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

File Name 12.D **Path Name** D:\MassHunter\GCMS\1\data\RBEL\240501 scan **Sample Name** 12 **Sample Type** Sample Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

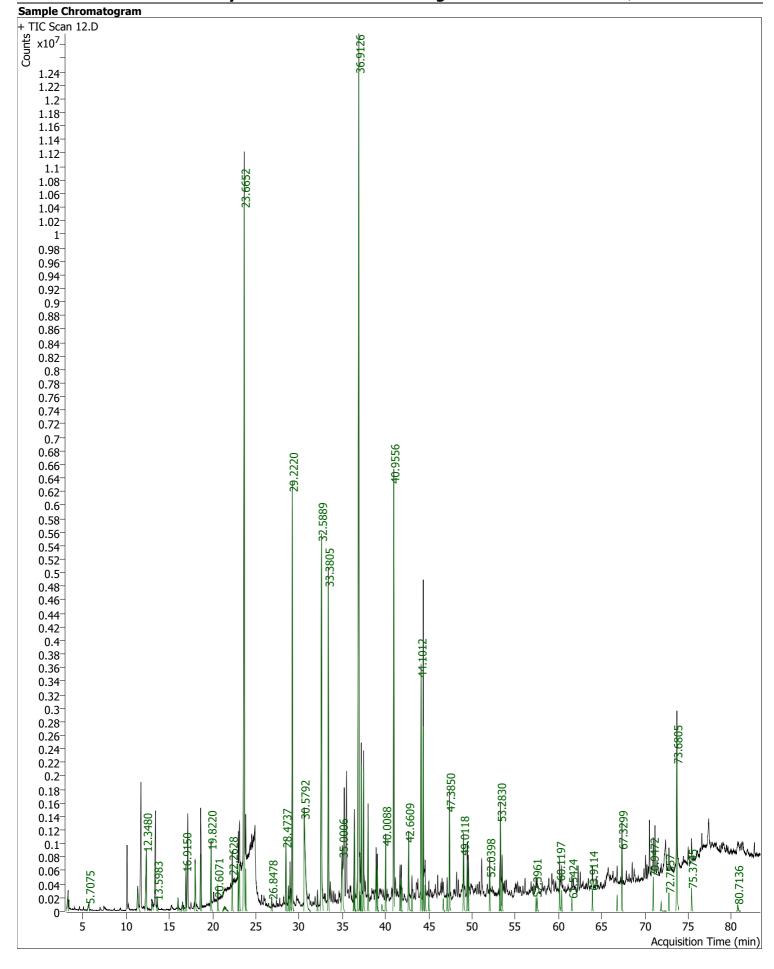
Acq. Date-Time 5/2/2024 4:45:06 AM **Instrument Name** GCMSD Dil. 1

Instrument Ne	anic Genab	DIII.	-	L		
Component R	「Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
3.2984	Propanoic acid	79-09-4	C3H6O2	1256319.7	99.1	
5.7075	Butanoic acid	107-92-6	C4H8O2	789556.9	97.0	
11.3424	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	2239579.2		
12.3480	Butyrolactone	96-48-0	C4H6O2	6030246.9	97.7	
12.9537	Methyltartronic acid	595-98-2	C4H6O5	946162.2	94.7	
13.5983	2,5-Hexanedione	110-13-4	C6H10O2	635144.0	93.9	
15.9946	2-Cyclopenten-1-one, 3-methyl-	2758-18-1	C6H8O	808024.4	97.8	
16.5198	3-Ethoxy-1,2-propanediol	1874-62-0	C5H12O3	785908.5	84.3	
16.9150	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2407522.4	85.3	
17.9758	Phenol	108-95-2	C6H6O	3330328.4	97.9	
18.6625	Diisoamyl ether	544-01-4	C10H22O	3178321.1	86.5	
19.8220	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	3907022.6	94.6	
20.6071	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	878018.7		
21.3606	1,3,5-Trioxane	110-88-3	C3H6O3	1063784.5	85.6	
22.2628	Phenol, 2-methyl-	95-48-7	C7H8O	2110366.8	94.1	
22.2626		106-62-7	C6H14O3	2180751.1	94.1 80.7	
	1-Propanol, 2-(2-hydroxypropoxy)- 1-Octanol					
23.1024		111-87-5	C8H18O	3997788.2	96.3	
23.6652	Phenol, 2-methoxy-	90-05-1	C7H8O2	56332737.3	98.1	
23.8347	Ethanone, 1-(2-thienyl)-	88-15-3	C6H6OS	2233327.4	96.4	
26.8478	Phenol, 2-ethyl-	90-00-6	C8H10O	765957.8	82.8	
28.4737	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	3455280.5	96.4	
28.7578	Naphthalene	91-20-3	C10H8	1002380.3	94.4	
28.9532	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	2311310.6	96.8	
29.2220	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	25372584.8	99.3	
30.5792	Catechol	120-80-9	C6H6O2	15446578.6	96.6	
32.1225	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	786039.4		
32.5889	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	30836242.2	94.9	
33.3805	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	19698698.7	96.2	
35.0006	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	6713262.2	87.7	
36.3392	Furan, tetrahydro-2-(methoxymethyl)-	19354-27-9	C6H12O2	1952918.8	82.9	
36.3402	2-Furanmethanol, tetrahydro-	97-99-4	C5H10O2	1900617.7		
36.3973	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	5478440.2	85.4	
36.9126	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	71049033.8	98.9	
36.9944	7-Chloro-1-(4-fluorophenyl)heptan-1-one	17135-47-6	C13H16ClFO	1070860.1	80.6	
36.9972	4-Ethylcatechol	1124-39-6	C8H10O2	1392961.7	80.4	
37.1189	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-	703-23-1	C9H10O3	864597.1	82.9	
37.1925	3,4-Dimethoxyphenol, 2-methylpropionate	1000447-30-5	C12H16O4	8494608.0	88.1	
37.4508	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	7611739.3	94.6	
37.9738	1,2,3-Trimethoxybenzene	634-36-6	C9H12O3	4908238.9	91.1	
38.9032	4-Ethylcatechol	1124-39-6	C8H10O2	3389965.7	94.0	
39.0415	Benzaldehyde, 3-hydroxy-4-methoxy-	621-59-0	C8H8O3	2555702.9	89.4	
39.5741	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	617714.8	86.3	
40.0088	Ethanone, 1-(2,3,4-trihydroxyphenyl)-	528-21-2	C8H8O4	3710020.7	84.3	
40.9556	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	28479046.8	93.9	
41.6667	Ethanone, 1-(2,3,4-trihydroxyphenyl)-	528-21-2	C8H8O4	1476330.1	84.4	
41.8053	3-Allyl-6-methoxyphenol	501-19-9	C10H12O2	1848757.9	83.1	
42.6609	Apocynin	498-02-2	C9H10O3	4413902.0	97.5	
43.0479	Benzene, 1,2,3-trimethoxy-5-methyl-	6443-69-2	C10H14O3	1009709.2	86.6	
44.1012	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	13211186.9	98.9	
44.3512	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	9156638.0	90.9	
44.3562	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	10228371.1	83.4	
44.5709	Flopropione	2295-58-1	C9H10O4	1639148.3	81.5	
45.0009	3,4-Dimethoxyphenylacetone	776-99-8	C11H14O3	788429.4	80.9	
46.6637	Butyrovanillone	64142-23-0	C11H14O3	783226.6	87.2	
47.1122	Phenol, 2-methoxy-4-methyl-6-[propenyl]-	201359-63-9	C11H14O2	1119199.9	80.9	
47.3850	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	5491974.8	93.9	
49.0118	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	3998859.5	91.4	
49.4471	2-Naphthalenol, 3-methoxy-	18515-11-2	C11H10O2	3312190.0	96.5	
49.5791	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	1976903.1	83.9	
52.0398	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C11H14O3 C10H12O4	2031066.2	95.9	
		3900-49-0	C10H12O4 C12H12O2	1446977.2		
53.2084	1,6-Dimethoxynaphthalene				83.6 96.5	
53.2830	Syringylacetone	19037-58-2	C11H14O4	5140229.7	96.5	
53.4711	Naphthalene, 2,3-dimethoxy-	10103-06-7	C12H12O2	2708270.4	86.5	
57.3961	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	828365.0	84.3	
	is story to tour state occurry and	Page 1 of 81		G	enerated at 11:35 A	M on 5/2/2024

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.
57.5199	Dihydrosyringenin	20736-25-8	C11H16O4	879674.5	92.1	
60.1197	n-Hexadecanoic acid	57-10-3	C16H32O2	1926956.5	88.9	
60.3580	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	1230707.6	89.7	
61.5424	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	735959.4	86.3	
63.9114	4,4'-Diisopropylbiphenyl	18970-30-4	C18H22	1229382.1	82.2	
66.7666	9,10-Anthracenedione, 1,4-dimethyl-	1519-36-4	C16H12O2	997926.7	80.8	
67.3299	Retene	483-65-8	C18H18	3743204.2	97.6	
70.9472	Methyl dehydroabietate	1235-74-1	C21H30O2	2014327.5	93.2	
71.8600	8-Isopropyl-1,3-dimethylphenanthrene	135886-06-5	C19H20	727560.7	83.5	
72.7557	1-(2,4-Dihydroxyphenyl)-2-(3,4- dimethoxyphenyl)ethanone	24126-98-5	C16H16O5	1060992.0	82.6	
73.6805	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	11809309.0	93.7	
75.3745	1-Octadecanol	112-92-5	C18H38O	1532124.5	90.2	
80.7136	5-Eicosene, (E)-	74685-30-6	C20H40	648546.6	82.6	
80.7138	3-Eicosene, (E)-	74685-33-9	C20H40	627284.8	82.7	



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1

0.75 0.5

0.25

3.15 3.2 3.25 3.3

Acquisition Time (min)

57.0

2

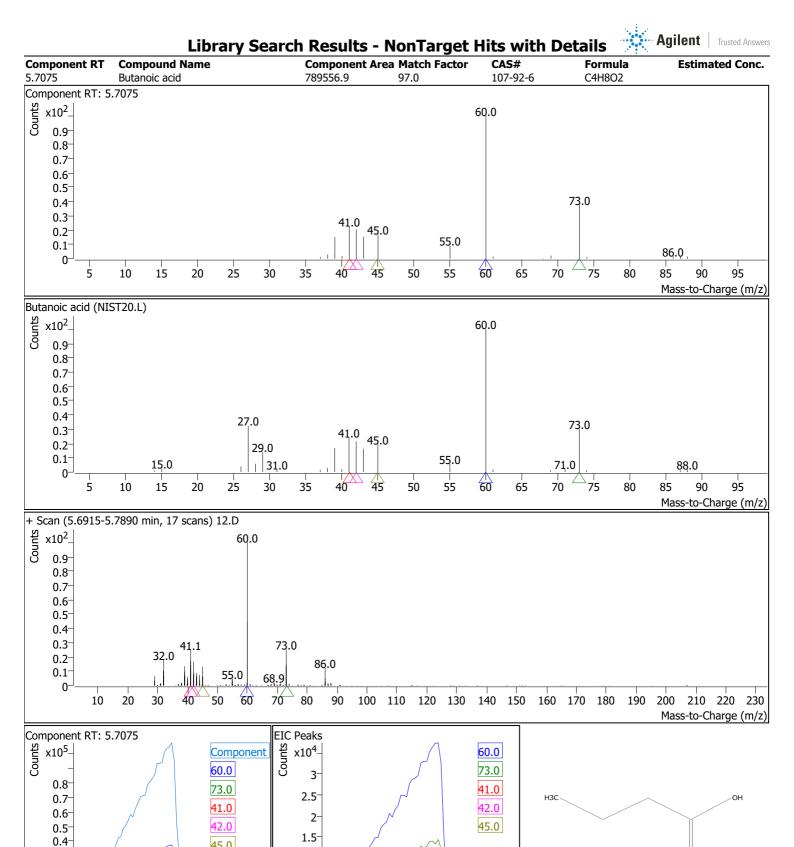
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3.15

3.2

3.25

3.3 Acquisition Time (min) CH3





5.6

5.7 Acquisition Time (min)

45.0

1

5.5

0.5

0.3

0.2-

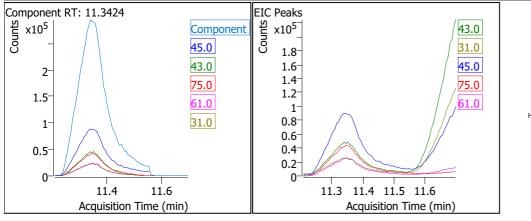
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5.5

5.6

5.7

--- 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 11.3424 1,2-Propanediol, 3-methoxy-2239579.2 88.3 C4H10O3 Component RT: 11.3424 v10² 0.9 45.0 0.8 0.7^{-} 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 0.2 33.0 88.0 0.1 75 10 15 20 25 30 55 60 65 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 (11.2334-11.5773 min, 57 scans) 12.D St x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4^{-} 75.0 0.3 31.0 0.2 61.0 0.1 88.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 11.3424 **EIC Peaks** x10⁵ Component 43.0



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56.0

1.25

0.75

0.5⁻ 0.25⁻ 0

12.2

12.3

12.4

Acquisition Time (min)

12.5

1

29.0

56.0

4

3

2

12.2

12.3

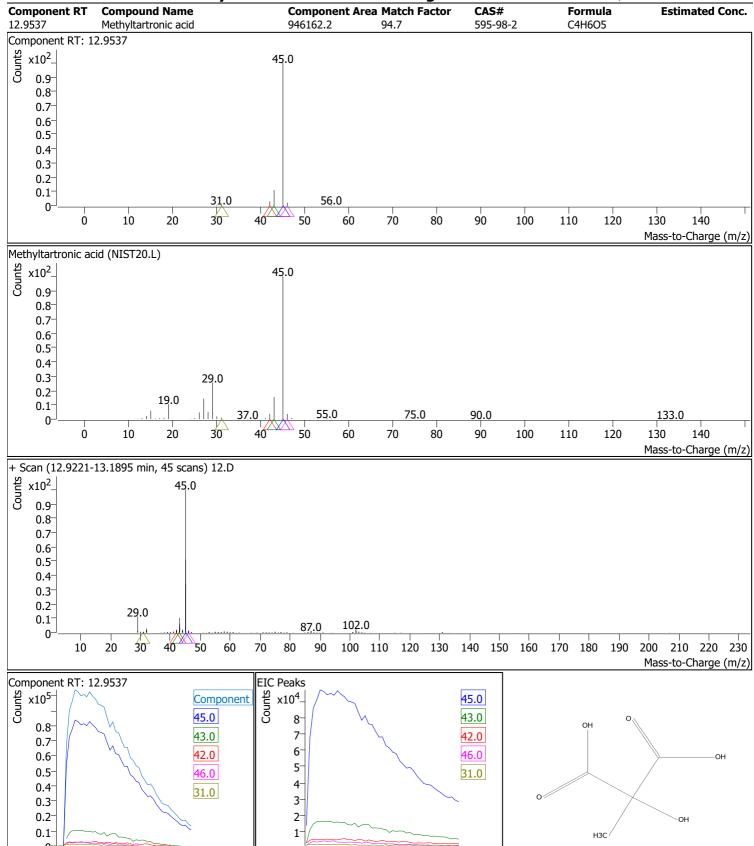
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Acquisition Time (min)

12.5

Library Search Results - NonTarget Hits with Details





13

13.1

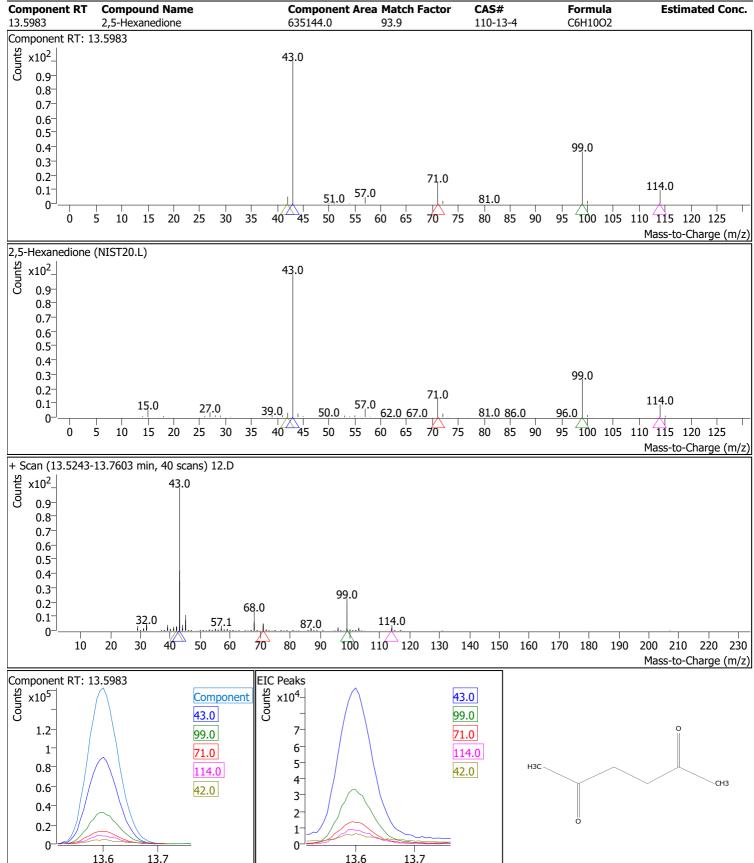
Acquisition Time (min)

13

13.1







Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2758-18-1 15.9946 2-Cyclopenten-1-one, 3-methyl-808024.4 97.8 C6H8O Component RT: 15.9946 v10² 0.9 96.0 0.8 0.7^{-} 67.0 0.6 0.5 53.0 81.0 0.4 39.0 0.3 0.2 65.0 0.1 65 10 15 20 25 30 35 45 50 55 75 80 85 90 100 105 110 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3-methyl- (NIST20.L) Counts x10²_ 0.9 96.0 0.8 0.7 0.6 0.5 67.0 0.4 53.0 81.0 0.3 39.0 0.2 27.0 0.1 56.0 51.0 99.0 10 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 105 110 Mass-to-Charge (m/z) + Scan (15.9274-16.1422 min, 36 scans) 12.D st x10² 0.9 96.0 0.8 0.7 0.6 67.0 0.5 0.4^{-} 81.0 53.0 39.0 0.3 0.2 32.0 0.1 117.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 15.9946 **EIC Peaks** st x10⁵-Counts x10⁴ 96.0 Component 96.0 67.0 3 1.2 67.0 53.0 CH3 81.0

16.1

Acquisition Time (min)

39.0

1

0.8

0.6

0.4

0.2

0

16

16.1

Acquisition Time (min)

53.0

81.0

39.0

2.5

1.5

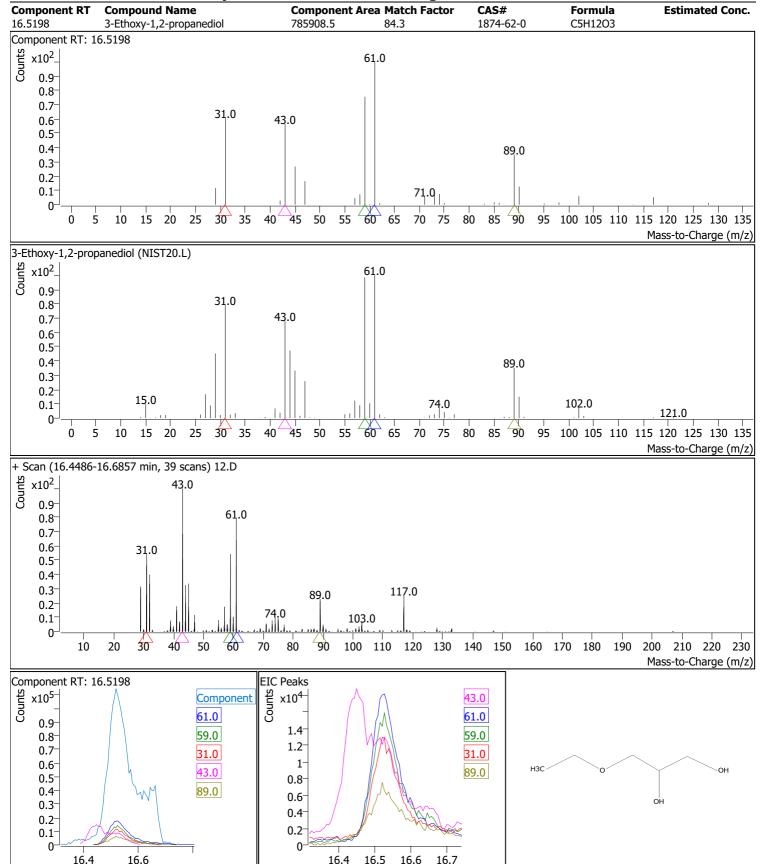
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1

2-

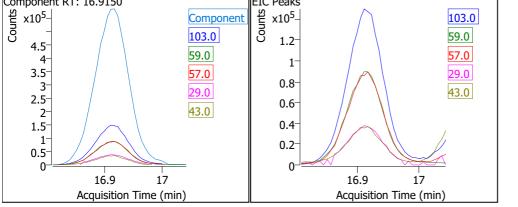






Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 53951-44-3 1,3-Dioxolane-4-methanol, 2-ethyl-2407522.4 85.3 C6H12O3 Component RT: 16.9150 v10² 0.9 103.0 0.8 0.7 59.0 0.6 0.5 0.4 0.3 29.0 43.0 131.0 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 (16.8106-17.0009 min, 33 scans) 12.D St x10² 0.9 103.0 0.8 0.7 57.0 0.6 0.5 0.4^{-} 0.3 31.0 0.2 131.1 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: 16.9150 Counts Counts x10⁵ x10⁵– 103.0 Component 103.0 59.0 1.2



... 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 17.9758 Phenol 3330328.4 97.9 C6H6O Component RT: 17.9758 v10² 0.9 94.0 0.8 0.7^{-} 0.6 0.5 0.4 66.0 0.3 0.2 39.0 0.1 63.0 55.0 50.0 0 ⁴95 25 40 10 15 20 30 35 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) Phenol (NIST20.L) St x10²_0.9 94.0 0.8 0.7 0.6 0.5 0.4 0.3 66.0 0.2 39.0 0.1 47.0 51.0 55.0 14.0 18.0 63.0 27.0 31.0 42.0 79.0 40 95 10 15 20 25 30 35 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) + Scan (17.9113-18.2912 min, 64 scans) 12.D St x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4^{-} 66.0 0.3 0.2 39.0 0.1 32.0 51.0 110.1 82.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 17.9758 EIC Peaks Counts Counts x10⁵-94.0 Component 94.0 66.0 2.25 5 66.0 65.0 2 1.75 39.0 65.0 4 1.5 39.0 40.0

18.1

18.2 Acquisition Time (min)

1.25

0.75 0.5

0.25

1

18

40.0

3

2-

1

18

18.1

Acquisition Time (min)

18.2

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18.65

18.7

Acquisition Time (min)

18.75

69.1

41.0

1.4

1.2

0.8

0.6

0.4

 0.2^{-}

1

71.0

69.1

41.0

5

4

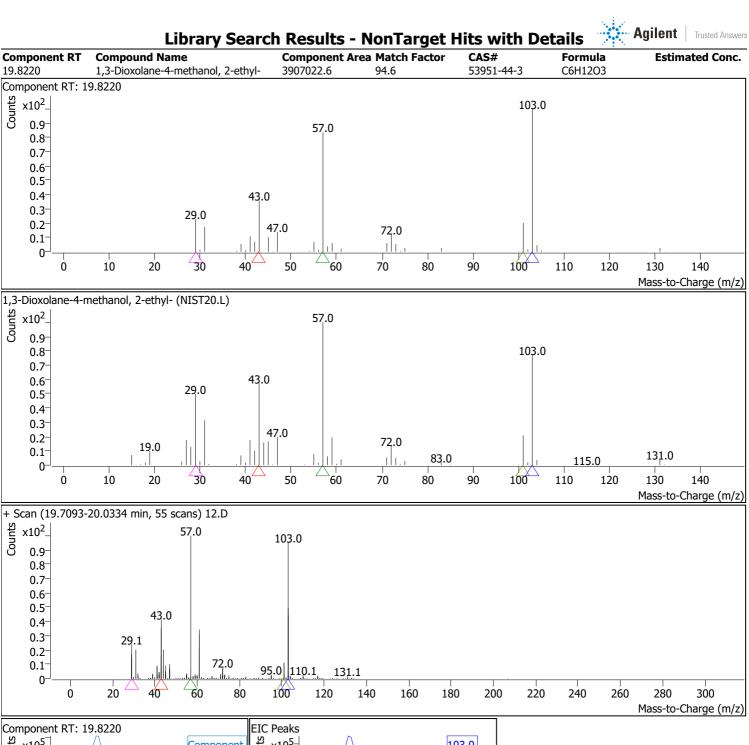
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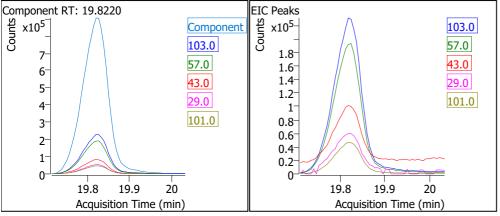
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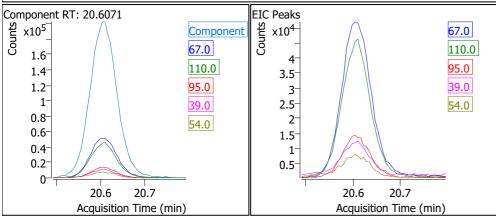
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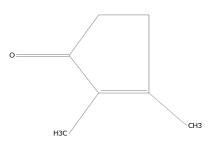
18.7





··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.6071 2-Cyclopenten-1-one, 2,3-dimethyl-878018.7 90.7 1121-05-7 C7H10O Component RT: 20.6071 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 95.0 39.0 0.2 54.0 41.0 81.0 65.0 0.1 95 110 15 20 30 35 40 45 50 55 60 65 80 85 100 105 115 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 67.0 0.8 110.0 0.7 0.6 0.5 0.4 0.3 39.0 95.0 27.0 0.2 53.0 81.0 0.1 51.0 65.0 32.0 91.0 99.0 110 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (20.5211-20.7588 min, 40 scans) 12.D St x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 67.0 110.1 0.3 31.0 0.2 0.1 81.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 20.6071 **EIC Peaks** Counts y x10⁵ x10⁴ 67.0 Component 67.0 110.0 1.6 4 110.0 95.0 1.4 3.5





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 21.3606 1,3,5-Trioxane 1063784.5 85.6 110-88-3 C3H6O3 Component RT: 21.3606 v10² 0.9 61.0 0.8 0.7 0.6 0.5 89.0 0.4 0.3 31.0 0.2 0.1 56.0 90 55 25 60 75 80 10 15 20 30 35 50 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 29.0 0.4 0.3 0.2 0.1 44.0 14.0 56.0 90 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 Mass-to-Charge (m/z) + Scan (21.1096-21.8231 min, 121 scans) 12.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 89.0 56.0 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: 21.3606 **EIC Peaks** Counts Counts x10⁴ Component 61.0 43.0 8 4.5 89.0 31.0 6 3.5 31.0 89.0 3 60.0 2.5



43.0

3

21.2

21.4

21.6

Acquisition Time (min)

2

21.2

21.4

21.6

Acquisition Time (min)

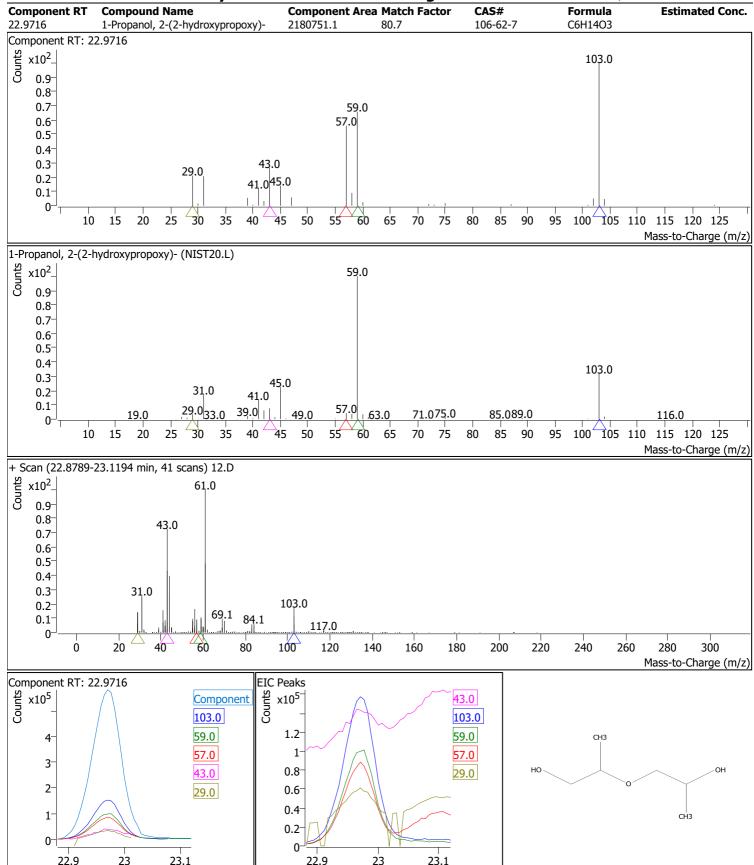
1.5

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 95-48-7 22.2628 Phenol, 2-methyl-2110366.8 C7H8O Component RT: 22.2628 v10² 0.9 108.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 90.0 0.2 103.0 0.1 55 75 85 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 58.0 ^{63.0} 68.0 74.0 90 100 105 110 115 120 10 15 25 30 35 40 50 55 60 65 70 75 80 85 95 Mass-to-Charge (m/z) + Scan (22.1740-22.3940 min, 37 scans) 12.D St x10²_ 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 107.0 0.2 77.0 0.1 90.0 **110** 10 20 30 40 50 60 70 80 100 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 22.2628 **EIC Peaks** Counts Counts x10⁵ 108.0 Component 108.0 107.0 0.9 107.0 0.8^{-} 77.0 3.5 0.7^{-} 77.0 79.0 3

 0.6^{-}







Acquisition Time (min)

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.1024 1-Octanol 3997788.2 96.3 111-87-5 C8H18O Component RT: 23.1024 v10² 0.9 56.0 41.0 0.8 69.1 0.7 84.1 0.6 0.5 0.4 0.3 0.2 0.1 55 100 105 110 115 120 125 130 135 140 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 95 100 105 110 115 120 125 130 135 140 55 20 25 35 40 45 50 60 65 70 75 80 85 90 Mass-to-Charge (m/z) + Scan (22.9588-23.2621 min, 52 scans) 12.D st x10² 0.9 61.0 43.0 0.8 0.7 0.6 0.5 0.4^{-} 31.0 0.3 0.2 103.0 69.1 84.1 0.1 117.0 60 Ó 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.1024 Counts x10⁵ Counts x10⁴ 56.0 Component 56.0 55.0 5 55.0 41.0 6 41.0 70.1 5

23.1

23.2

Acquisition Time (min)

69.1

70.1

3

2

1

23

23.1

23.2

Acquisition Time (min)

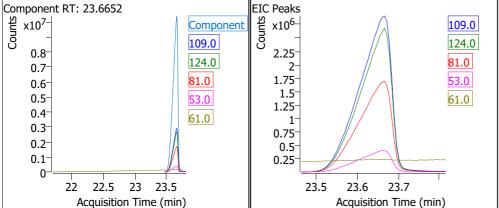
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3

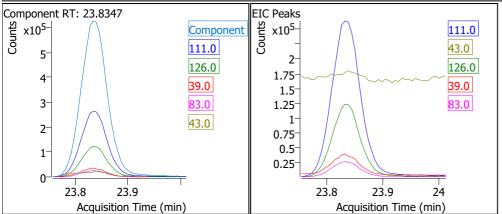
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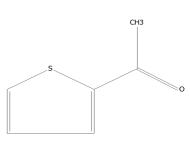
23

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6652 Phenol, 2-methoxy-56332737.3 98.1 C7H8O2 Component RT: 23.6652 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 61.0 0.1 39.0 60 80 110 10 20 30 40 50 70 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) Counts 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 15.0 60 110 10 20 30 40 50 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4642-23.8151 min, 60 scans) 12.D st x10² 0.9 124.0 109.0 81.0 0.8 0.7 0.6 0.5 43.0 0.4^{-} 61.0 0.3 53.0 0.2 31.0 39.0 0.1 77.0 95.0 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: 23.6652 EIC Peaks Counts Counts x10⁶ 109.0 Component 109.0 124.0 0.8 2.25 124.0 81.0 0.7 2



··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 88-15-3 23.8347 Ethanone, 1-(2-thienyl)-2233327.4 96.4 C6H6OS Component RT: 23.8347 v10² 0.9 111.0 0.8 0.7 0.6 0.5 126.0 0.4 0.3 0.2 39.0 83.0 0.1 57.0 40 70 110 10 20 30 80 90 100 120 130 140 Mass-to-Charge (m/z) Ethanone, 1-(2-thienyl)- (NIST20.L) st x10² 0.9 111.0 0.8 0.7 0.6 0.5 126.0 0.4 0.3 39.0 0.2 43.0 83.0 0.1 57.0 63.0 69.074.0 27.032.0 97.0 110 10 20 30 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.7505-24.0113 min, 44 scans) 12.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 0.2 31.0 111.0 126.0 0.1 55.0 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: 23.8347 EIC Peaks Counts Counts x10⁵-111.0 Component 111.0 43.0 СНЗ 5 2





Library Search Results - NonTarget Hits with Details ··· Agilent | Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-00-6 26.8478 Phenol, 2-ethyl-765957.8 82.8 C8H10O Component RT: 26.8478 v10² 0.9 107.0 0.8 0.7 0.6 0.5 122.0 0.4 77.0 0.3 0.2 117.0 0.1 132.0 55 65 75 80 85 90 95 100 105 110 115 120 125 130 135 60 Mass-to-Charge (m/z) Phenol, 2-ethyl- (NIST20.L) Counts x10²_ 0.9 107.0 0.8 0.7 0.6 122.0 0.5 0.4 0.3 77.0 0.2 86.0 ^{91.0} 0.1 39.0 51.0 103.0 27.0 65.0 18.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (26.7643-26.9724 min, 35 scans) 12.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 43.0 122.1 0.3 61.0 77.0 0.2 32.0 0.1 53.0 91.0 132.1 151.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 26.8478 **EIC Peaks** st x10⁵ Counts x10⁴ 107.0 Component 107.0 122.0 4 1.4 3.5 122.0 77.0 1.2 3-77.0 117.0 1

26.8

26.9 Acquisition Time (min)

79.0

2.5

1.5

0.5

2-

1

117.0

79.0

0.8

0.6

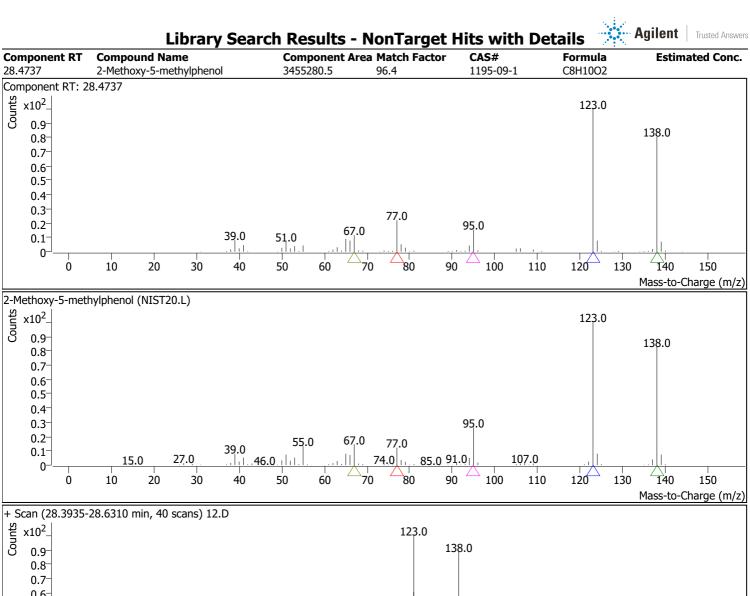
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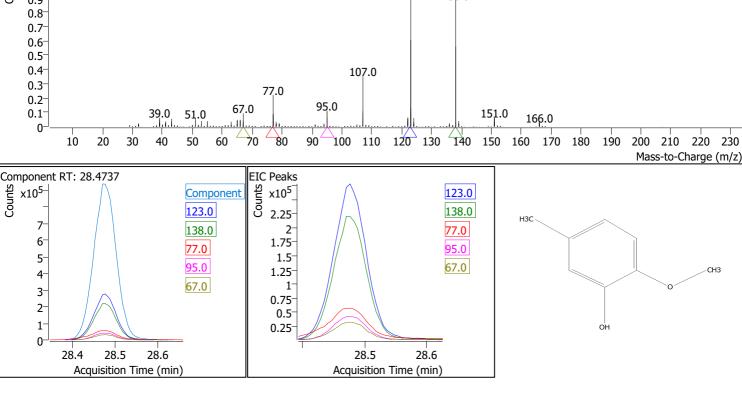
0.2

0

26.8

26.9





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28.8

Acquisition Time (min)

28.9

126.0

1.25

0.75

0.5

28.7

28.8

Acquisition Time (min)

28.9

0.25

1

102.0

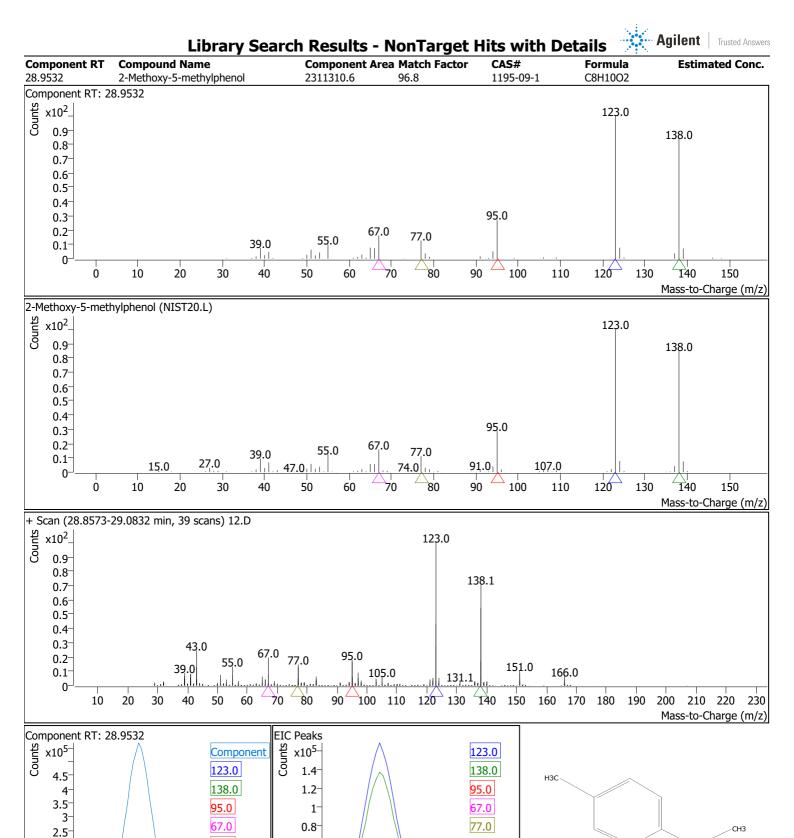
126.0

0.6

0.4

0.2

28.7



29

Acquisition Time (min)

77.0

1.5

0.5

1

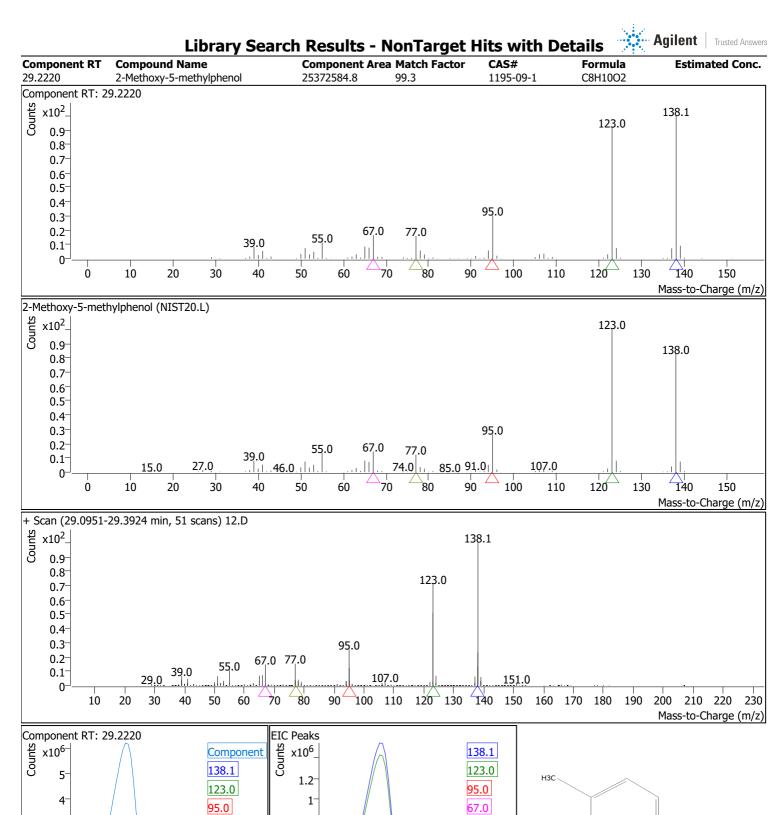
28.9

29 Acquisition Time (min) 0.6

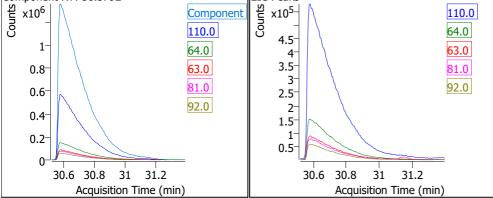
0.4

0.2

28.9



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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.** 786039.4 1450-72-2 32.1225 Ethanone, 1-(2-hydroxy-5-90.9 C9H10O2 methylphenyl)-Component RT: 32.1225 x10²_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 0.3 77.0 0.2^{-} 0.1 51.0 107.0 0-____80 150 0 10 20 30 40 50 60 70 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 150.0 0.5 0.4 0.3 107.0 0.2 77.0 43.0 51.0 0.1 27.0 63.0 85.091.0 131.0 121.0 0 130 150 10 20 30 40 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0407-32.2287 min, 32 scans) 12.D st x10² 0.9 135.0 0.8 0.7 0.6 0.5 0.4 150.0 0.3 43.0 0.2 77.0 96.0 165.0 180.0 0.1 32.0 53.0 67.0 121.1 0 _____80 140 200 220 260 Ó 20 40 60 100 120 160 180 240 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 32.1225 Counts Counts x10⁵x10⁴ 135.0 Component НО 135.0 150.0 7 1.6 150.0 77.0 6 **Н3С** 1.4 136.0 77.0 1.2 5 136.0 79.0 1 4 0.8

32.1 32.15

Acquisition Time (min)

79.0

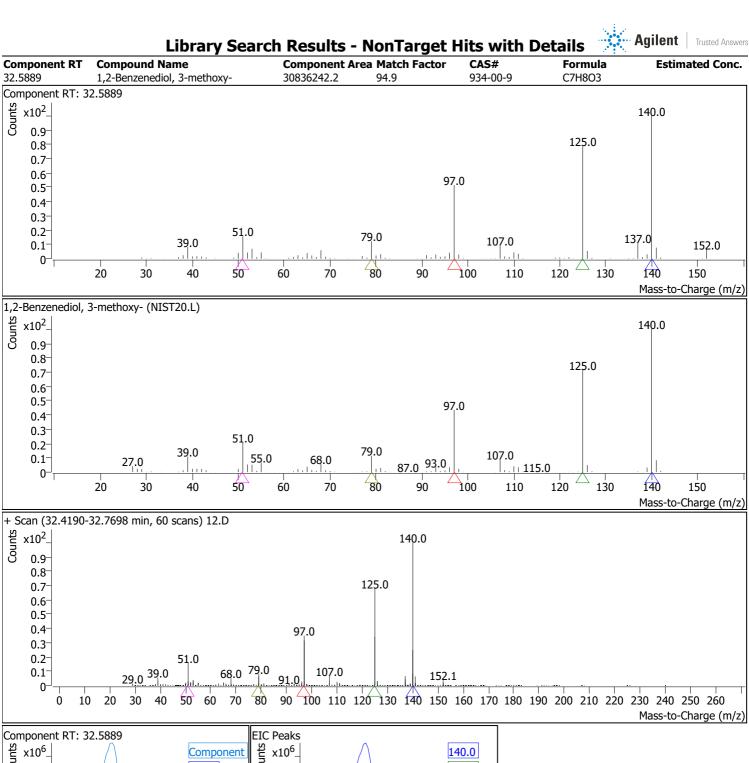
32.1 32.15 32.2

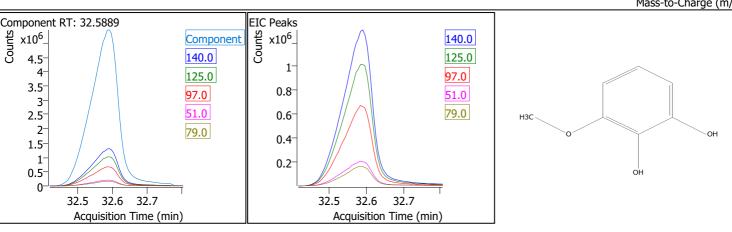
Acquisition Time (min)

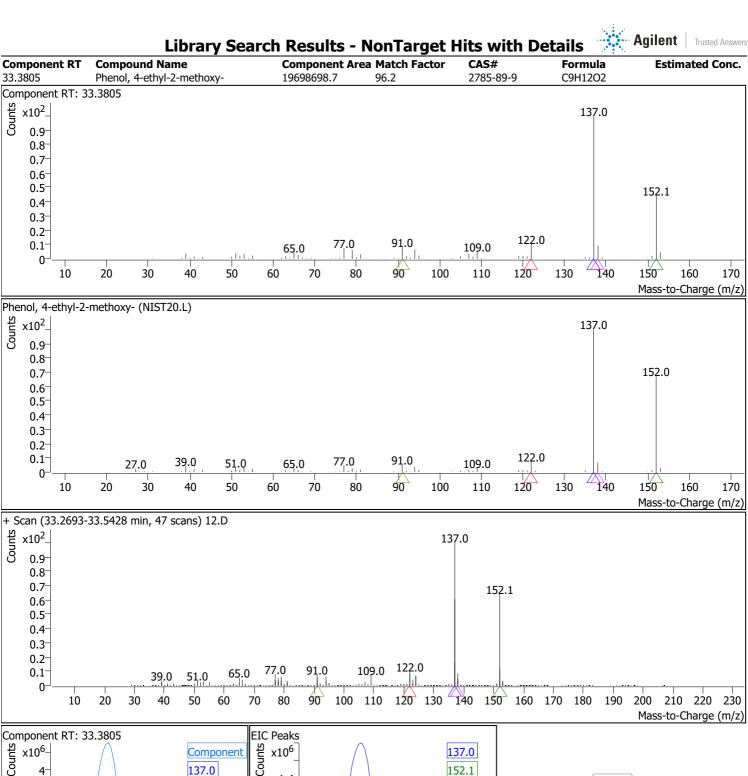
0.6

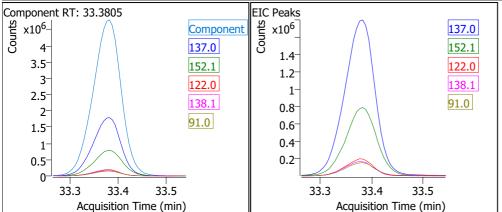
0.4 0.2 3-

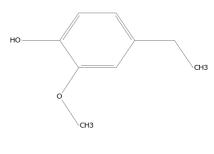
2











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35

35.1 35.2

Acquisition Time (min)

77.0

4

3

2

1

35

35.2

Acquisition Time (min)

77.0

137.0

0.8

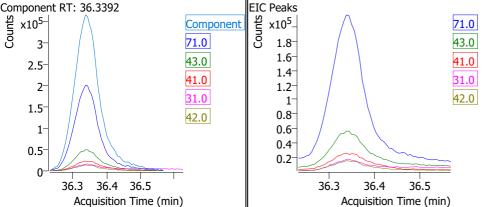
0.6

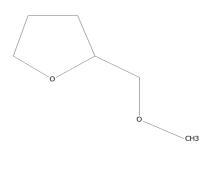
0.4

0.2

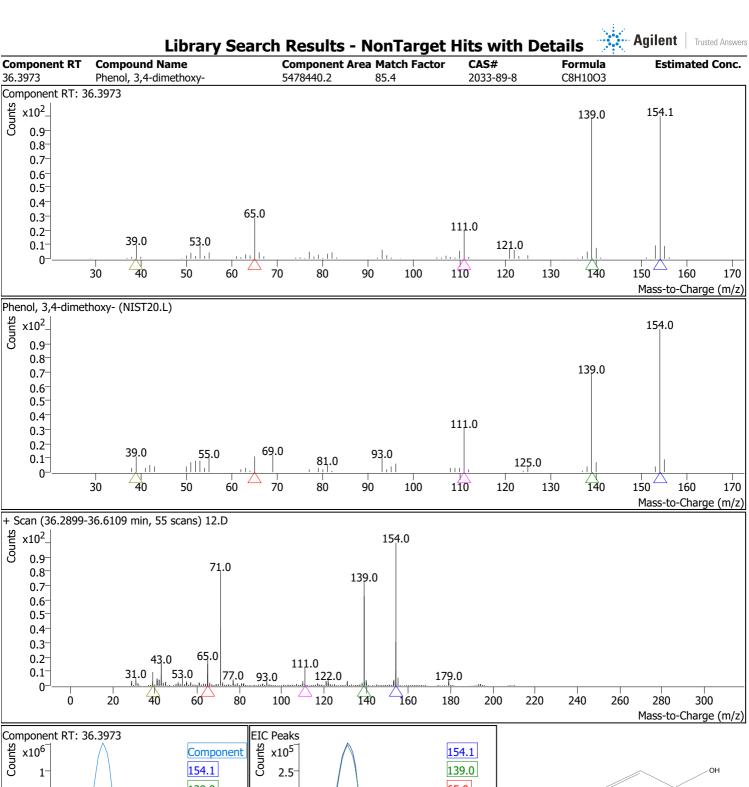
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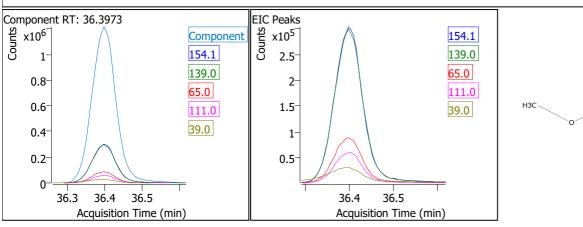
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 36.3392 Furan, tetrahydro-2-(methoxymethyl)- 1952918.8 82.9 19354-27-9 C6H12O2 Component RT: 36.3392 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 0.1 31.0 57.0 95 100 105 110 115 120 125 30 35 60 65 Mass-to-Charge (m/z) Furan, tetrahydro-2-(methoxymethyl)- (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 0.1 58.0 15.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (36.2363-36.5693 min, 57 scans) 12.D st x10² 0.9 154.0 71.0 0.8 139.0 0.7^{-} 0.6 0.5 0.4^{-} 0.3 43.0 65.0 0.2 111.0 0.1 31.0 53.0 77.0 122.0 93.0 179.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 36.3392 **EIC Peaks** Counts x10⁵ x10⁵-71.0 Component 71.0 43.0 1.8 1.6 43.0 41.0 2.5 1.4



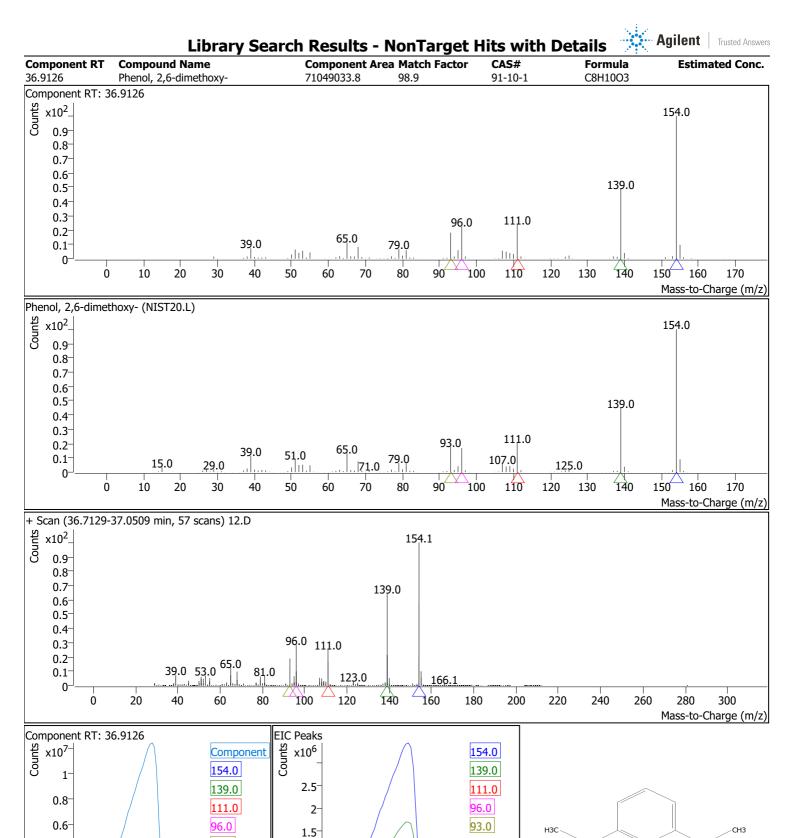


-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 97-99-4 36.3402 2-Furanmethanol, tetrahydro-1900617.7 83.9 C5H10O2 Component RT: 36.3402 v10² 0.9 71.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 41.0 31.0 0.1 57.0 10 15 25 30 35 55 60 65 70 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 (36.2363-36.5693 min, 57 scans) 12.D st x10² 0.9 154.0 71.0 0.8 139.0 0.7 0.6 0.5 0.4^{-} 0.3 43.0 65.0 0.2 111.0 0.1 31.0 53.0 77.0 122.0 93.0 179.0 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 36.3402 **EIC Peaks** Counts x10⁵-71.0 Component 71.0 43.0 1.8 1.6 43.0 41.0 2.5 1.4





CH3



93.0

1

36.8

36.9

Acquisition Time (min)

0.5

0.4

0.2

0

36.8

36.9

Acquisition Time (min)

37

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1070860.1 36.9944 7-Chloro-1-(4-fluorophenyl)heptan-1-80.6 17135-47-6 C13H16CIFO Component RT: 36.9944 x10²_ 123.0 0.9 8.0 0.7 0.6 138.0 0.5 0.4 0.3 0.2^{-} 0.1 95.0 0-120 100 140 220 240 0 20 40 60 80 160 180 200 260 Mass-to-Charge (m/z) 7-Chloro-1-(4-fluorophenyl)heptan-1-one (NIST20.L) $x10^{2}$ 123.0 0.9 0.8 138.0 0.7 0.6 0.5 0.4 0.3 95.0 0.2 0.1 75.0 55.0 151.0 41.0 109.0 165.0177.0189.0 207.0 242.0 0 120 140 240 20 40 60 80 100 160 180 200 220 260 Mass-to-Charge (m/z) + Scan (36.9439-37.1164 min, 30 scans) 12.D st x10² 123.0 154.0 0.8 0.7 138.0 0.6 0.5 0.4 0.3 166.1 51.0 65.0 77.0 0.2 179.0 111.0 0.1 0 120 140 200 220 260 Ó 20 40 60 80 100 160 180 240 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 36.9944 Counts Counts x10⁵ $x10^{5}$ 123.0 Component 138.0 123.0 1.2 1.75 138.0 95.0 1 1.5 124.0 124.0 1.25 0.8

37

37.05

Acquisition Time (min)

37.1

120.0

95.0

120.0

0.6

 0.4°

0.2

1

0.75

0.5

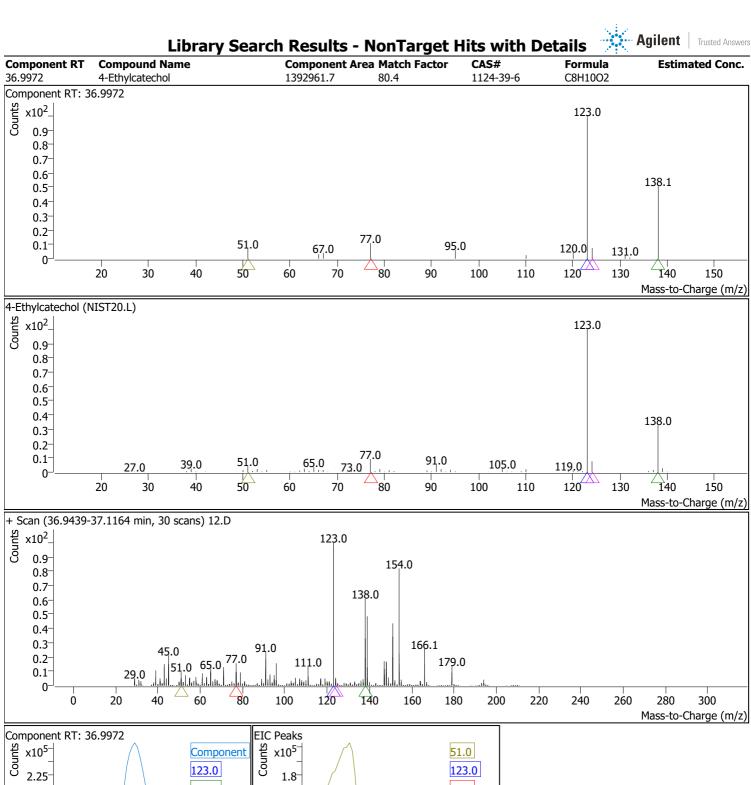
36.9

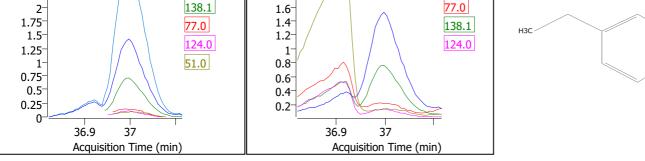
37

Acquisition Time (min)

37.1

0.25





··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 864597.1 703-23-1 37.1189 Ethanone, 1-(2-hydroxy-6-82.9 C9H10O3 methoxyphenyl)-Component RT: 37.1189 x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 166.0 0.4 0.3 0.2^{-} 136.0 91.0 0.1 108.0 0-90 150 170 30 40 50 60 70 80 100 110 120 130 140 160 180 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-6-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 166.0 0.5 0.4 0.3 0.2 136.0 108.0 0.1 93.0 43.0 65.0 77.0 121.0 0 150 90 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (37.0391-37.2765 min, 40 scans) 12.D $x10^{2}$ 154.0 0.9 0.8 0.7 0.6 139.0 0.5 0.4 0.3 111.0 0.2 39.0 53.0 65.0 77.0 0.1 123.0 166.1179.0 0 Ó 40 60 80 140 200 220 260 300 20 100 120 160 180 240 280 Mass-to-Charge (m/z) Component RT: 37.1189 **EIC Peaks** Counts Counts x10⁵x10⁵_ 151.0 Component 166.0 151.0 1.8 1 СНЗ 166.0 91.0 1.6 1.4 0.8 152.0 152.0 1.2 136.0 136.0 0.6 CH3 1 91.0

37.2

Acquisition Time (min)

 0.4°

0.2

37.1

0.8

0.6 0.4

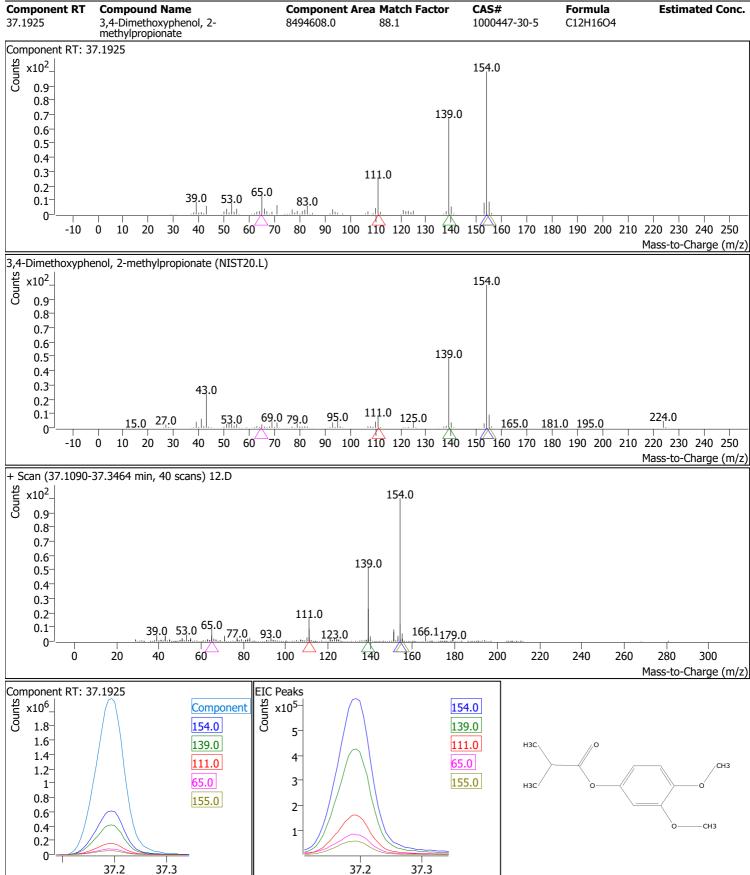
0.2

37.1

37.2

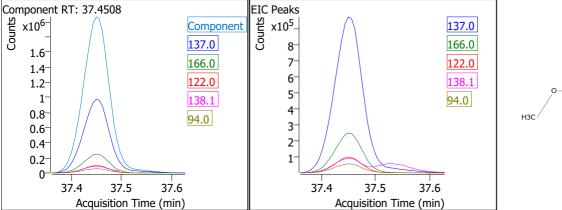






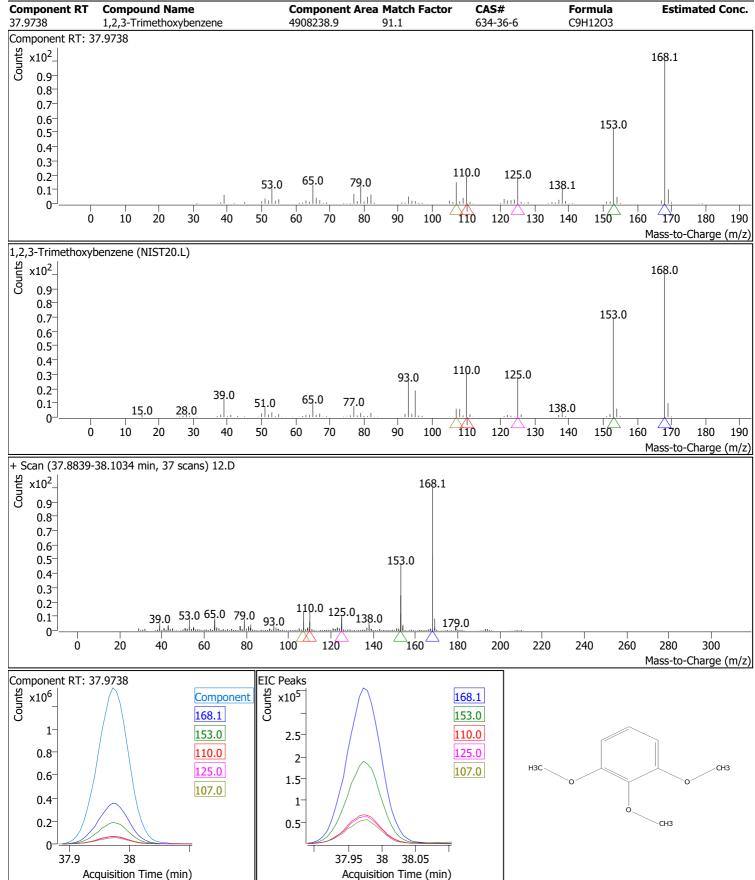
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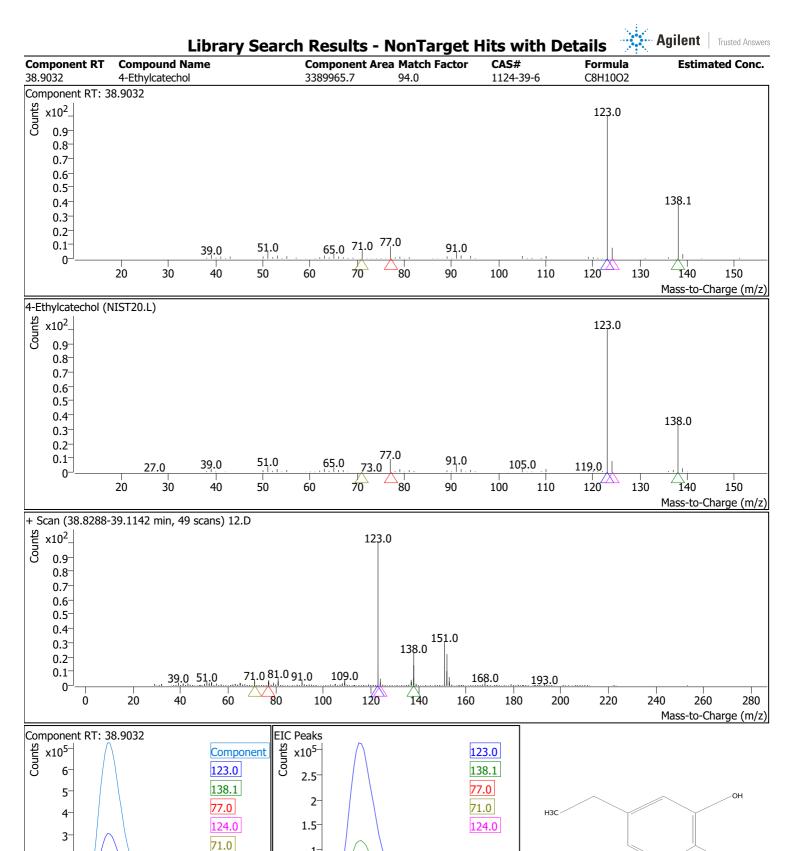
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2785-87-7 37.4508 Phenol, 2-methoxy-4-propyl-7611739.3 94.6 C10H14O2 Component RT: 37.4508 v10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 77.0 51.0 65,0 160 170 50 120 10 20 30 40 60 70 80 100 110 130 180 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 (37.3601-37.6200 min, 44 scans) 12.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 0.1 39.0 51.0 65.0 77.0 154.0 179.0 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: 37.4508 Counts Counts x10⁵-137.0 Component 137.0 166.0 8-1.6 166.0 7 122.0 1.4











39

Acquisition Time (min)

39.1

1

0.5

38.9

2

1

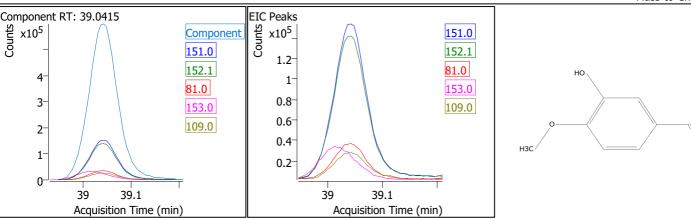
38.9

39

Acquisition Time (min)

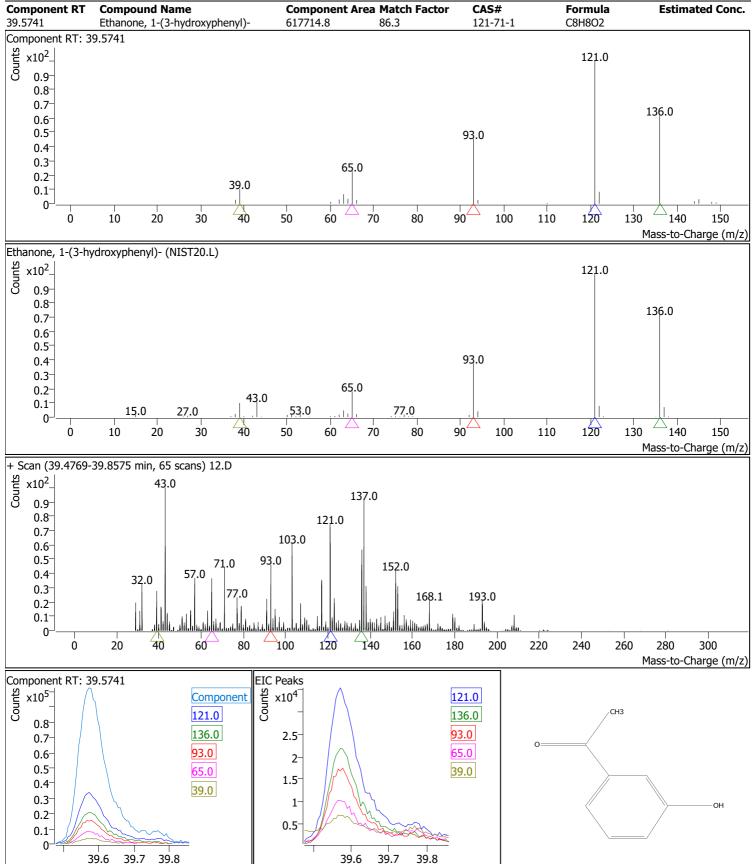
39.1

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 621-59-0 39.0415 Benzaldehyde, 3-hydroxy-4-methoxy-2555702.9 89.4 C8H8O3 Component RT: 39.0415 v10² 0.9 151.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 81.0 109.0 0.2 65.071.0 0.1 80 110 10 20 30 60 100 120 130 140 150 160 170 Mass-to-Charge (m/z) Benzaldehyde, 3-hydroxy-4-methoxy- (NIST20.L) st x10²_ 0.9-151.0 0.8 0.7 0.6 0.5 0.4 81.0 0.3 109.0 0.2 123.0 39.0 0.1 15.0 119.0 128.0 137.0 74.0 110 10 20 30 40 50 60 70 80 90 100 120 130 150 160 170 Mass-to-Charge (m/z) + Scan (38.9477-39.1915 min, 42 scans) 12.D st x10² 0.9 151.0 0.8 123.0 0.7 0.6 0.5 0.4^{-} 0.3 81.0 0.2 109.0 138.1 39.0 51.0 168.0 71.0 0.1 91.0 193.0 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z)





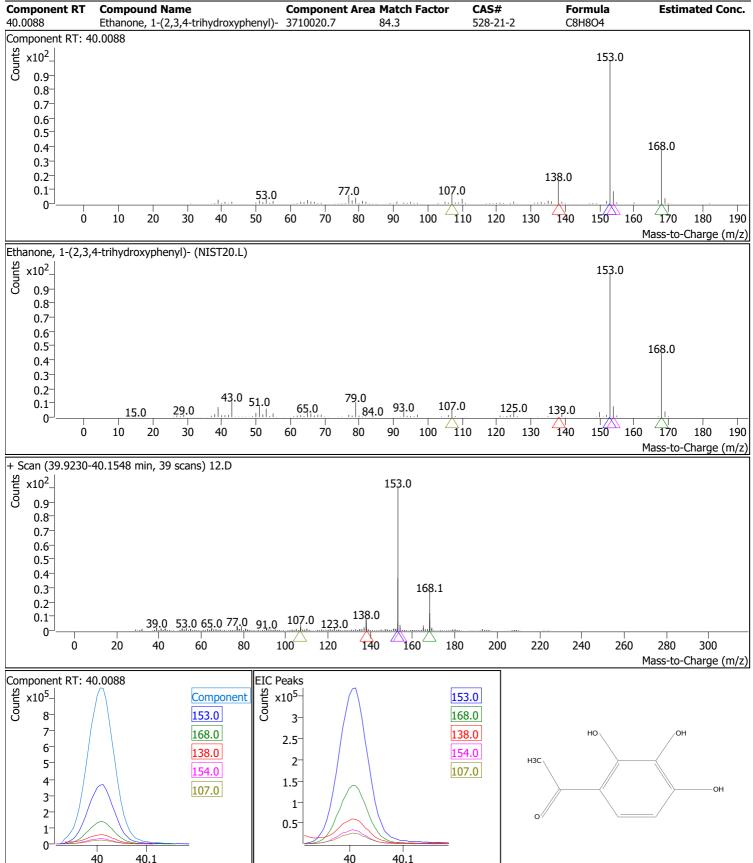




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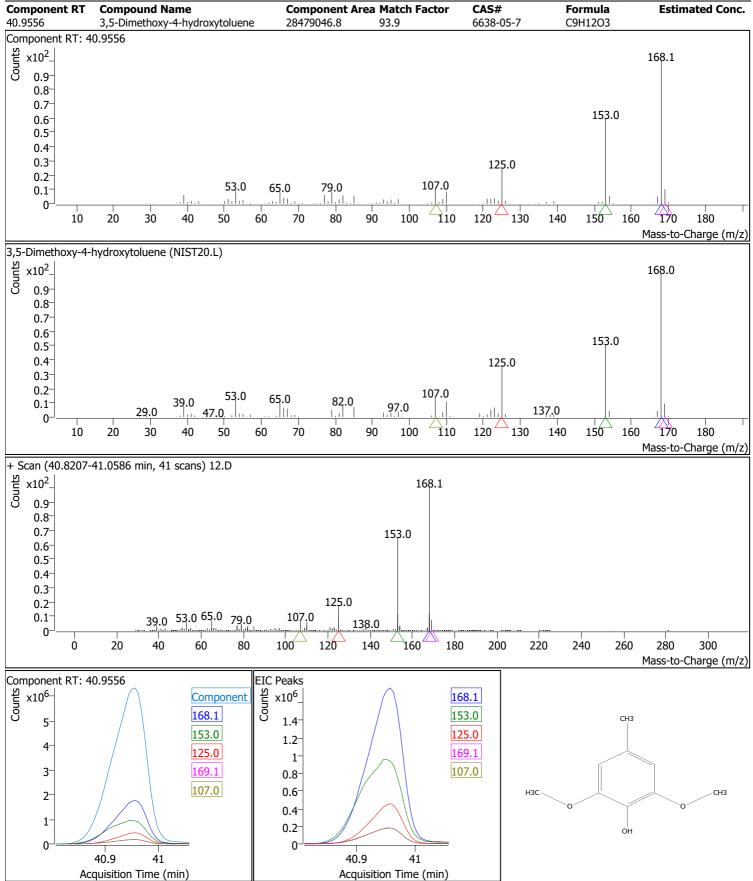




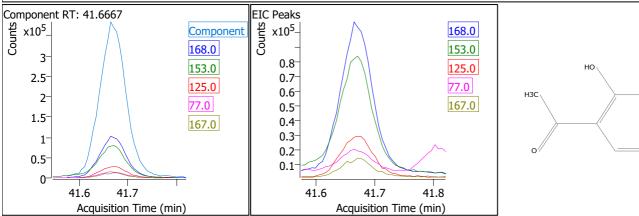
Acquisition Time (min)

Library Search Results - NonTarget Hits with Details

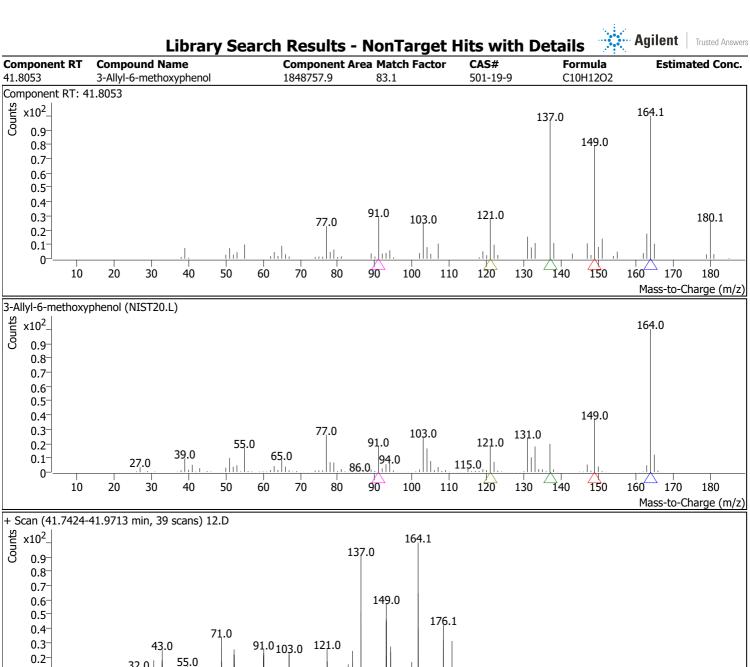


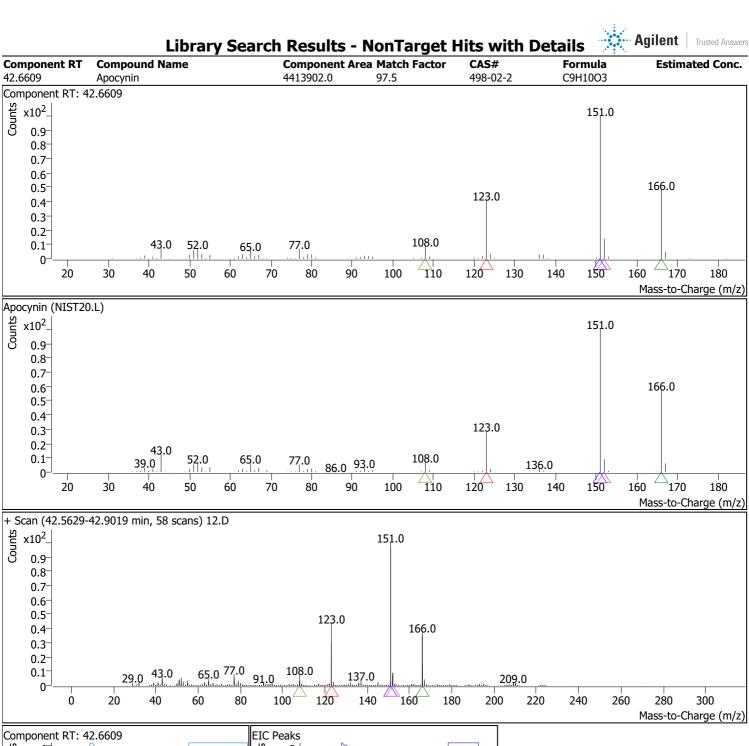


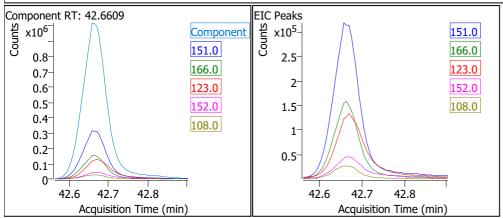
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 528-21-2 41.6667 Ethanone, 1-(2,3,4-trihydroxyphenyl)-1476330.1 C8H8O4 Component RT: 41.6667 $x10^{2}$ 168.0 0.9 153.0 0.8 0.7^{-} 0.6 0.5 0.4 125.0 0.3 0.2 77.0 0.1 20 30 60 70 80 90 100 110 120 130 140 150 160 180 Mass-to-Charge (m/z) Ethanone, 1-(2,3,4-trihydroxyphenyl)- (NIST20.L) st v10² 0.9 153.0 168.0 0.8 0.7 0.6 0.5 0.4 0.3 79.0 0.2 51.0 0.1 125.0 65.0 93.0 107.0 139.0 170 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 180 Mass-to-Charge (m/z) + Scan (41.5759-41.8197 min, 42 scans) 12.D St x10² 0.9 168.1 0.8 0.7 0.6 153.0 0.5 0.4 137.0 0.3 107.0 125.0 0.2 91.0 187.1 ^{43.0} 55.0 0.1 202.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 41.6667 Counts Counts x10⁵ x10⁵-168.0 Component 168.0 153.0 3



-OH

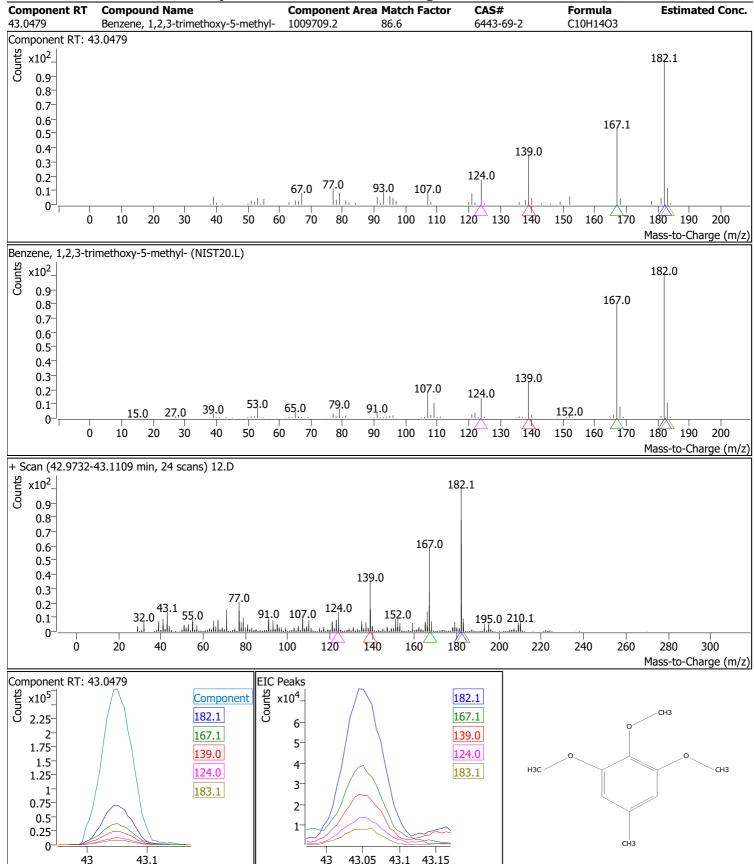






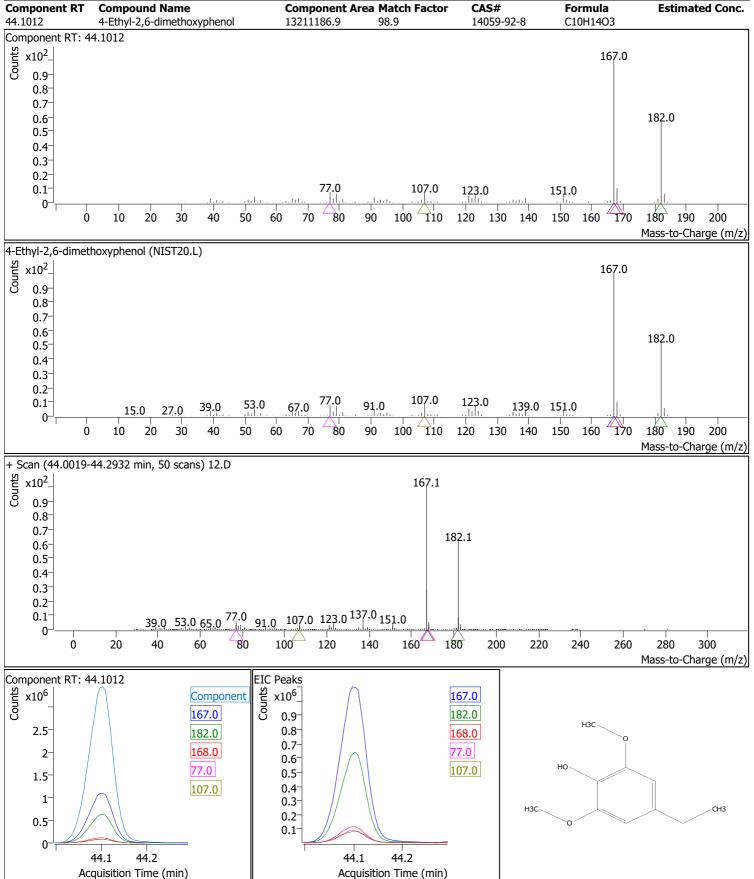
Library Search Results - NonTarget Hits with Details



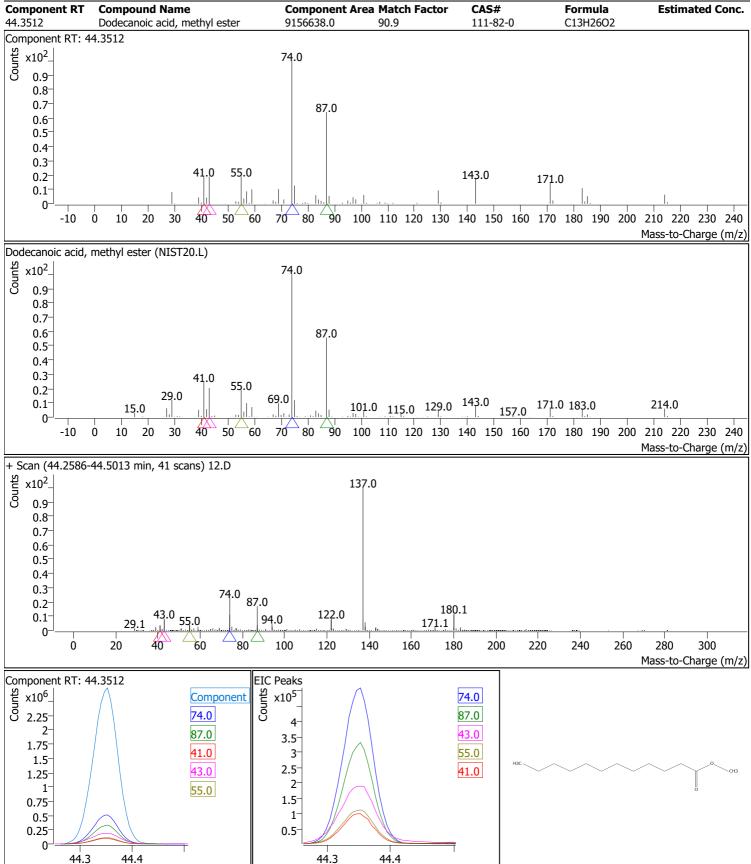


Acquisition Time (min)





Library Search Results - NonTarget Hits with Details Component Area Match Factor CAS# Formula Estimated Conc.



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.** 2-Propanone, 1-(4-hydroxy-3-44.3562 10228371.1 83.4 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3562 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 122.0 94.0 0.1 65.0 77.0 <u>53</u>.0 120 140 180 20 30 40 50 60 70 80 100 110 130 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 85.0⁹1.0 131.0 147.0 164.0 173.0 0 100 130 180 20 30 50 60 80 110 120 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2412-44.4419 min, 34 scans) 12.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 74.0 87.0 0.3 0.2 43.0 55.0 180.1 122.0 0.1 171.1 0 120 140 180 200 Ó 20 40 60 100 160 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3562 **EIC Peaks** Counts Counts x10⁶ x10⁶ 137.0 Component 180.0 137.0 1.8 180.0 122.0 1.6 0.8 1.4 138.0 122.0 1.2

44.4

Acquisition Time (min)

44.5

94.0

0.6

0.4

0.2

44.3

138.0

94.0

1

 0.8^{-}

0.6 0.4

0.2

44.3

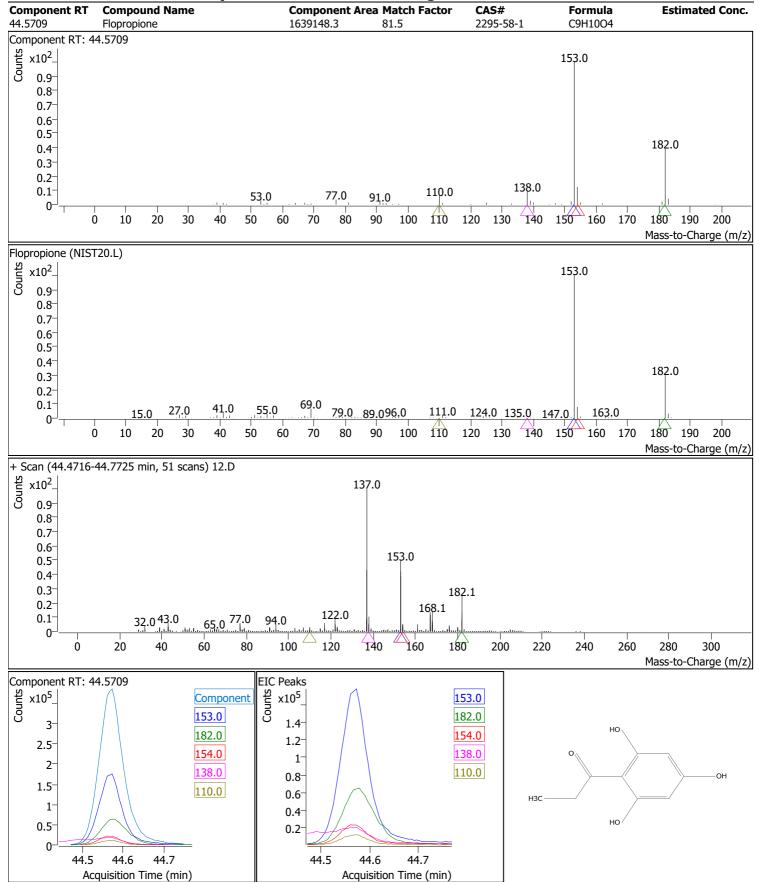
44.4

Acquisition Time (min)

44.5

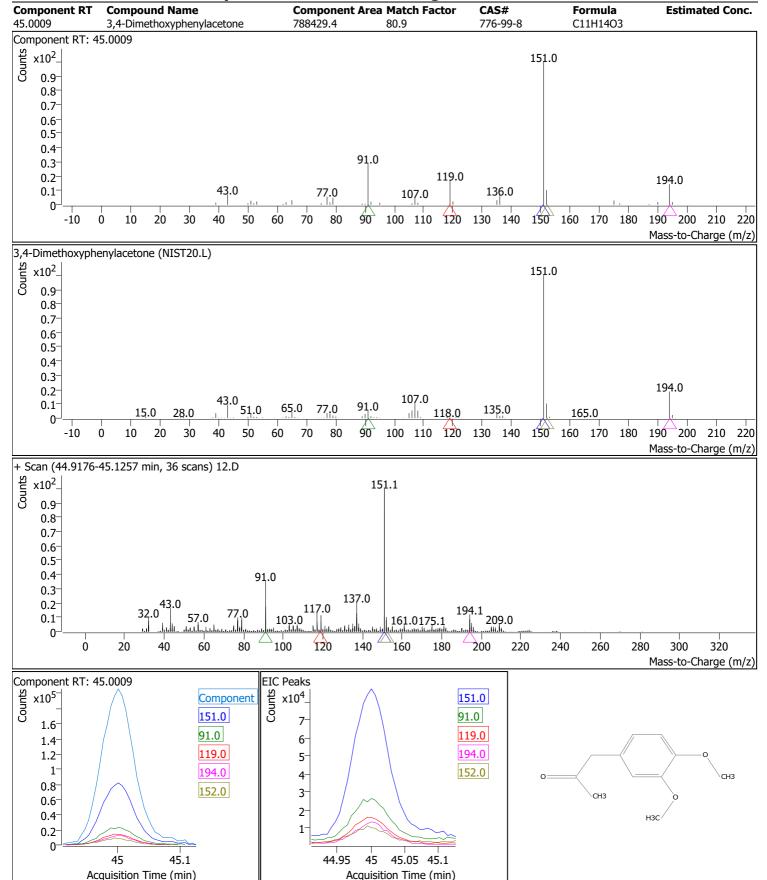






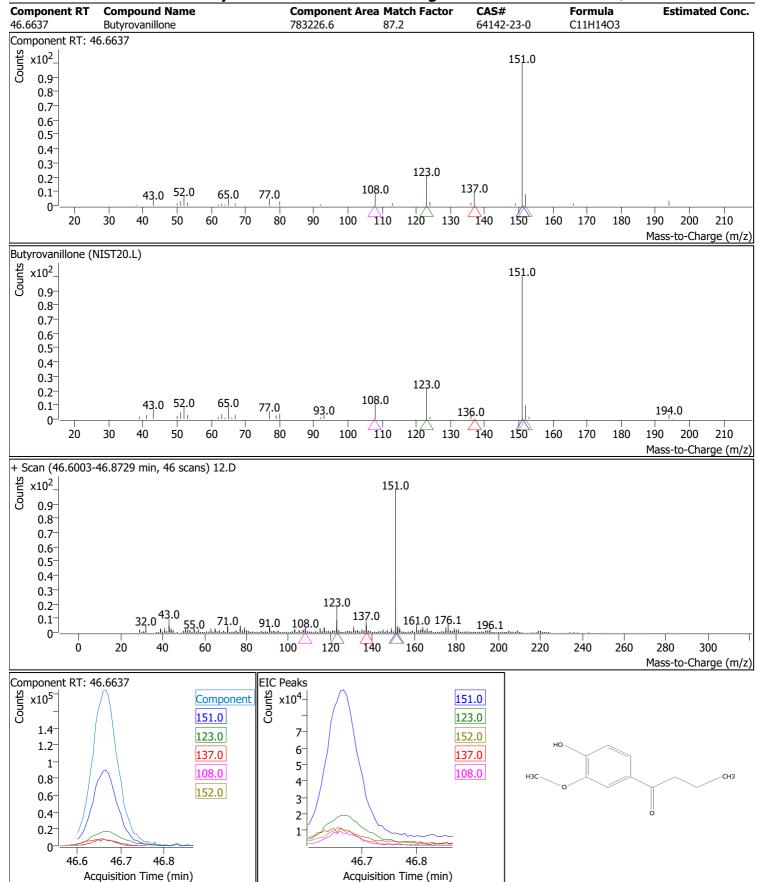












··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 47.1122 Phenol, 2-methoxy-4-methyl-6-1119199.9 80.9 201359-63-9 C11H14O2 [propenyl]-Component RT: 47.1122 x10²_ 178.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 135.0 0.3 146.0 107.0 91.0 163.0 0.2^{-} 77.0 117.0 0.1 0-150 180 30 40 50 60 70 80 90 100 110 120 130 140 160 170 190 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 0 150 180 30 50 60 70 80 90 100 110 120 130 140 160 170 190 Mass-to-Charge (m/z) + Scan (47.0322-47.2484 min, 37 scans) 12.D st x10² 178.1 0.8 0.7 0.6 0.5 150.0 0.4 135.0 0.3 77.0 91.0 167.0 117.0 0.2 39.0 194.1 65.0 0.1 0 140 0 20 40 60 80 100 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 47.1122 **EIC Peaks** Counts Counts x10⁴_ x10⁵ 178.0 Component 150.0 178.0 2.25 CH3 3.5 150.0 135.0 1.75 3-107.0 135.0 1.5 2.5



47.1

47.2

Acquisition Time (min)

146.0

146.0

107.0

2-

1

1.5

0.5

1.25

0.75

0.5

47.1

47.2

Acquisition Time (min)

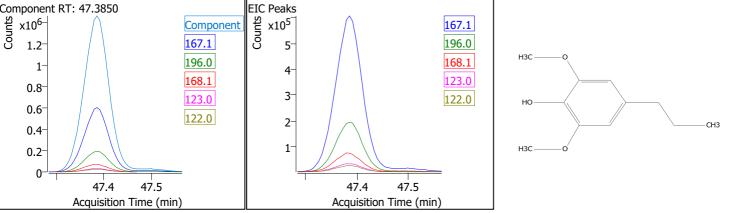
0.25

1

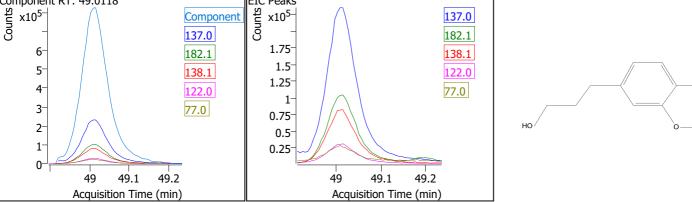
-CH3

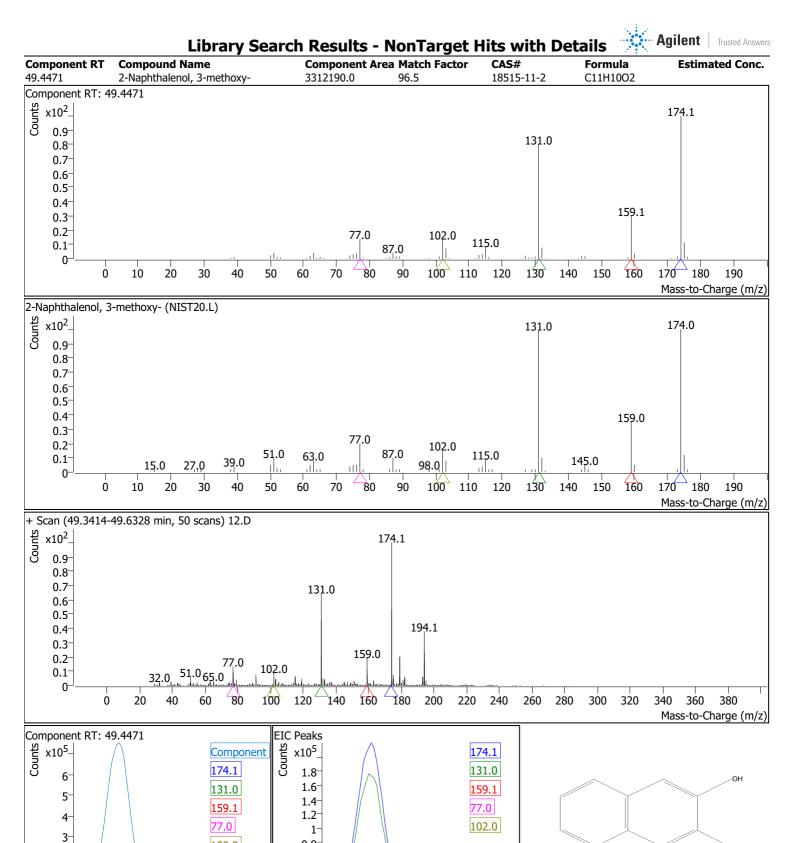
но

--- 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 47.3850 2,6-Dimethoxy-4-propylphenol 5491974.8 93.9 C11H16O3 Component RT: 47.3850 y x10² 0.9 167.1 0.8 0.7 0.6 0.5 0.4 196.0 0.3 0.2 0.1 123.0 77.0 175.0 53.0 190 200 120 130 140 150 160 170 180 10 20 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 29.0 39.0 106.0 151.0 181.0 120 130 140 150 160 170 180 190 200 10 20 50 60 70 100 110 Mass-to-Charge (m/z) + Scan (47.2841-47.5635 min, 48 scans) 12.D st x10² 0.9 167.1 0.8 0.7^{-} 0.6 0.5 0.4^{-} 196.1 0.3 151.1 0.2 0.1 65.0 77.0 91.0 107.0 123.0 137.0 43.0 175.0 29.1 200 20 40 60 80 100 120 140 160 180 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 47.3850 x10⁵ 167.1 Component



··· 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 49.0118 Benzenepropanol, 4-hydroxy-3-3998859.5 91.4 C10H14O3 methoxy-Component RT: 49.0118 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 91.0 157.1 107.0 0.1 0-**140** 180 10 20 30 40 50 60 70 90 100 110 120 130 150 160 170 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) Counts $x10^{2}$ 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 0.1 31.0 39.0 53.0 149.0 164.0 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 (48.9137-49.1511 min, 40 scans) 12.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 182.1 0.4 0.3 158.1 0.2 $39.0\,\,{}^{51.0}\,\,{}^{65.0}\,\,{}^{77.0}\,\,{}^{91.0}\,\,{}^{107.0}\,\,{}^{122.0}$ 0.1 149.0 167.0 0 80 100 180 220 20 40 60 120 140 160 200 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 49.0118 **EIC Peaks** Counts Counts x10⁵ x10⁵ 137.0 Component 182.1 137.0 1.75 6 182.1 138.1 1.5 5 122.0 138.1





49.5

Acquisition Time (min)

49.6

102.0

2

1

49.4

49.5

Acquisition Time (min)

49.6

0.8

0.6

49.4

CH3

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49.55

49.6

Acquisition Time (min)

0.4

 0.2^{-1}

1.5⁻

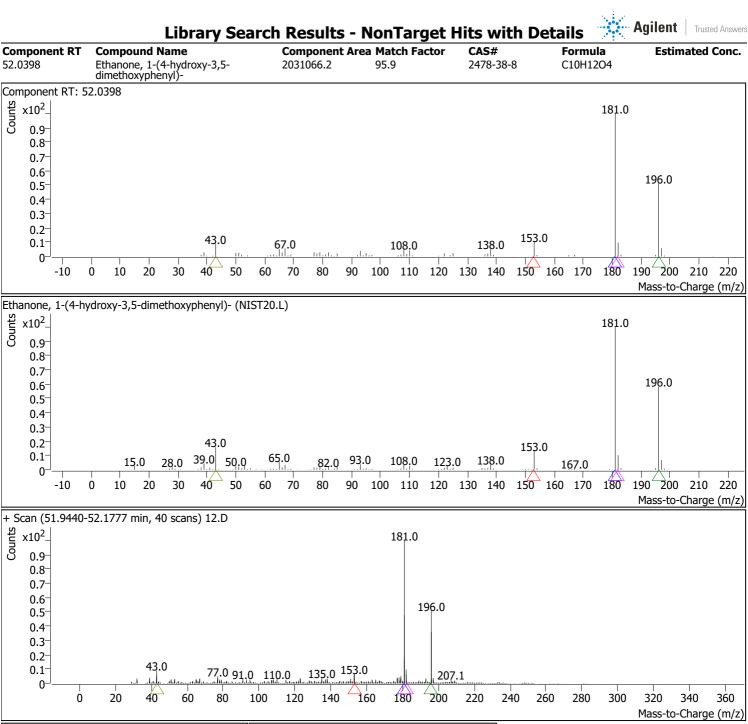
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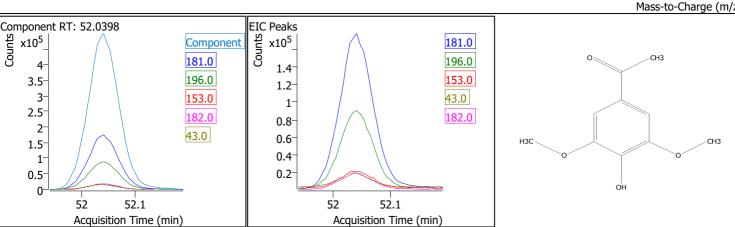
49.6

Acquisition Time (min)

49.7

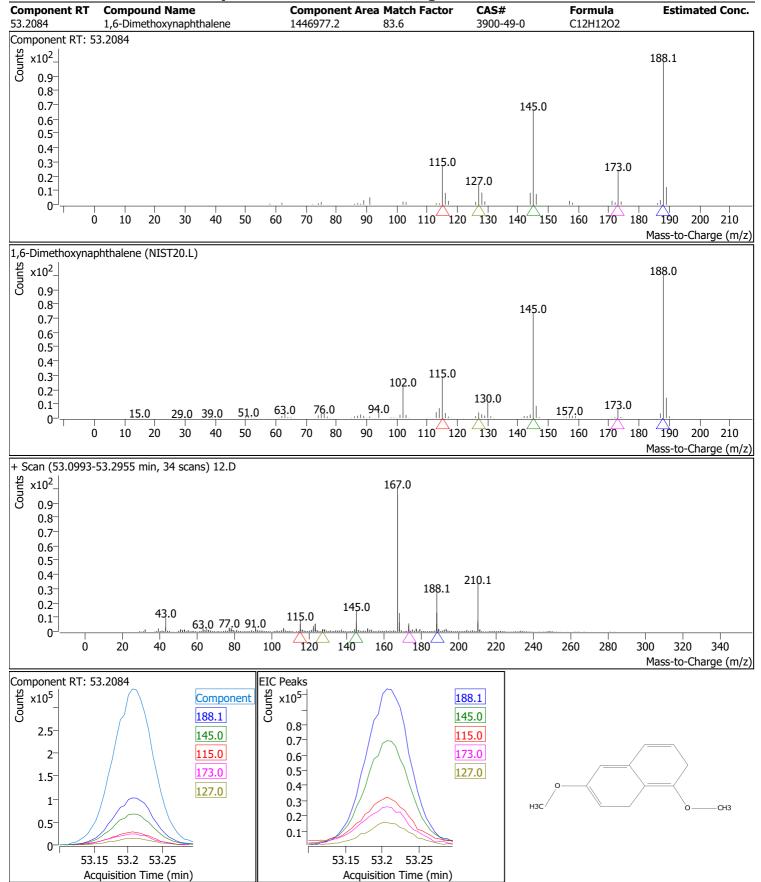
НЗС





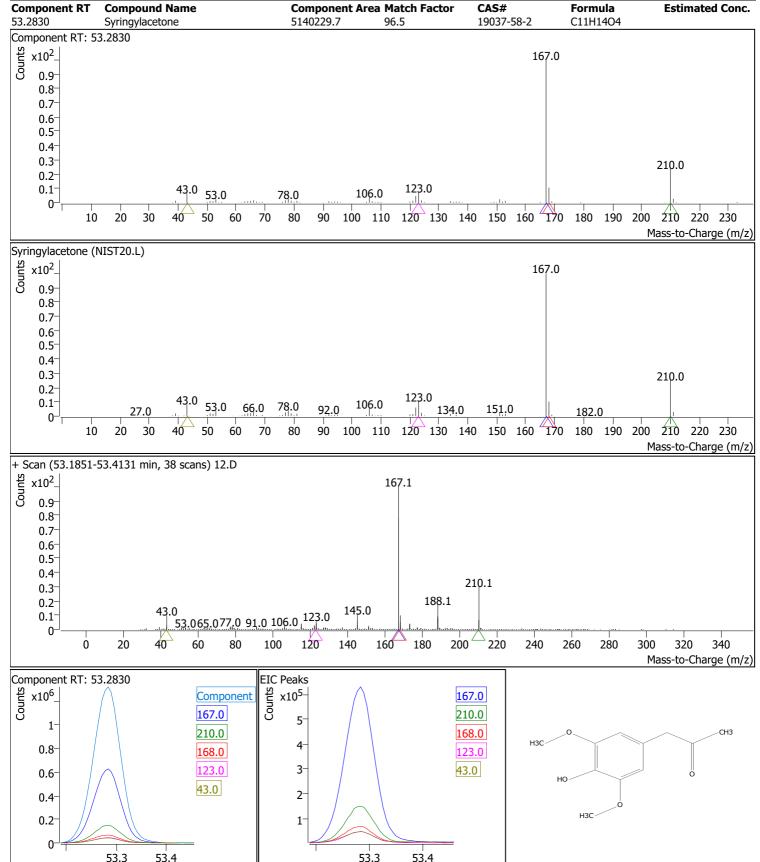




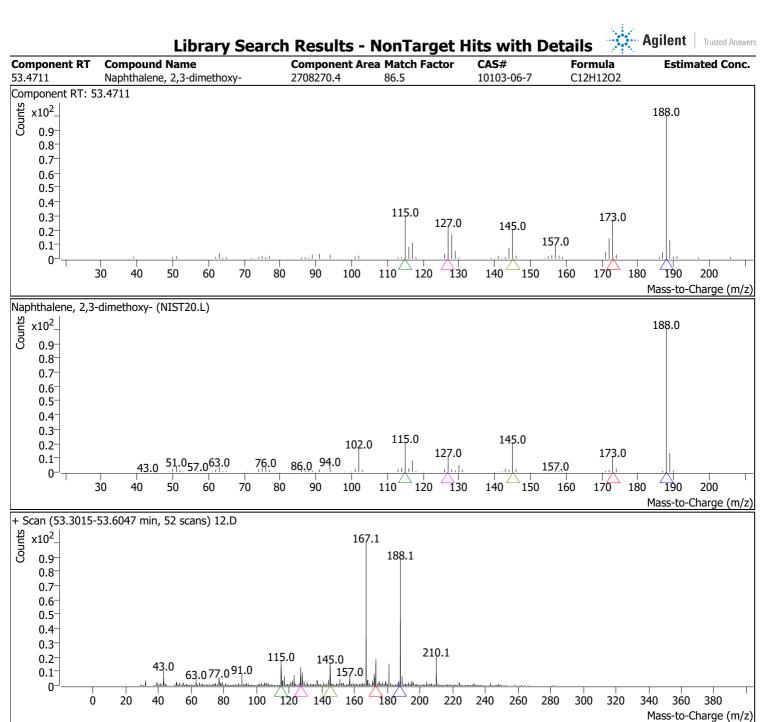


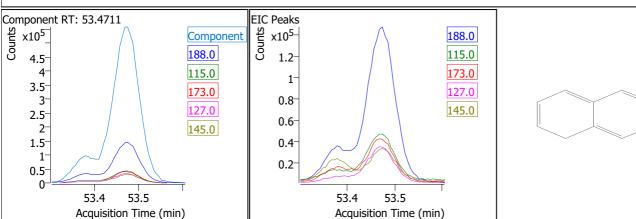






Acquisition Time (min)





CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-57.3961 828365.0 84.3 1000197-14-1 C19H28 Component RT: 57.3961 $x10^{2}$ 241.1 159.1 0.9 0.8 0.7 0.6 0.5 0.4 185.1 0.3 256.1 213.1 0.2 117.0129.0 143.0 0.1 0 40 140 160 180 240 260 0 20 60 80 100 120 200 220 280 Mass-to-Charge (m/z) 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro- (NIST20.L) $x10^{2}$ 241.0 0.9 0.8 0.7 159.0 0.6 0.5 0.4 256.0 185.0 0.3 0.2-213.0 129.0 143.0 0.1 199.0 115.0 55.0 91.0 171.0 69.0 225.0 0 240 20 100 140 160 220 60 80 120 180 200 260 280 Mass-to-Charge (m/z) + Scan (57.3151-57.5113 min, 34 scans) 12.D Counts x10²_ 159.1 0.9 241.2 0.8 0.7 0.6 212.1 168.0 0.5 202.1 0.4 77.0 91.0 0.3 185.1 115.0 141.0 0.2 256.2 0.1 180 160 200 220 240 260 0 20 40 60 80 100 120 140 280 300 320 340 360 380 Mass-to-Charge (m/z) Component RT: 57.3961 EIC Peaks 00 x10⁵ Counts x10⁴ 241.1 Component СНЗ 241.1 159.1 1.6 3 159.1 185.1 1.4 2.5 1.2 185.1 213.1 2-1 256.1 256.1

57.4 57.45

Acquisition Time (min)

1.5

0.5

1

57.35

213.1

0.8

0.6

0.4

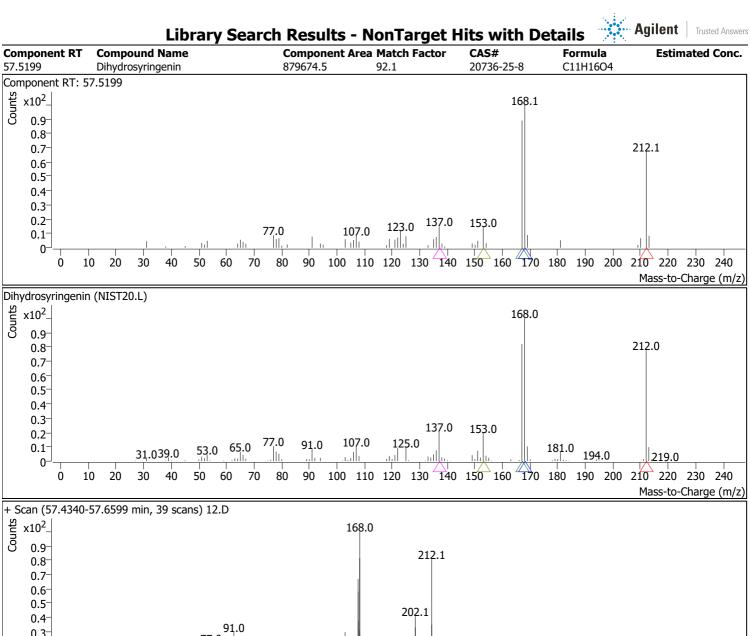
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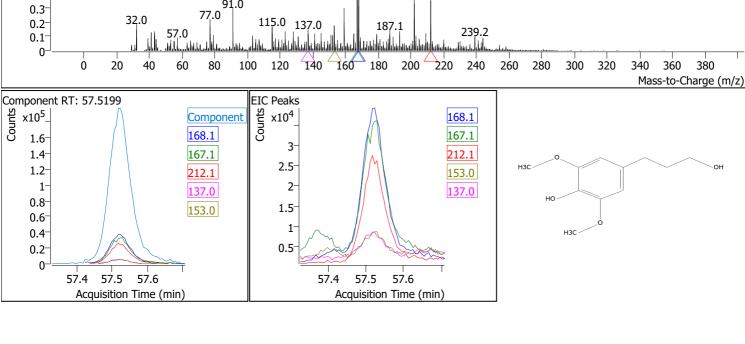
57.4

Acquisition Time (min)

СНЗ

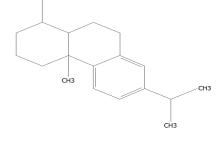
СНЗ





--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 60.1197 n-Hexadecanoic acid 1926956.5 88.9 57-10-3 C16H32O2 Component RT: 60.1197 $x10^{2}$ 73.0 0.9 60.0 0.8 43.0 0.7^{-} 55.0 256.1 0.6 129.0 0.5 0.4 0.3 0.2 0.1 0 20 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) n-Hexadecanoic acid (NIST20.L) st x10² 0.9 43.0 60.0 0.8 0.7 0.6 0.5 29.0 256.0 0.4 129.0 0.3 97.0 213.0 0.2 115.0 157.0 171.0 185.0 0.1 143.0 227.0 199.0 40 20 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) + Scan (60.0224-60.3356 min, 53 scans) 12.D St x10² 0.9 73.0 43.1 0.8 0.7 241.2 57.1 0.6 0.5 256.2 0.4^{-} 129.0 159.1 213.1 0.3 185.1 32.0 83.1 0.2 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 -20 Mass-to-Charge (m/z) EIC Peaks Component RT: 60.1197 Counts Counts x10⁴ 73.0 Component 73.0 43.0 3 3.5 60.0 60.0 2.5 3

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-60.3580 1230707.6 89.7 1000197-14-1 C19H28 Component RT: 60.3580 $x10^{2}$ 159.1 241.1 0.9 0.8 0.7 0.6 0.5 0.4 185.1 256.1 0.3 117.0 143.0 0.2 0.1 0 40 140 160 200 240 0 20 60 80 100 120 180 220 260 280 Mass-to-Charge (m/z) 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro- (NIST20.L) $x10^{2}$ 241.0 0.9 0.8 0.7 159.0 0.6 0.5 0.4 256.0 185.0 0.3 0.2-213.0 129.0 143.0 199.0 0.1 55.0 91.0 115.0 171.0 69.0 225.0 0 240 20 100 140 220 60 80 120 160 180 200 260 280 Mass-to-Charge (m/z) + Scan (60.2762-60.4827 min, 35 scans) 12.D Counts x10² 241.2 0.9 159.1 0.8 0.7 0.6 0.5 0.4 185.1 0.3 128.0 256.2 0.2 41.1 91.0 213.1 0.1 160 180 200 240 220 260 280 300 360 380 400 -20 0 20 40 60 80 100 120 140 320 340 420 440 Mass-to-Charge (m/z) Component RT: 60.3580 EIC Peaks Counts x10⁴x10⁵ 159.1 Component СНЗ 159.1 241.1 2.5 4.5 241.1 185.1 2 3.5 185.1 256.1 3



60.4

Acquisition Time (min)

242.1

1.5

1-

0.5

60.3

60.4

Acquisition Time (min)

256.1

242.1

2.5

1.5

1 0.5

60.3

2

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-735959.4 61.5424 86.3 1000197-14-1 C19H28 Component RT: 61.5424 $x10^{2}$ 159.1 241.1 0.9 0.8 0.7 0.6 0.5 0.4 185.1 256.1 0.3 117.0129.0 143.0 213.1 0.2 0.1 0 140 160 180 220 240 0 20 40 60 80 100 120 200 260 280 Mass-to-Charge (m/z) 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro- (NIST20.L) $x10^{2}$ 241.0 0.9 0.8 0.7 159.0 0.6 0.5 0.4 256.0 185.0 0.3 0.2-213.0 129.0 143.0 199.0 0.1 55.0 91.0 115.0 171.0 69.0 225.0 0 240 20 100 140 220 60 80 120 160 180 200 260 280 Mass-to-Charge (m/z) + Scan (61.4478-61.6319 min, 31 scans) 12.D Counts x10² 241.2 0.9 0.8 159.1 0.7 0.6 0.5 0.4 117.0 141.1 0.3 43.0 256.2 185.1 0.2 55.0 32.0 103.0 196 1 0.1 180 200 240 260 160 220 280 300 320 360 380 0 20 40 60 80 100 120 140 340 400 420 Mass-to-Charge (m/z) Component RT: 61.5424 EIC Peaks Sounts x10⁵ Counts x10⁴ 241.1 Component СНЗ 159.1 159.1 1.4 241.1 185.1 2.5 1.2 185.1 256.1 2 1 256.1 242.1

61.55

Acquisition Time (min)

1.5

1

0.5

242.1

0.8

0.6

0.4

0.2

61.5

61.55

Acquisition Time (min)

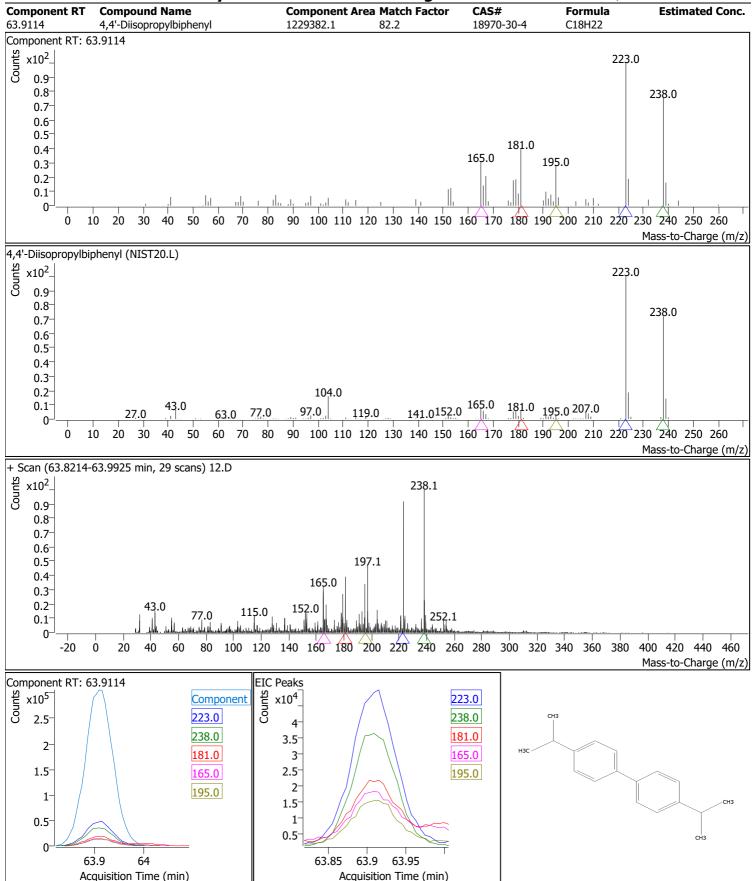
61.6

СНЗ

СНЗ

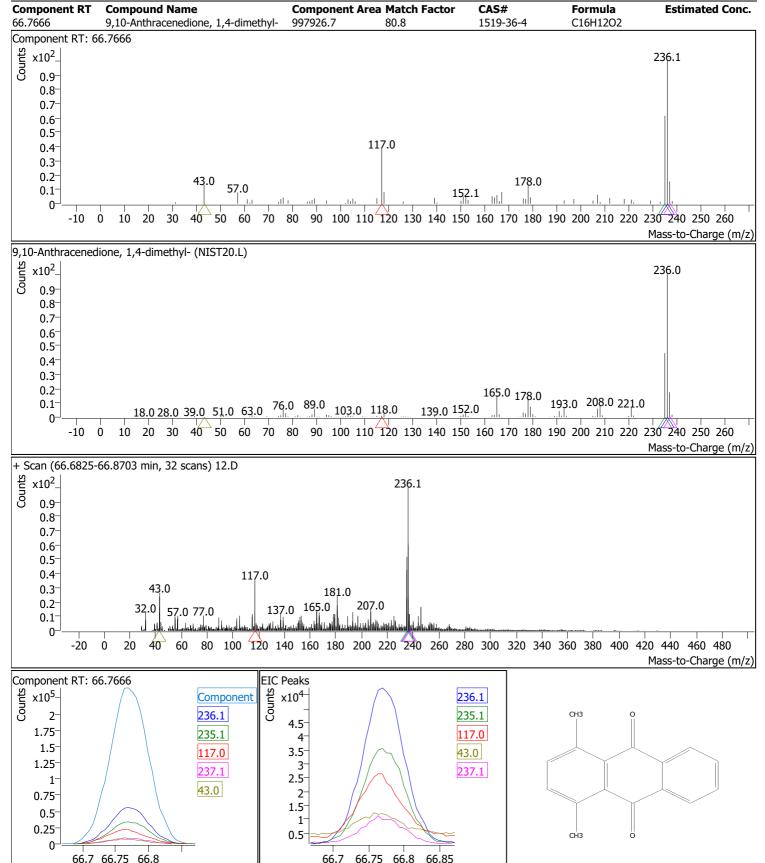






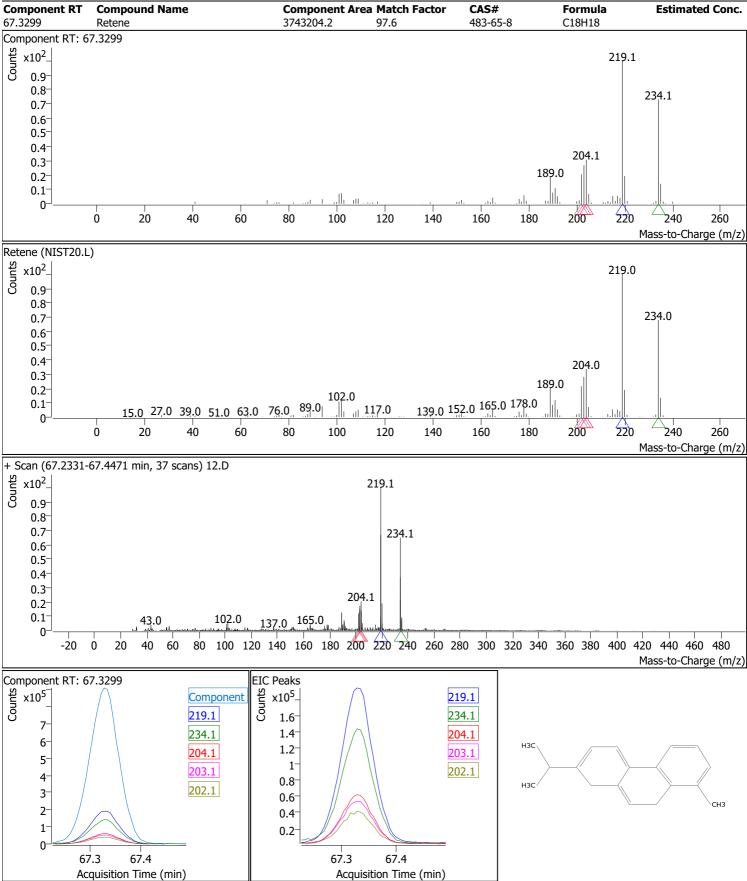




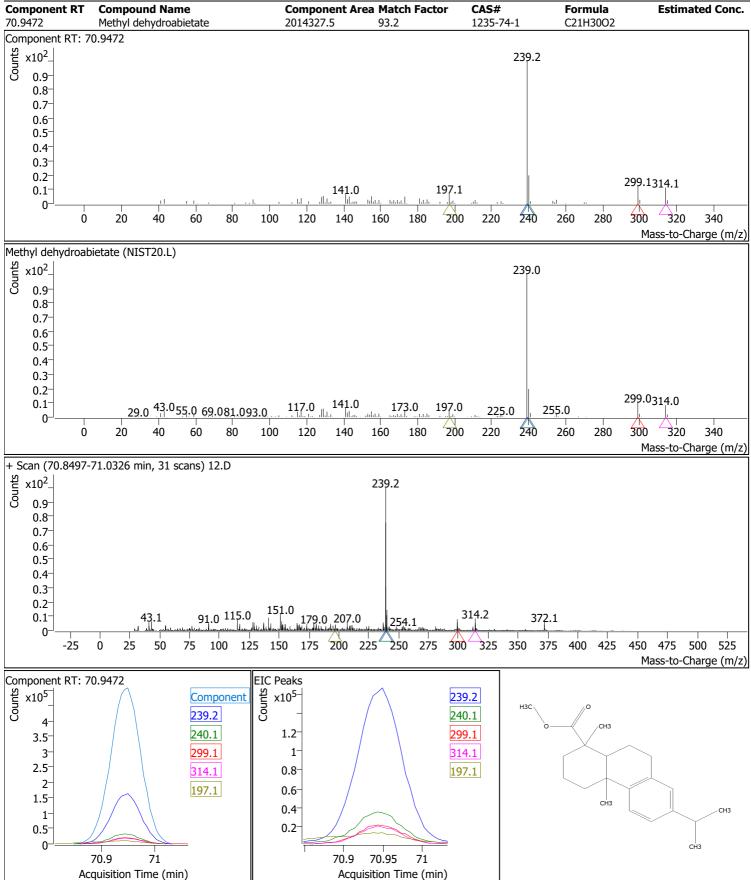


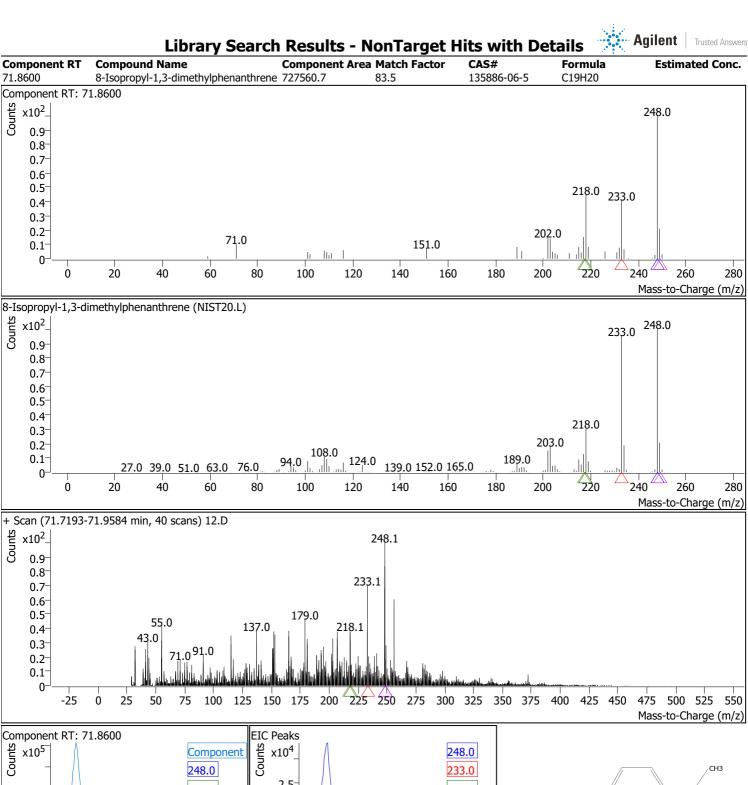
Acquisition Time (min)

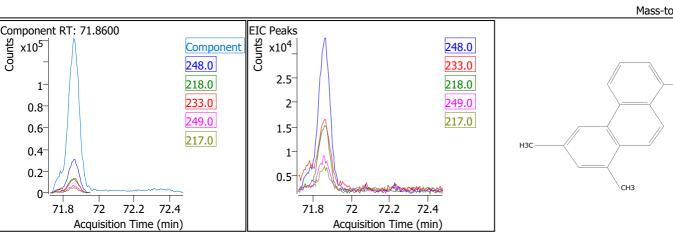




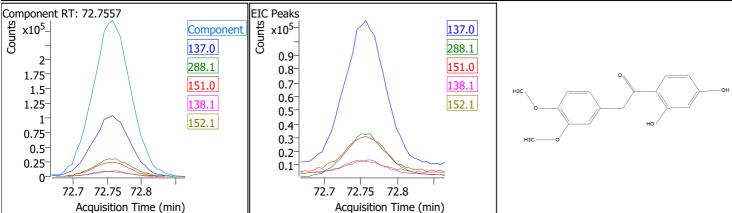


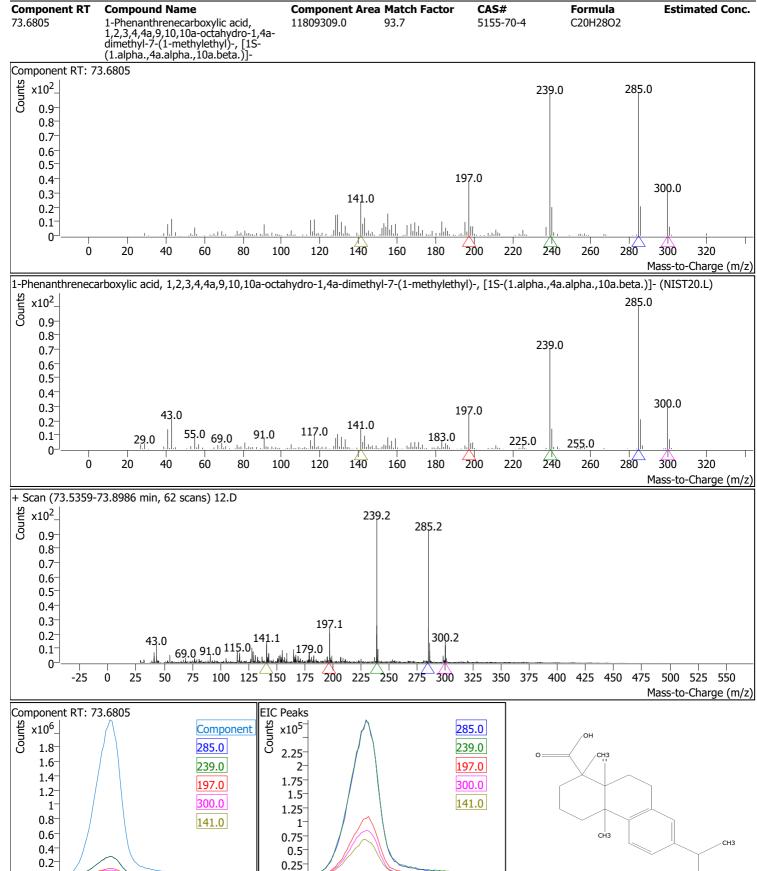






Library Search Results - NonTarget Hits with Details ··· Agilent | Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1-(2,4-Dihydroxyphenyl)-2-(3,4-dimethoxyphenyl)ethanone 1060992.0 72.7557 82.6 24126-98-5 C16H16O5 Component RT: 72.7557 Counts x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 288.1 0.3 151.0 0.2^{-} 0.1 122.0 77.0 94.0 140 -20 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) 1-(2,4-Dihydroxyphenyl)-2-(3,4-dimethoxyphenyl)ethanone (NIST20.L) x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 151.0 0.2 288.0 0.1 81.0 107.0 15.027.039.0 53.065.0 259.0 213.0228.0 n 300 -20 20 40 60 80 100 120 140 160 180 200 220 240 260 280 320 Mass-to-Charge (m/z) + Scan (72.6814-72.8640 min, 31 scans) 12.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 151.0 179.0 0.3 288.1 0.2 165.0 79.0 115.0 239.1 0.1 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 -25 25 50 100 125 Mass-to-Charge (m/z) Component RT: 72.7557 **EIC Peaks** x10⁵ 137.0 x10⁵ Component





73.7

73.8 Acquisition Time (min)

73.6

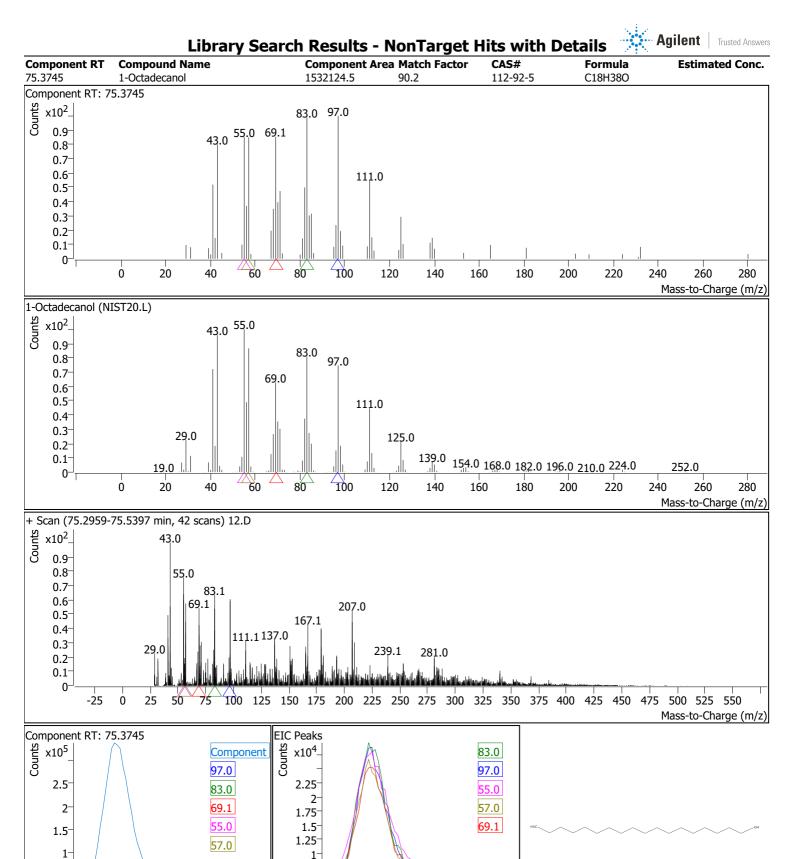
73.6

73.7

73.8

Acquisition Time (min)

СНЗ



75.4

75.5 Acquisition Time (min)

0.75

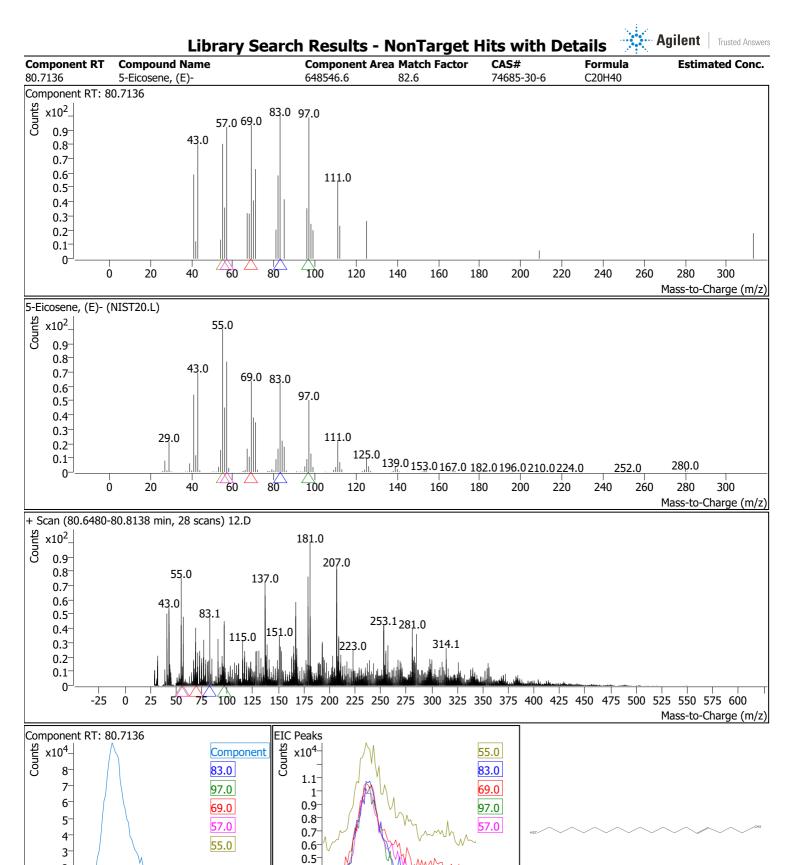
0.5 0.25

0.5

0

75.4

75.5



80.7 80.8 80.9

Acquisition Time (min)

0.4

0.3

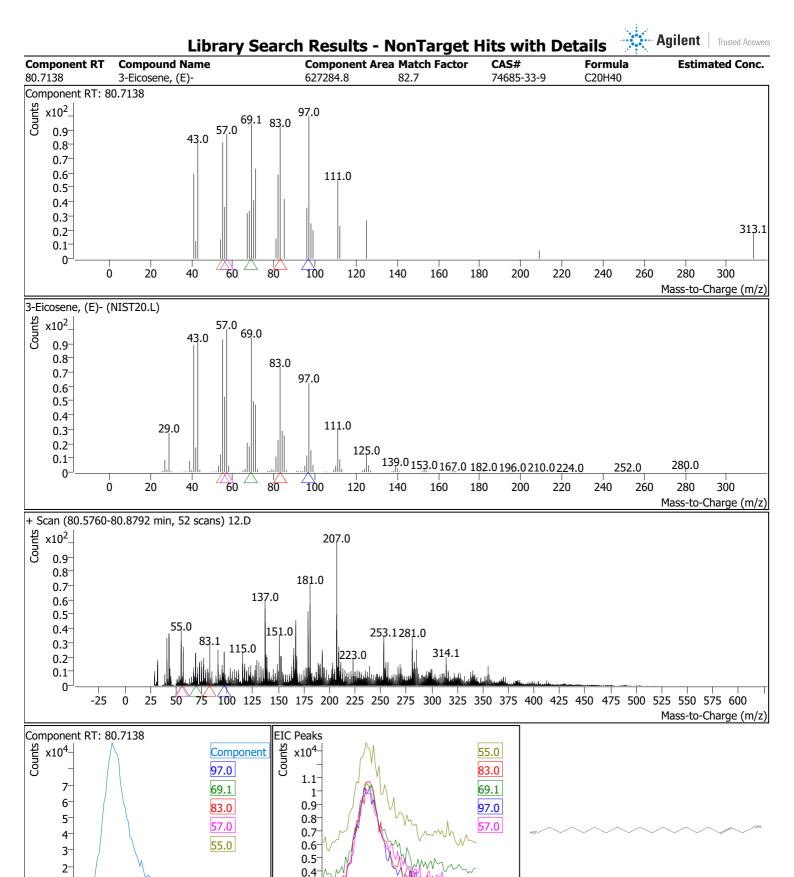
2

1

80.8

Acquisition Time (min)

81



80.7 80.8 80.9

Acquisition Time (min)

81

0.3⁻ 0.2⁻

1

80.8

Acquisition Time (min)

81