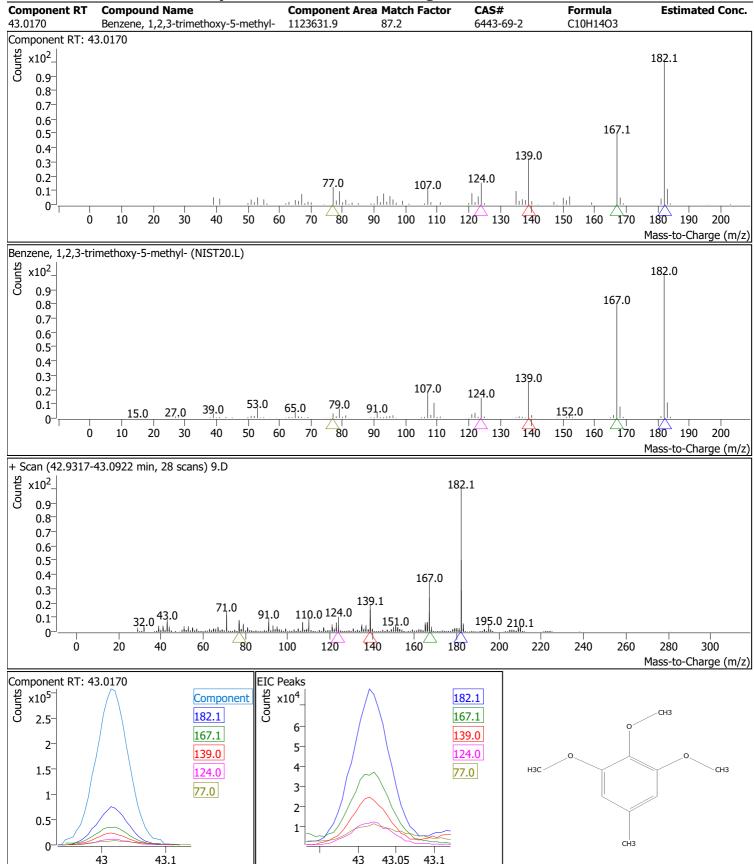




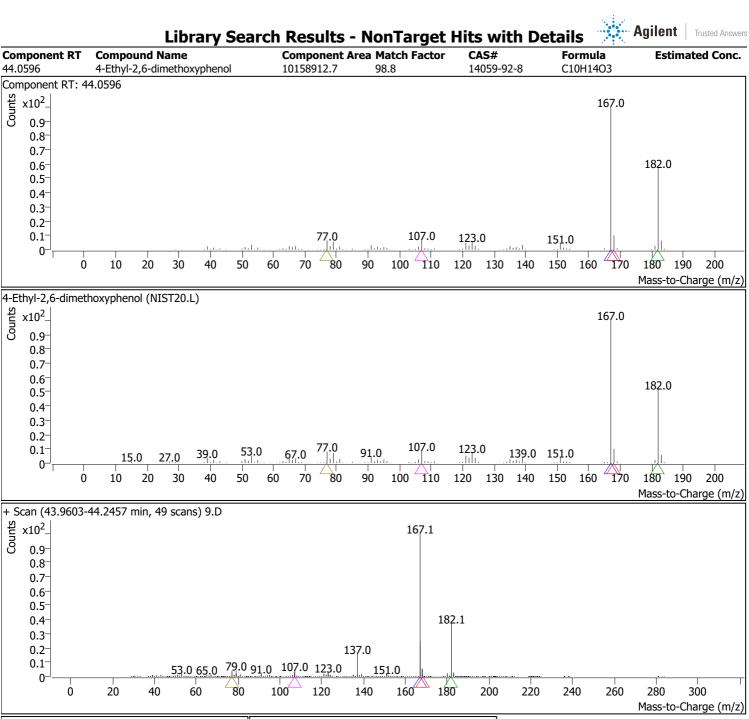
Acquisition Time (min)

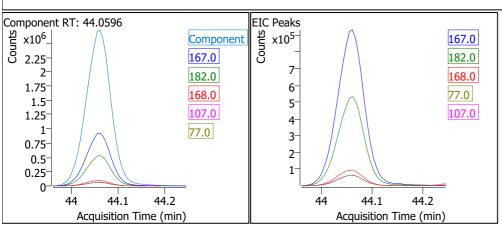


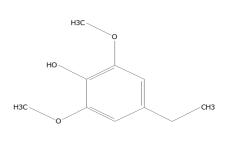




Acquisition Time (min)







··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 44.3023 2-Propanone, 1-(4-hydroxy-3-13134927.4 95.7 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3023 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.1 0.2 122.0 94.0 0.1 51.0 66.0 77.0 0-120 180 20 30 50 60 70 80 90 100 110 130 140 150 160 170 190 200 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 (44.1835-44.3765 min, 33 scans) 9.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 74.0 0.3 180.1 87.0 0.2 43.0 55.0 66.0 122.0 0.1 94.0 115.1 129.1 171.1 0 140 180 Ó 20 40 60 80 100 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3023 **EIC Peaks** Counts Counts x10⁶ x10⁶ 137.0 Component 180.1 137.0 1.2 2.5 180.1 122.0 1 2-122.0 138.1 0.8

44.25

44.3

Acquisition Time (min)

94.0

1.5

1

0.5

44.3

44.4

Acquisition Time (min)

138.1

94.0

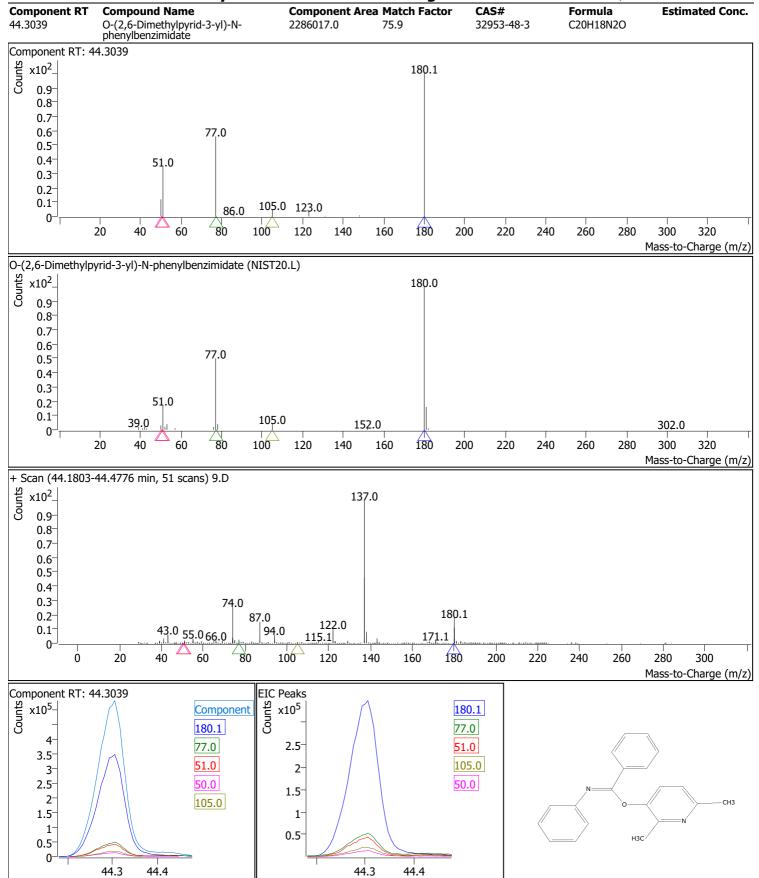
0.6

0.4

 0.2^{-1}

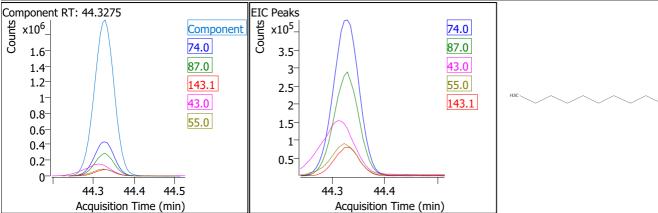
Library Search Results - NonTarget Hits with Details





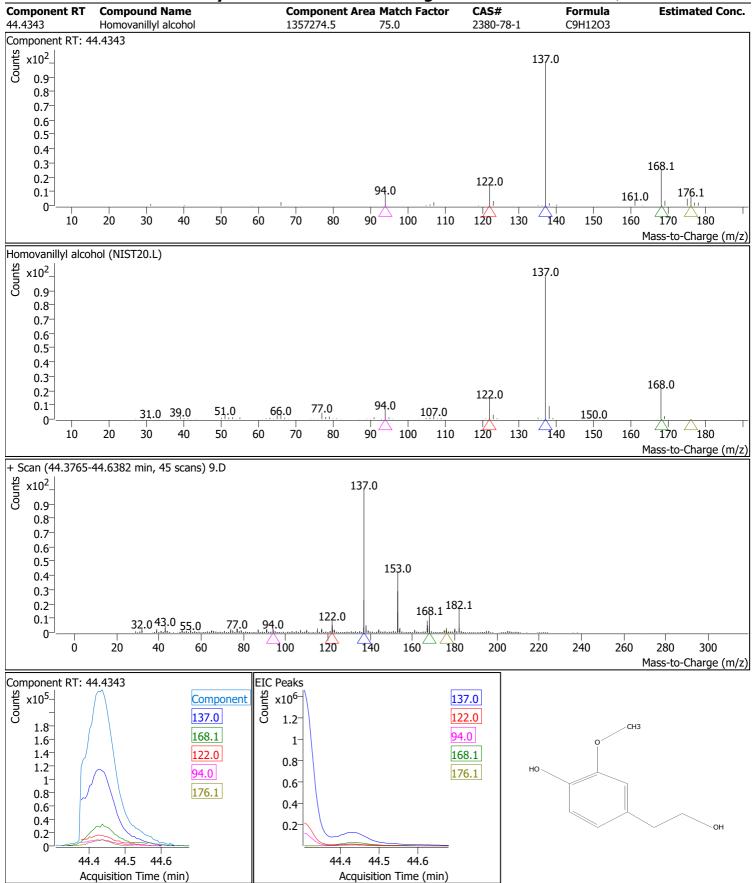
Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3275 Dodecanoic acid, methyl ester 6793335.9 93.8 111-82-0 C13H26O2 Component RT: 44.3275 v10² 0.9 74.0 0.8 0.7^{-} 87.0 0.6 0.5 0.4 0.3 143.1 43.0 55.0 171.1 183.1 0.2 69.1 0.1 20 50 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 10 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10²_ 0.9 74.0 0.8 0.7 87.0 0.6 0.5 0.4 0.3 0.2 55.0 29.0 69.0 214.0 0.1 101.0 115.0 129.0 83.0 10 20 30 50 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) + Scan (44.2398-44.5133 min, 47 scans) 9.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 74.0 180.1 0.2 87.0 122.0 43.0 55.0 66.0 0.1 153.0 171.1 115.1 129.1 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3275 **EIC Peaks** x10⁵-74.0 Component



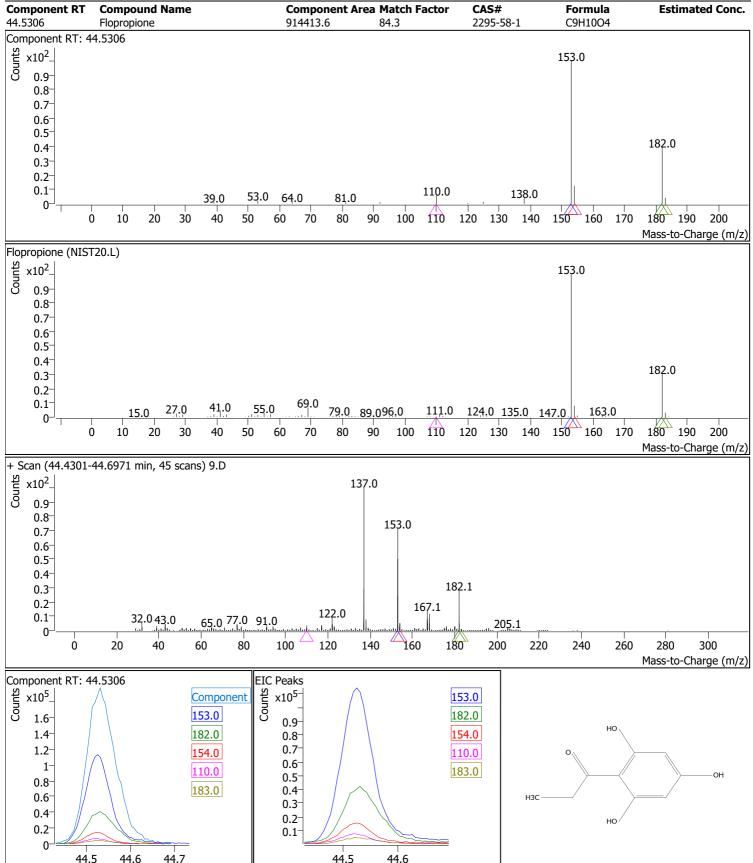








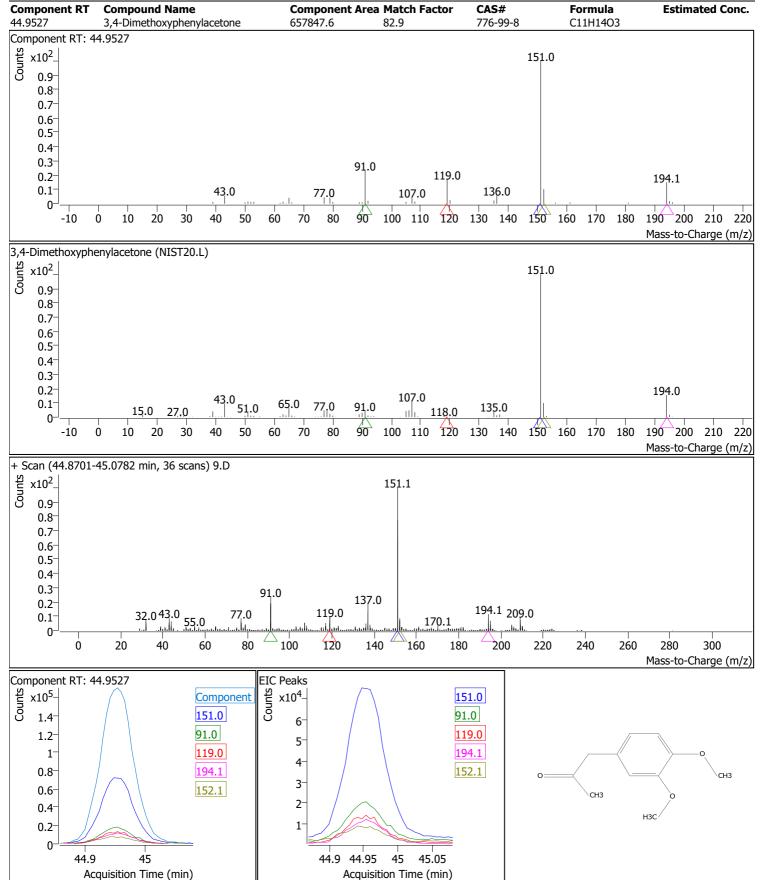


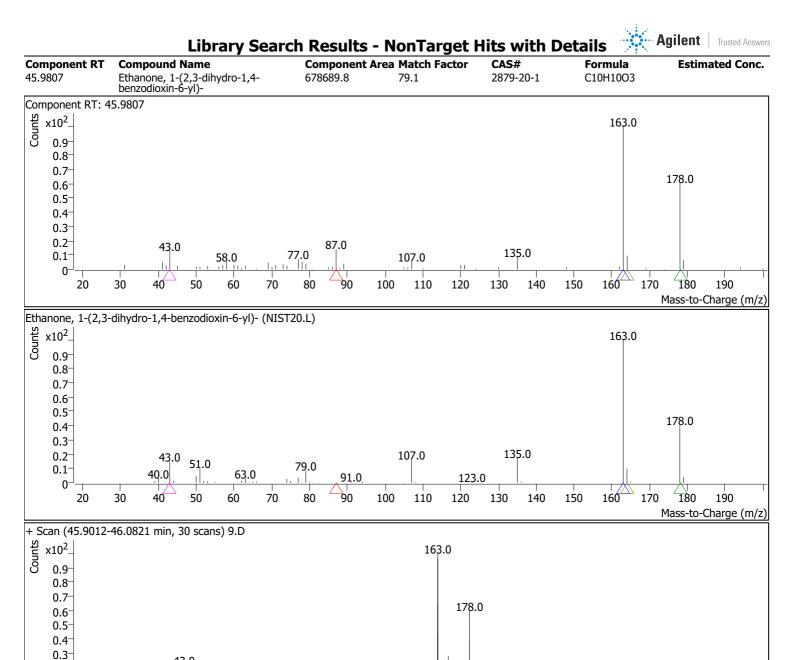


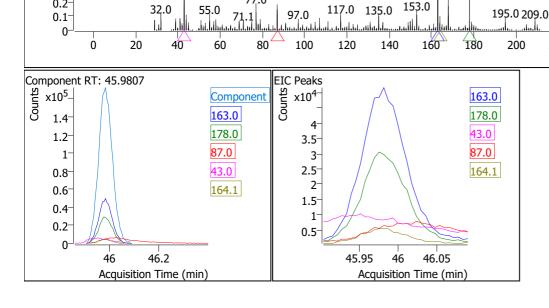
Acquisition Time (min)





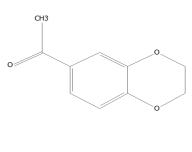






77.0

0.2



260

280

300 Mass-to-Charge (m/z)

220

240

--- 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 46.4694 633294.3 78.2 C10H12O3 methoxyphenyl)-Component RT: 46.4694 x10² 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 123.0 108.0 170.0 0.1 52.0 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 (46.3826-46.5409 min, 27 scans) 9.D x10². 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 123.0 180.1 165.0 0.1 65.0 77.0 91.0 107.0 32.0 44.0 137.0 209.1 0 Ó 40 180 260 300 20 60 80 100 120 140 160 200 220 240 280 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 46.4694 Counts Counts x10⁴. x10⁵ 151.0 Component СНЗ 180.0 151.0 6 1.2 180.0 123.0 5 1 152.0 123.0

46.45

46.5

Acquisition Time (min)

108.0

4

3

2-

46.4

152.0

108.0

46.5

Acquisition Time (min)

8.0

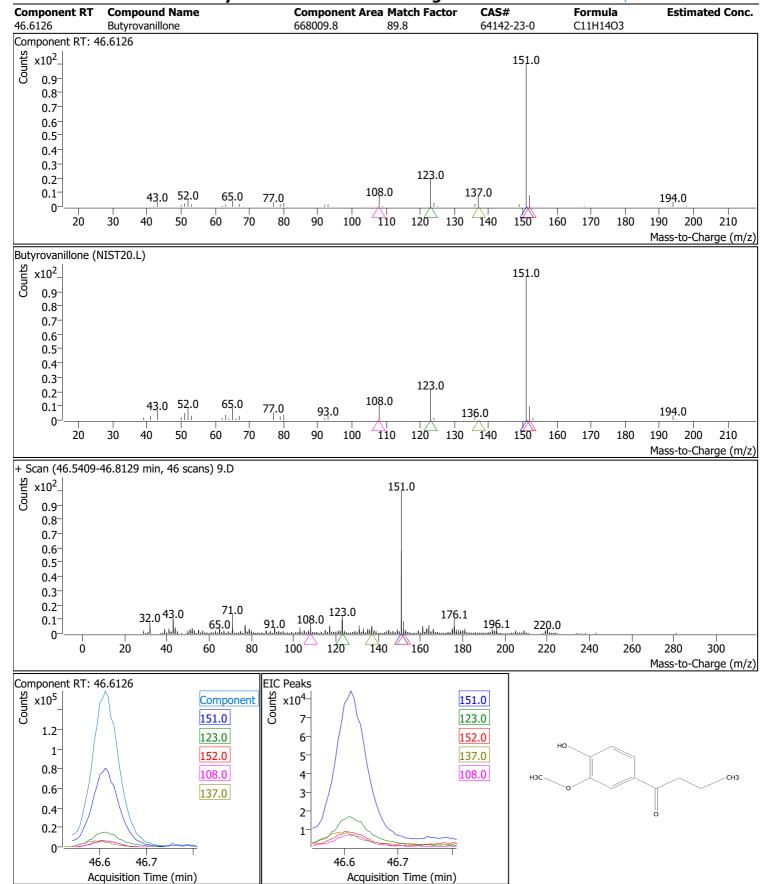
0.6

0.4⁻ 0.2⁻ 0⁻

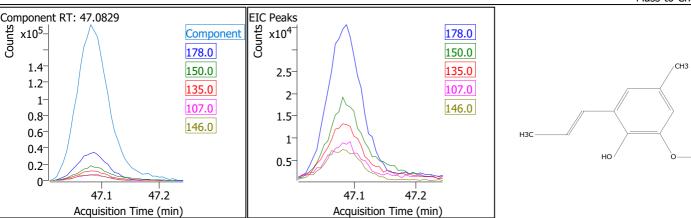
нзс







··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 750062.3 201359-63-9 47.0829 Phenol, 2-methoxy-4-methyl-6-76.5 C11H14O2 [propenyl]-Component RT: 47.0829 x10²_ 178.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 135.0 0.3 107.0 146.0 163.0 194.1 91.0 0.2 117.0 0.1 0-180 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 190 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-methyl-6-[propenyl]- (NIST20.L) $x10^{2}$ 178.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 91.0 135.0 163.0 0.2 117.0 145.0 131.0 77.0 65.0 107.0 0.1 43.0 51.0 84.0 |151.0 0 180 150 30 50 60 70 80 90 100 110 120 130 140 160 170 190 Mass-to-Charge (m/z) + Scan (47.0111-47.2483 min, 39 scans) 9.D st x10² 178.1 0.8 0.7 0.6 0.5 150.0 0.4 0.3 77.0 91.0 117.1 135.0 32.0 0.2 163.1 194.1 0.1 0 140 180 300 20 40 60 80 100 120 160 200 220 240 260 280 320 340 Mass-to-Charge (m/z) Component RT: 47.0829 **EIC Peaks** Counts Counts x10⁵x10⁴ 178.0 Component 150.0 178.0 CH3 1.4 150.0 135.0 2.5 1.2 107.0 135.0



-CH3

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 6766-82-1 47.3469 2,6-Dimethoxy-4-propylphenol 4507386.4 92.4 C11H16O3 Component RT: 47.3469 v10² 0.9 167.0 0.8 0.7 0.6 0.5 0.4 196.0 0.3 151.0 0.2 0.1 123.0 136.0 77.0 190 200 120 130 140 150 160 170 10 20 50 60 70 100 110 Mass-to-Charge (m/z) 2,6-Dimethoxy-4-propylphenol (NIST20.L) Counts x10²_ 0.9 167.0 0.8 0.7 0.6 0.5 0.4 0.3 196.0 0.2 0.1 77.0 53.0 29.0 39.0 106.0 151.0 181.0 120 130 140 150 160 170 180 190 200 10 20 50 60 70 80 100 110 Mass-to-Charge (m/z) + Scan (47.2500-47.5339 min, 48 scans) 9.D st x10² 0.9 167.1 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 196.1 0.2 151.0 0.1 123.0 137.0 32.043.0 65.0 77.0 91.0 179.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 47.3469 EIC Peaks Counts x10⁶ Counts 167.0 Component 167.0 196.0 1 3.5 **H3C** 196.0 151.0 0.8 3 151.0 168.0 2.5



47.4

Acquisition Time (min)

47.5

123.0

HO

нзс

0.6

0.4

0.2

47.3

47.4

Acquisition Time (min)

47.5

168.0

123.0

2-

1.5

0.5

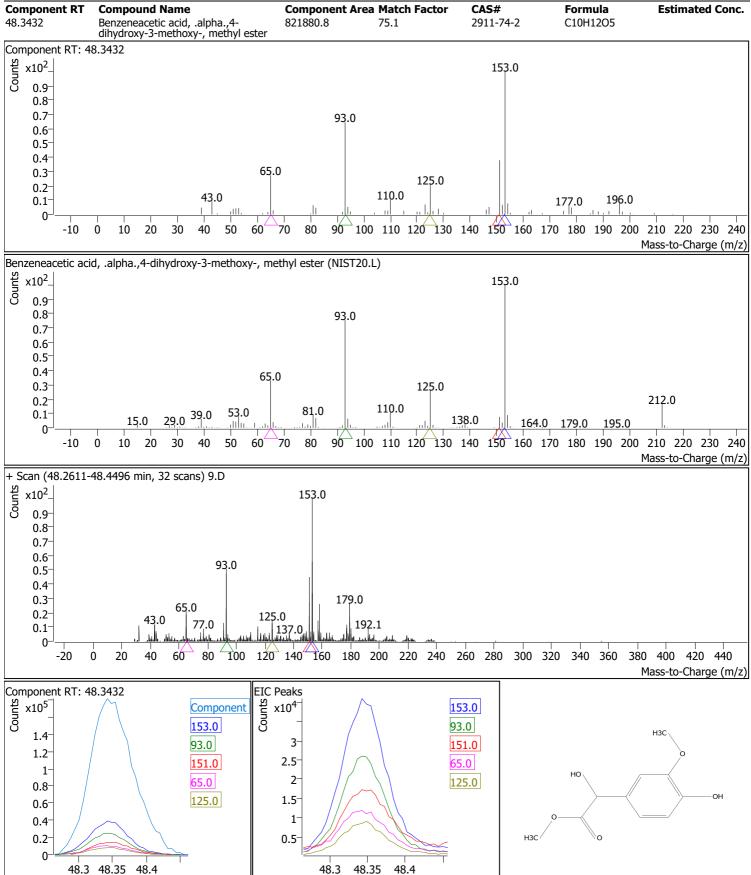
1

47.3

-CH3

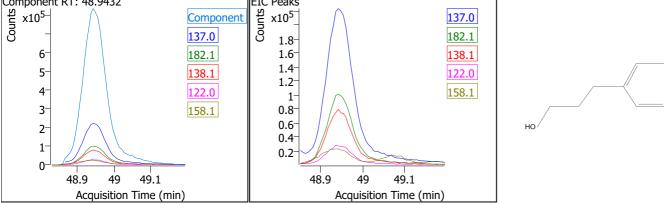
Library Search Results - NonTarget Hits with Details

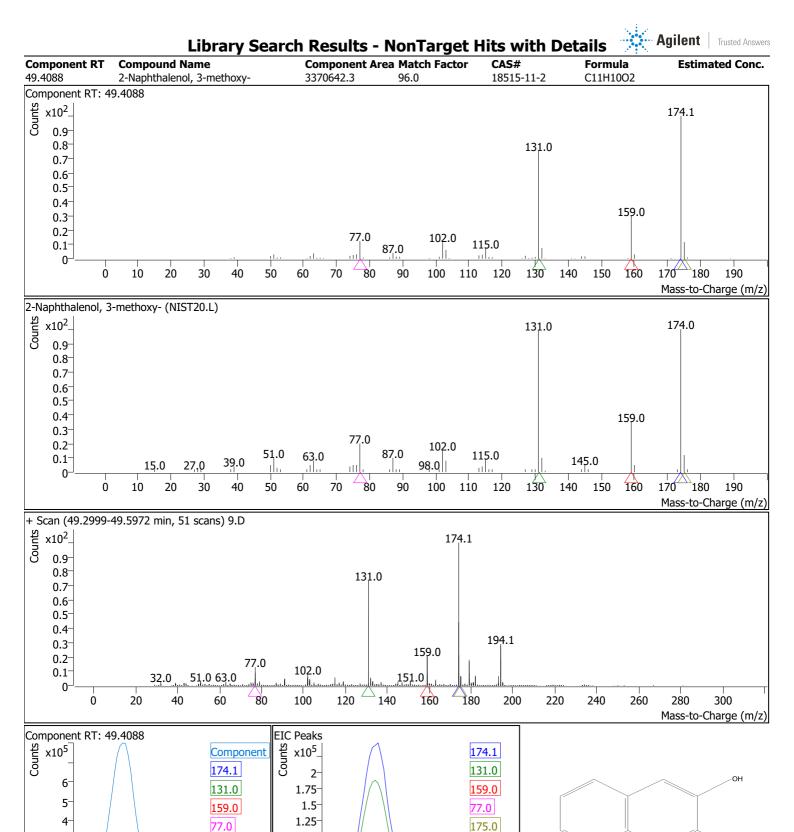




Acquisition Time (min)

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 48.9432 Benzenepropanol, 4-hydroxy-3-3855643.1 89.1 C10H14O3 methoxy-Component RT: 48.9432 x10² 137.0 0.9 8.0 0.7 0.6 0.5 182.1 0.4 0.3 0.2^{-} 122.0 158.1 77.0 91.0 107.0 0.1 0-140 160 10 20 30 40 50 60 70 80 90 100 110 120 130 150 170 180 190 200 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 0 160 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 190 200 Mass-to-Charge (m/z) + Scan (48.8658-49.1928 min, 56 scans) 9.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 182.1 0.4 0.3 0.2 158.1 77.0 91.0 0.1 122.0 32.0 51.0 0 140 160 180 300 20 40 60 80 100 120 200 220 240 260 280 320 340 360 380 Mass-to-Charge (m/z) Component RT: 48.9432 **EIC Peaks** Counts Counts x10⁵ 137.0 x10⁵ Component 137.0 182.1 1.8 6 182.1 1.6 138.1 1.4 5 138.1 122.0





49.5

Acquisition Time (min)

1

0.75

0.5

0.25

175.0

3

2

1

49.4

49.5

Acquisition Time (min)

CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 49.5436 (E)-2,6-Dimethoxy-4-(prop-1-en-1-1940729.7 88.2 20675-95-0 C11H14O3 yl)phenol Component RT: 49.5436 x10²_ 194.0 0.9 8.0 0.7 0.6 0.5 179.0 0.4 0.3 91.0 0.2^{-} 77.0 119.0 133.0 151.0 163.0 0.1 0-0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 200 210 220 Mass-to-Charge (m/z) (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol (NIST20.L) $x10^{2}$ 194.0 0.9 0.8 0.7 0.6 0.5 0.4 91.0 0.3 119.0 77.0 131.0 179.0 0.2 65.0 151.0 105.0 53.0 39.0 0.1 163.0 ا 97.0 27.0 85.0 0 90 180 10 20 40 50 60 70 80 100 110 120 130 140 150 160 170 190 200 210 220 Mass-to-Charge (m/z) + Scan (49.4426-49.6209 min, 31 scans) 9.D x10²_ 194.1 0.9 0.8 0.7 0.6 179.1 0.5 0.4 0.3 131.0 77.0 91.0 0.2 163.1 105.0 119.0 0.1 32.043.0 65.0 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 49.5436 **EIC Peaks** Counts Counts x10⁵x10⁵-194.0 Component 179.0 194.0 0.9 3.5 **Н3С** 179.0 91.0 0.8 3 193.0 91.0 0.7^{-} 2.5 0.6^{-} 193.0 119.0 НО 2 0.5^{-} 119.0 0.4^{-} 1.5

49.6

Acquisition Time (min)

0.3

0.2

0.1

49.5

1

49.5

49.6

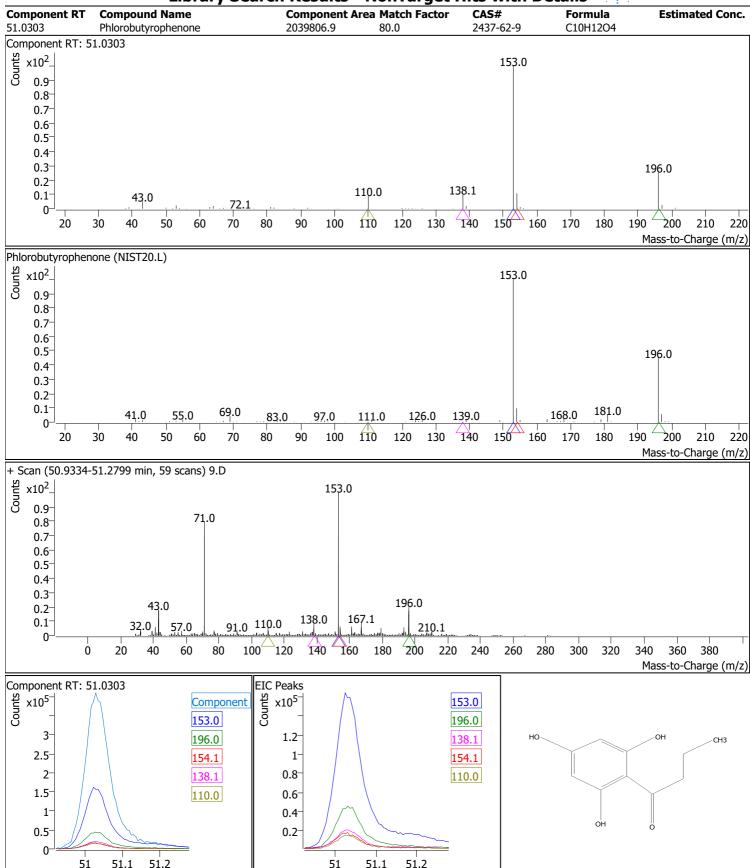
Acquisition Time (min)

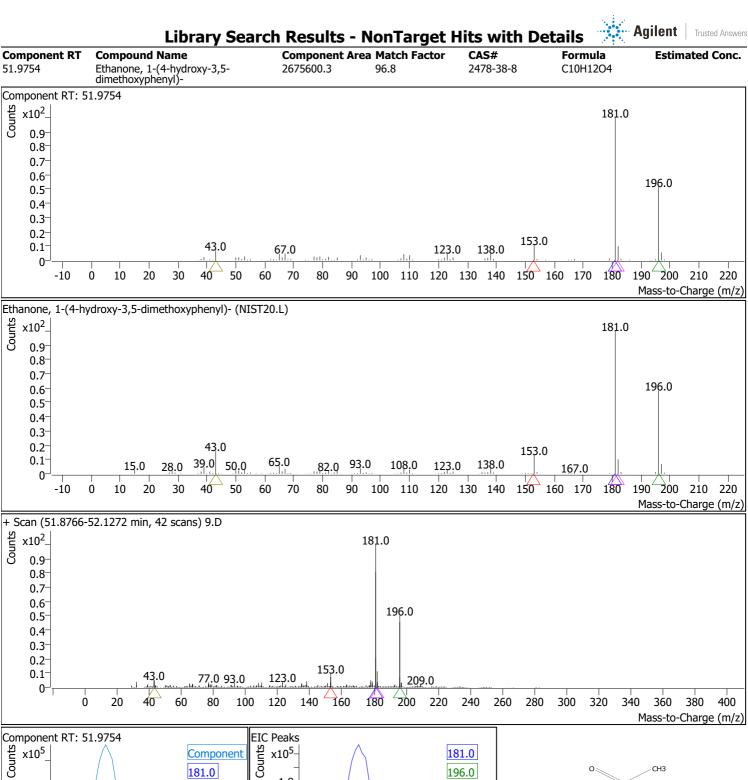
0.5

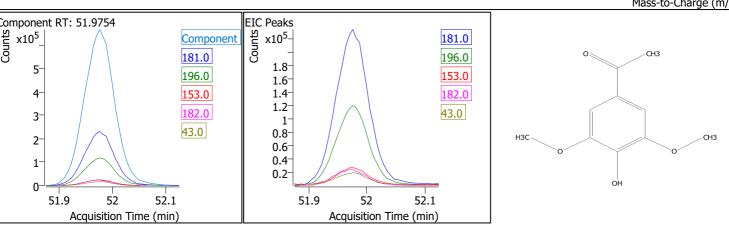
НЗС





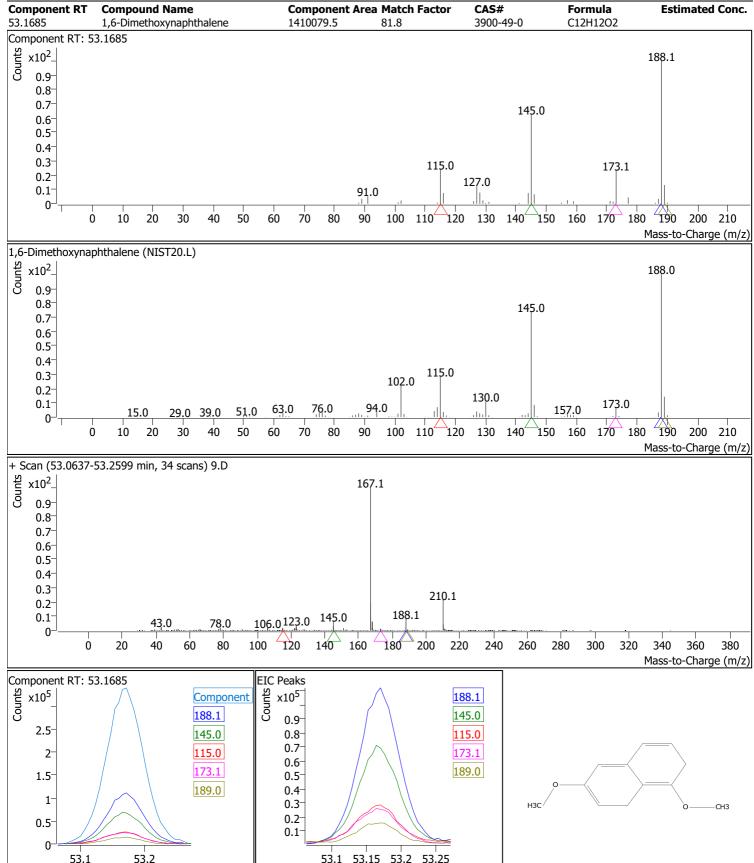






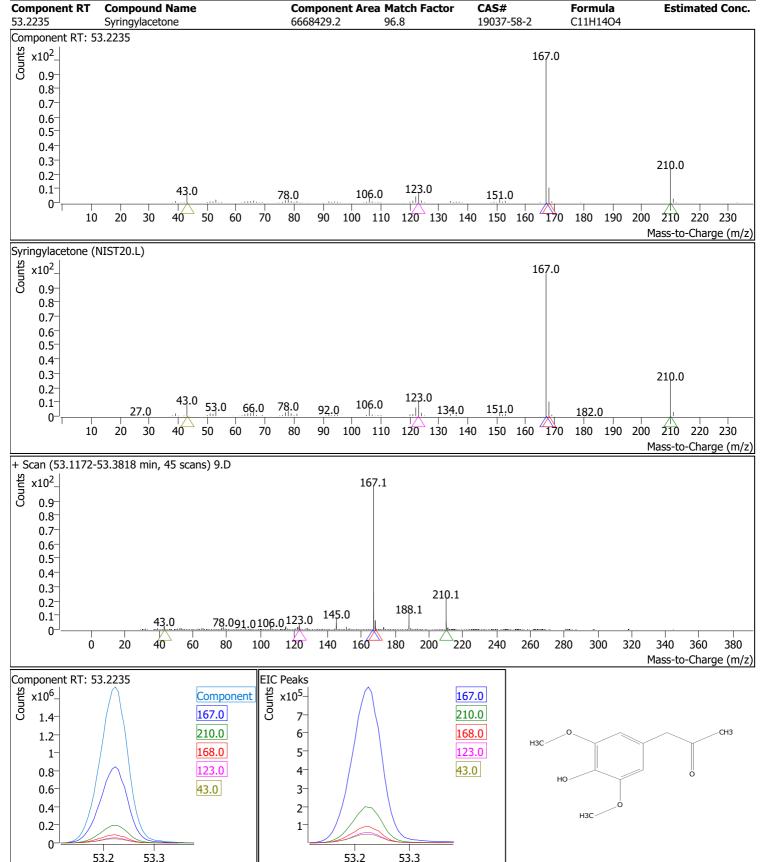


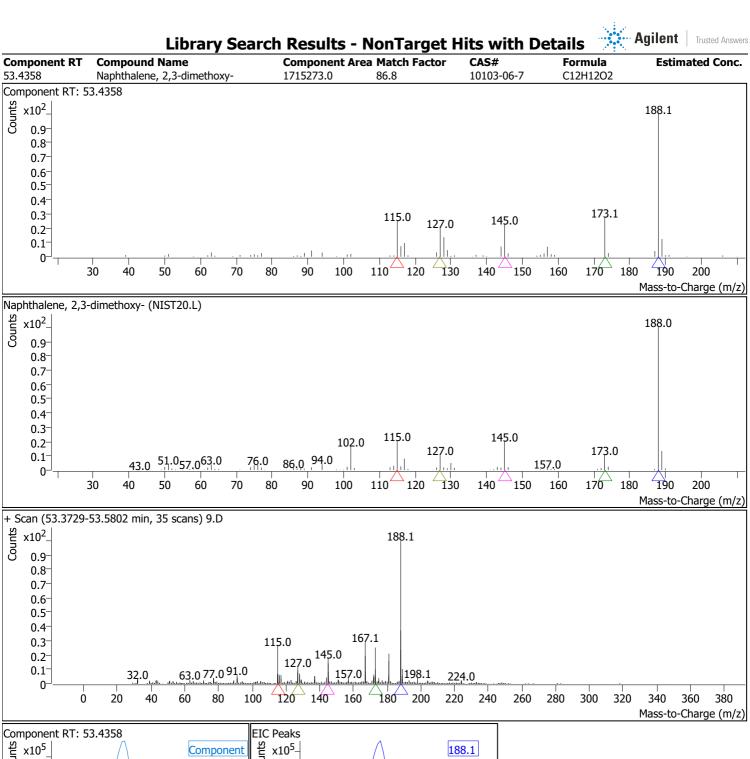


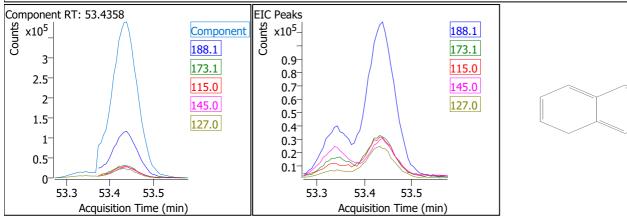








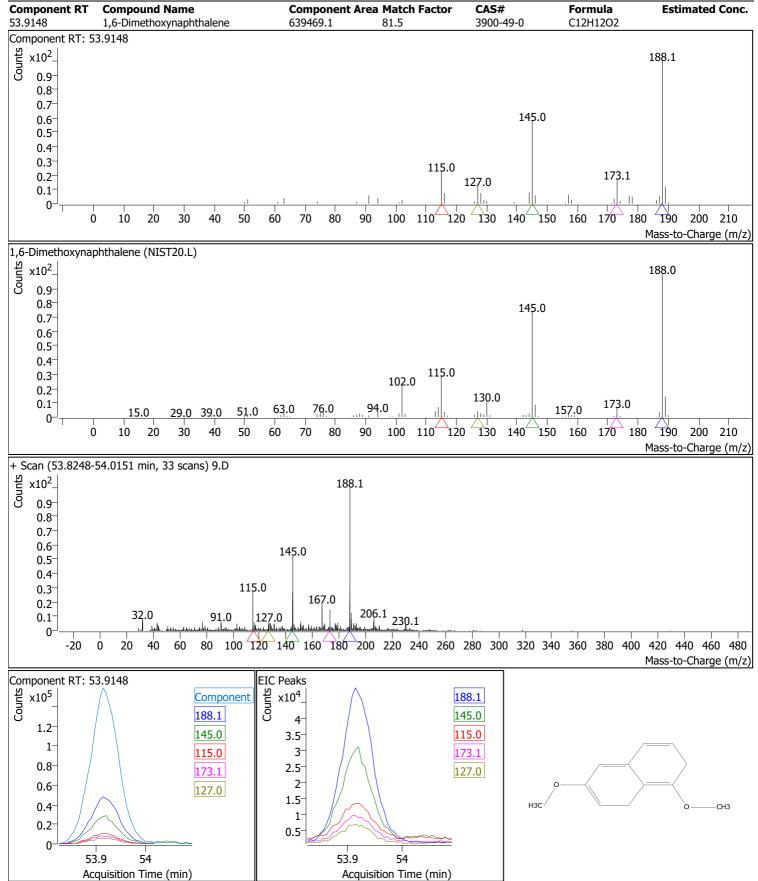


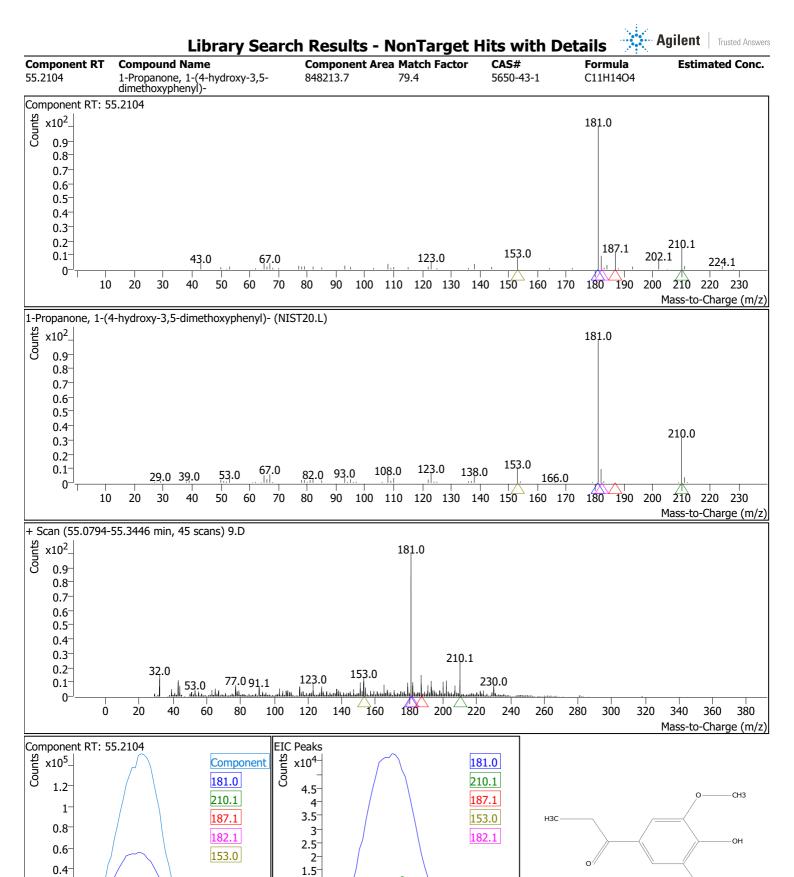


CH3











Acquisition Time (min)

1

55.1

0.5

0.2

0¹ 55.1

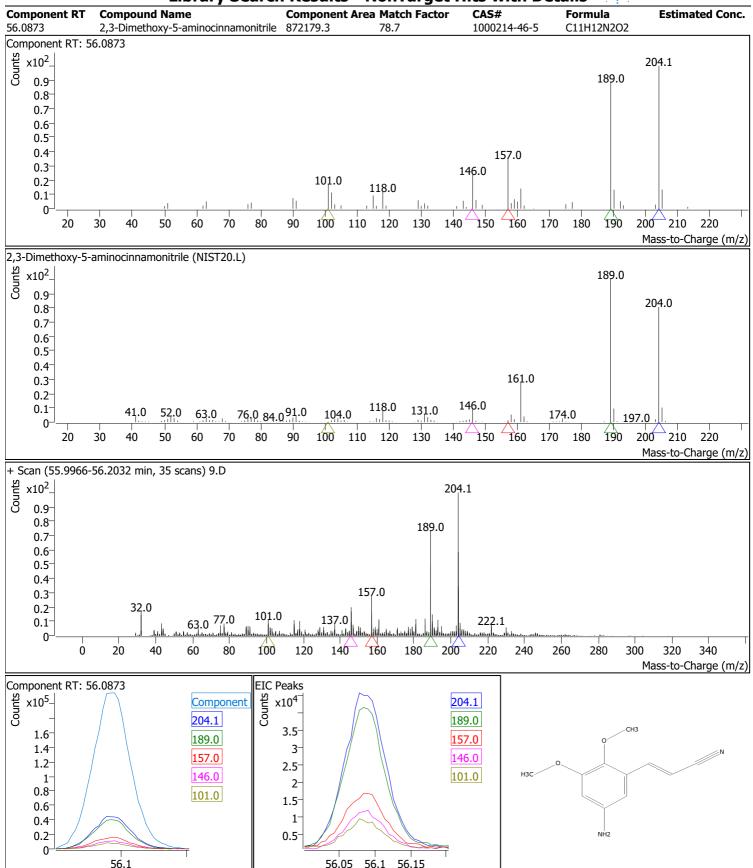
55.2

Acquisition Time (min)

-CH3

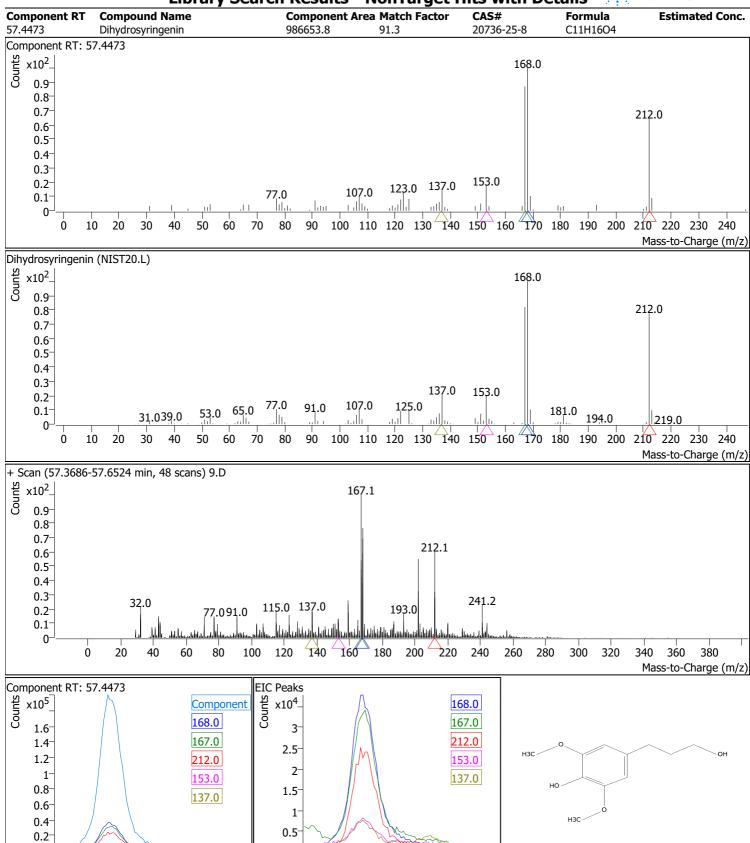












57.5

Acquisition Time (min)

57.6

57.4

57.5

Acquisition Time (min)

57.6

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62.2

62.3

Acquisition Time (min)

2

1

1.5

0.5

183.1

8.0

0.6

0.4

0.2

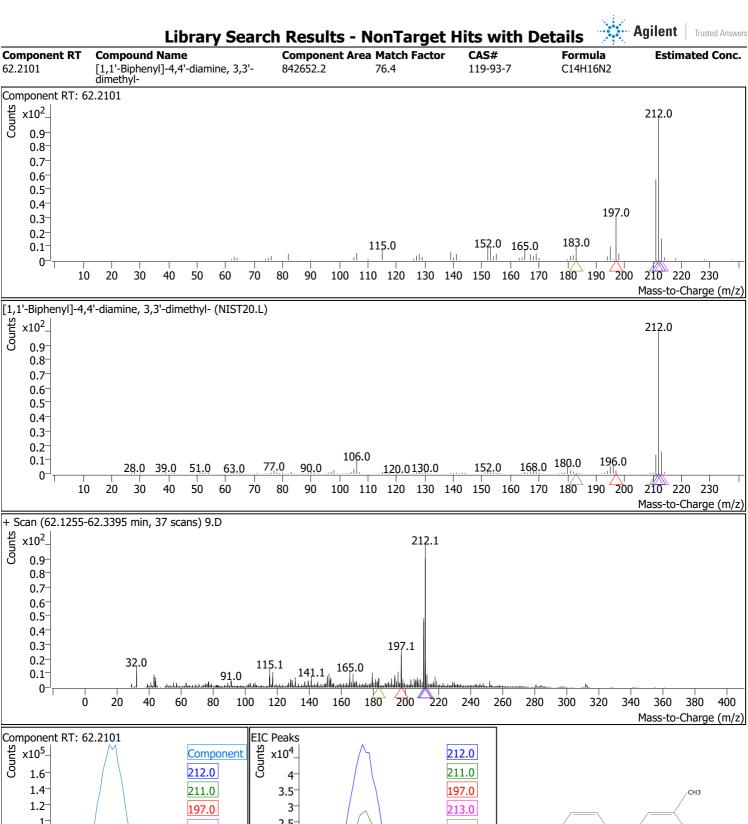
62.2

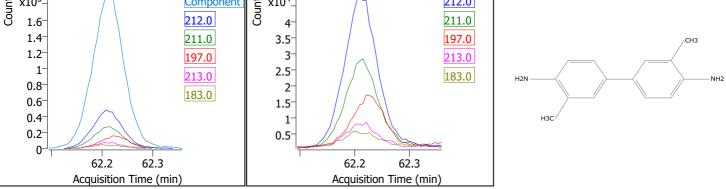
62.3

Acquisition Time (min)

нзс

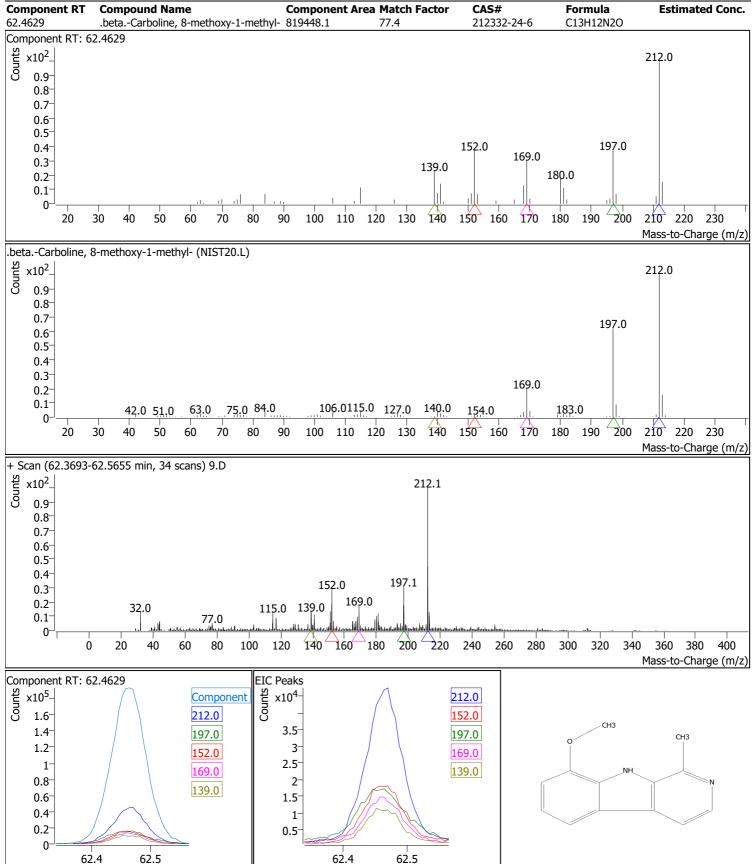
H2N





Library Search Results - NonTarget Hits with Details

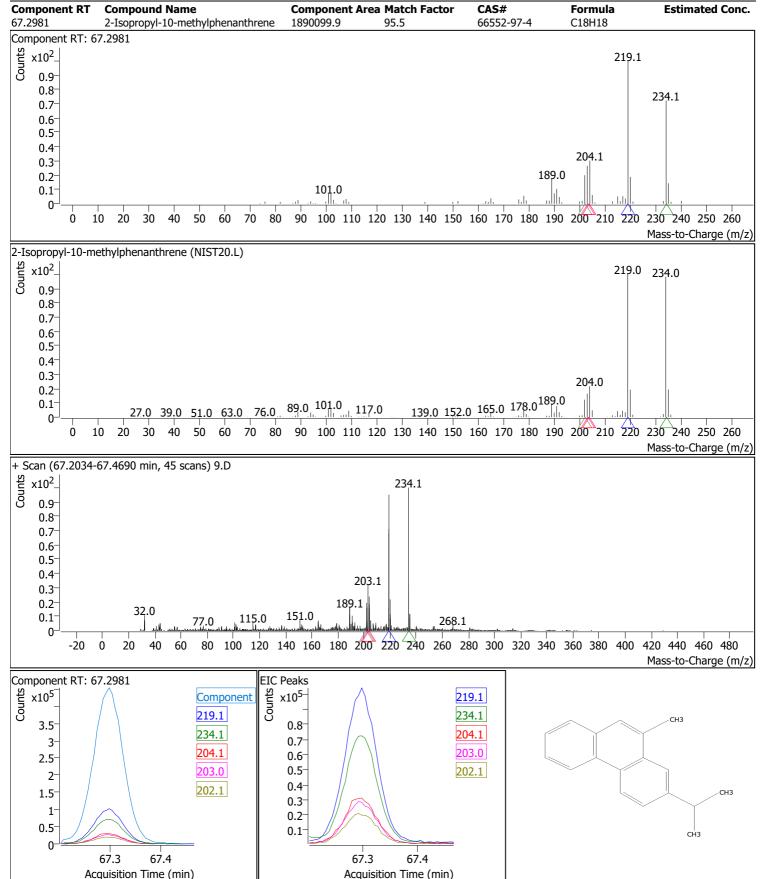




Acquisition Time (min)

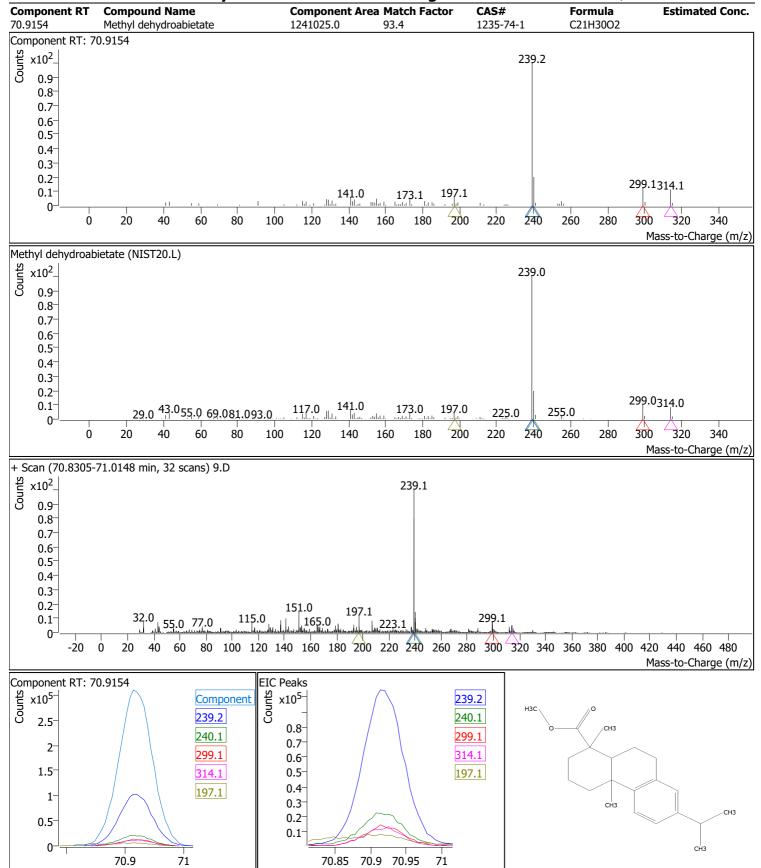
Library Search Results - NonTarget Hits with Details

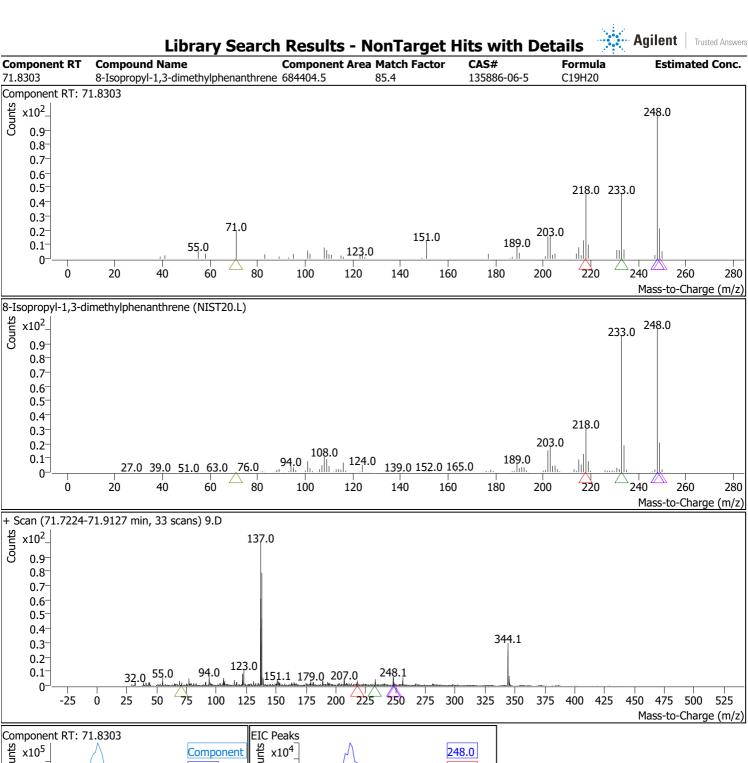


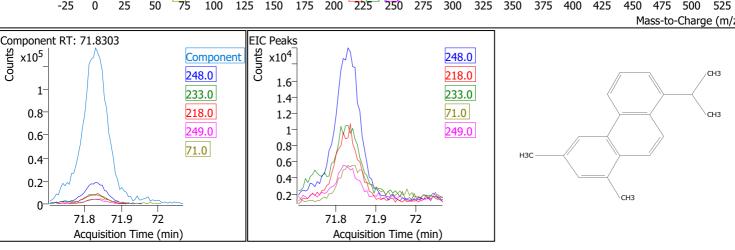






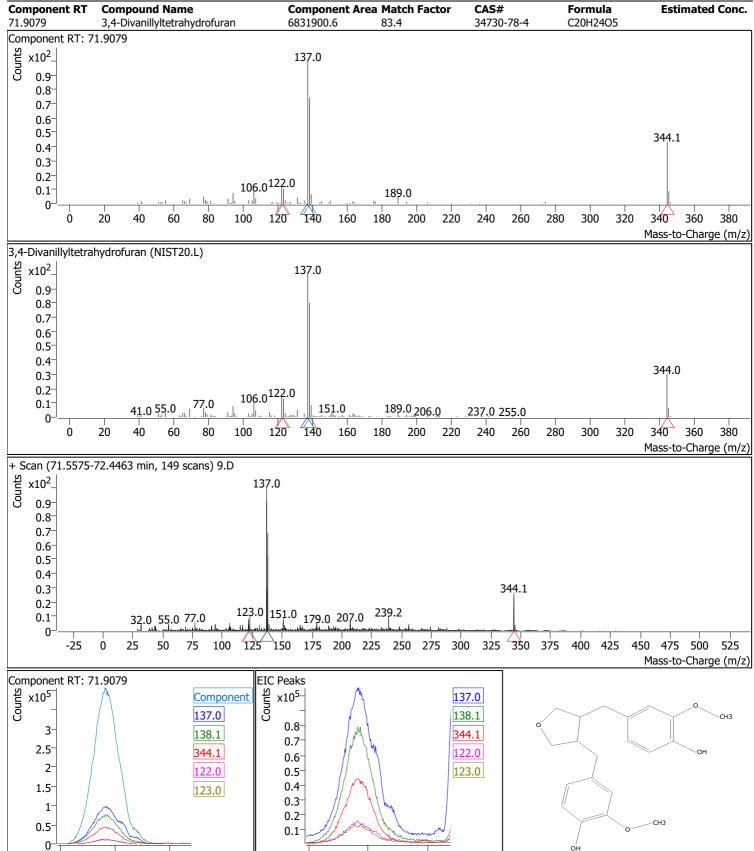










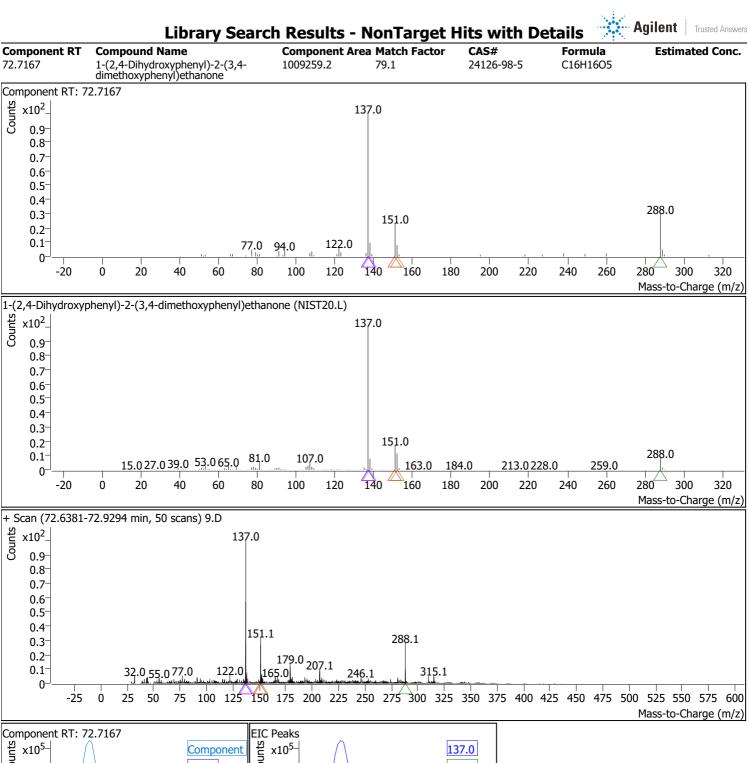


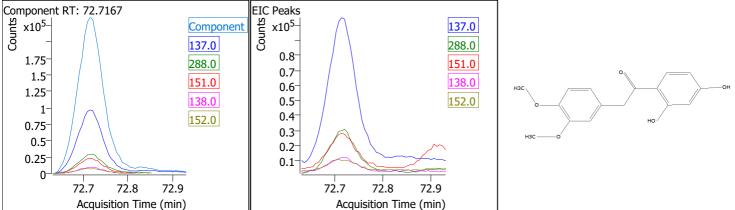
Acquisition Time (min)

72

Acquisition Time (min)

72.5





Compound Name Component RT Component Area Match Factor 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.)]-73.6259 10433003.5 5155-70-4 C20H28O2 Component RT: 73.6259 $x10^{2}$ 285.0 239.0 0.9 0.8 0.7 0.6 0.5 197.0 0.4^{-} 300.0 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 0.2 141.0 117.0 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 (73.4765-73.7976 min, 55 scans) 9.D 돌 x10². 285.2 0.9 0.8 0.7 239.2 0.6 0.5 197.1 0.4 0.3 300.2 0.2 141.0 43.1 0.1 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 25 75 -25 0 50 100 125 Mass-to-Charge (m/z) Component RT: 73.6259 EIC Peaks x10⁶ x10⁵ 285.0 Component 285.0 239.0 2 СНЗ 1.4 239.0 197.0 1.75 1.2

73.6

73.7

Acquisition Time (min)

300.0

141.0

73.8

197.0

300.0

141.0

73.8

1

0.8

0.6

0.4

0.2

73.6

73.7

Acquisition Time (min)

1.5

1.25

0.75

0.5

0.25

1

СНЗ

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor Component RT Compound Name** CAS# **Formula Estimated Conc.** 77.2394 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-541806.4 85.9 65996-50-1 C6H5N3O2 dione Component RT: 77.2394 x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 123.0 0.1 80.0 95.0 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 80.0 108.0 0 55 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 60 Mass-to-Charge (m/z) + Scan (77.1389-77.4223 min, 48 scans) 9.D x10². 167.0 0.9 151.0 0.8 0.7 0.6 0.5 0.4 0.3 181.0207.0 304.1 0.2 253.1 137.0 281.0 32.0,55.077.0 0.1 328.2 239.1 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 50 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 77.2394 St x10₂ Counts x10⁴ 151.0 Component 152.1 151.0 0.8 152.1 123.0 6 0.7^{-} 95.0 123.0

77.3

Acquisition Time (min)

51.0

5

4

3-

2

77.2

51.0

95.0

77.1 77.2 77.3 77.4

Acquisition Time (min)

0.6

0.5

0.4

0.3

0.2