Library Search Results - NonTarget Hits with Details



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

240502 data.uaf **Analysis File Name**

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

D:\MassHunter\GCMS\1\data\RBEL\240501 scan **File Name** 14.D **Path Name Sample Name** 14 **Sample Type** Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

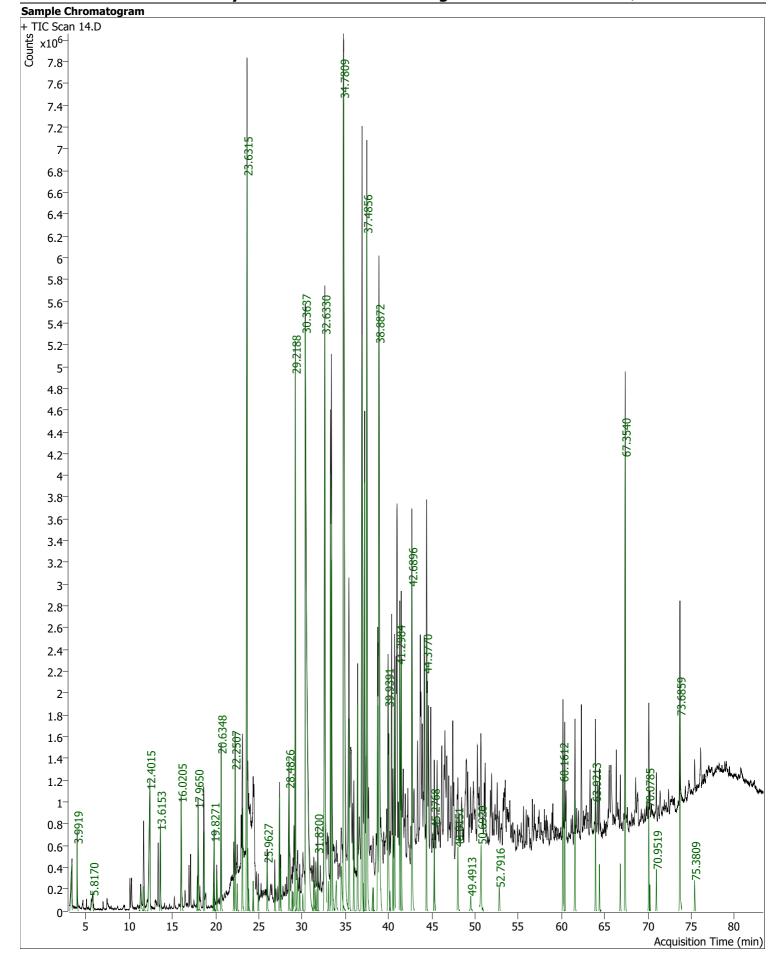
Acq. Date-Time 5/2/2024 7:46:43 AM **Instrument Name** GCMSD Dil. 1

			_			
Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
3.3936	Propanoic acid	79-09-4	C3H6O2	2778218.2	97.0	
3.9919	Propylene Glycol	57-55-6	C3H8O2	1492931.4	93.6	
5.8170	Butanoic acid	107-92-6	C4H8O2	1371472.6	87.0	
11.3347	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	1512487.0	87.0	
11.7291	2-Cyclopenten-1-one, 2-methyl-	1120-73-6	C6H8O	1014767.9	94.0	
12.4015	Butyrolactone	96-48-0	C4H6O2	9079644.3	97.6	
13.6153	2,5-Hexanedione	110-13-4	C6H10O2	3203555.7	96.5	
16.0205	2-Cyclopenten-1-one, 3-methyl-	2758-18-1	C6H8O	4829125.0	98.0	
17.8907	2-Cyclopenten-1-one, 3,4-dimethyl-	30434-64-1	C7H10O	997163.7	91.9	
17.9650	Phenol	108-95-2	C6H6O	4555984.7	97.2	
18.6617	Diisoamyl ether	544-01-4	C10H22O	2709097.1	87.4	
19.7612	2-Cyclopenten-1-one, 3,4-dimethyl-	30434-64-1	C7H10O	1072973.5	91.1	
19.8261	Propanoic acid, anhydride	123-62-6	C6H10O3	1068101.8	86.4	
19.8271	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2718055.8	93.8	
20.1347	3,6-Heptanedione	1703-51-1	C7H12O2	1327930.7	90.4	
20.6348	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	6074252.1	96.0	
22.0998	2-Cyclopenten-1-one, 3,4,5-trimethyl-	55683-21-1	C8H12O	1209804.7	94.1	
22.2507	Phenol, 2-methyl-	95-48-7	C7H8O	5293552.1	97.8	
22.5003	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	1004786.4	93.5	
23.1051	1-Octanol	111-87-5	C8H18O	4330003.4	93.8	
23.6315	Phenol, 2-methoxy-	90-05-1	C7H8O2	30767973.4	98.3	
23.7289	2-Cyclopenten-1-one, 2,3,4-trimethyl-	28790-86-5	C8H12O	2505961.1	90.5	
23.8300	Ethanone, 1-(2-thienyl)-	88-15-3	C6H6OS	776311.3	91.0	
24.3378	2-Cyclopenten-1-one, 3,4,5-trimethyl-	55683-21-1	C8H12O	1034472.6	86.4	
24.3380	2-Ethyl-3-methylcyclopent-2-en-1-one	1000423-46-8	C8H12O	1047351.0	87.3	
24.9386	Phenol, 2,5-dimethyl-	95-87-4	C8H10O	746808.7	95.6	
25.9627	2-Ethyl-3-methylcyclopent-2-en-1-one	1000423-46-8	C8H12O	1912440.1	91.2	
26.8468	Phenol, 2-ethyl-	90-00-6	C8H10O	1071359.8	92.3	
27.3827	Phenol, 2,4-dimethyl-	105-67-9	C8H10O	3882447.9	98.8	
27.5167	Phenol, 2,5-dimethyl-	95-87-4	C8H10O	1543933.7	97.5	
28.4826	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	4330808.3	95.1	
28.8421	Phenol, 2,3-dimethyl-	526-75-0	C8H10O	682887.8	91.5	
28.9574	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	668228.1	85.6	
29.2188	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	19499468.1	98.5	
29.4972	Octanoic acid	124-07-2	C8H16O2	2222956.8	94.4	
29.7328	Phenol, 3,4-dimethyl-	95-65-8	C8H10O	951301.7	92.7	
30.0870	Phenol, 3,4,5-trimethyl-	527-54-8	C9H12O	648930.6	88.0	
30.3637	Catechol	120-80-9	C6H6O2	65503490.7	98.7	
31.3539	Phenol, 2,4,6-trimethyl-	527-60-6	C9H12O	1661599.7	86.3	
31.3552	Phenol, 3-ethyl-5-methyl-	698-71-5	C9H12O	1629054.7	86.1	
31.5858	m-Guaiacol	150-19-6	C7H8O2	886403.4	86.8	
31.6095	Benzene, 1-ethyl-4-methoxy-	1515-95-3	C9H12O	736245.3	85.1	
31.8200	Benzene, 1-ethyl-4-methoxy-	1515-95-3	C9H12O	1985448.7	95.6	
32.6330	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	35219553.0	97.6	
33.0436	3,5-Dimethoxytoluene	4179-19-5	C9H12O2	973055.2	88.1	
33.2772	1,2-Benzenediol, 3-methyl-	488-17-5	C7H8O2	29487251.2	96.3	
33.3909	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	14119940.2	91.9	
33.9590	Nonanoic acid	112-05-0	C9H18O2	2233804.3	88.5	
34.5473	Hydroquinone	123-31-9	C6H6O2	4089737.7	91.6	
34.7809	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	70268551.5	97.9	
35.4166	1,3-Benzenediol, 2,5-dimethyl-	488-87-9	C8H10O2	9033536.0	91.1	
35.9752	3-Methoxy-5-methylphenol	3209-13-0	C8H10O2	3113413.6	95.0	
36.4196	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	8030761.4	88.6	
36.9177	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	25776347.2	94.6	
37.1290	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-	703-23-1	C9H10O3	928707.8	85.1	
37.2384 37.4856	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	17993408.5	89.2	
37.4856	1,3-Benzenediol, 2,5-dimethyl-	488-87-9	C8H10O2	30511359.0	92.8 95.5	
38.1844	n-Decanoic acid	334-48-5 5672 07 4	C10H20O2	1067149.3	85.5	
38.2267	2,6-Dimethoxytoluene	5673-07-4	C9H12O2	786800.4	89.2	
38.7326	1,3-Benzenediol, 4,5-dimethyl-	527-55-9	C8H10O2	9228419.3	91.2	
38.8872	4-Ethylcatechol	1124-39-6	C8H10O2	33656563.4	96.1	
39.9391	1,3-Benzenediol, 4,5-dimethyl-	527-55-9	C8H10O2	11120641.6	89.8	
40.1639	4-Formyl-3,5-dimethyl-1H-pyrrole-2-carbonitrile	1000296-05-3	C8H8N2O	757262.7	87.5	
40.5010	1,3-Benzenediol, 4-propyl-	18979-60-7	C9H12O2	2774085.0	90.2	

Library Search Results - NonTarget Hits with Details Agilent Trusted Answers



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Component	t RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
40.6868	4-Methoxy-2,6-dimethylphenol	2431-91-6	C9H12O2	8794778.3	86.4	
41.2984	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	10663387.7	90.7	
41.4560	1,4-Benzenedicarboxaldehyde, 2,5-dimethyl-	7044-92-0	C10H10O2	10145575.8	85.2	
42.6896	1,3-Benzenediol, 4-propyl-	18979-60-7	C9H12O2	14007415.2	86.5	
44.3770	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	7644054.6	93.2	
45.2768	Benzofuran, 5-methoxy-6,7-dimethyl-	35355-35-2	C11H12O2	3244496.8	86.7	
45.2768	2,2'-Isopropylidenedifuran	17920-88-6	C11H12O2	3222981.3	85.8	
48.0151	1-Methyl-2-naphthol	1076-26-2	C11H10O	3001062.8	93.3	
49.4913	3,4,5-Trihydroxyphthalaldehyde	16790-41-3	C8H6O5	795778.9	85.6	
50.6920	3,4-dihydroxyphenyl-2-propanone	1000378-94-2	C9H10O3	4067860.1	88.3	
52.7916	1,8-Naphthyridine, 2,4,7-trimethyl-	14757-44-9	C11H12N2	1253420.5	85.9	
60.1612	n-Hexadecanoic acid	57-10-3	C16H32O2	5177133.8	90.8	
60.3656	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	3895614.3	92.0	
61.5501	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	4299622.6	91.0	
63.9213	3,4'-Diisopropylbiphenyl	61434-46-6	C18H22	4111694.5	86.1	
64.3733	Heptadecane, 2,6,10,15-tetramethyl-	54833-48-6	C21H44	1599453.9	87.0	
66.7896	9,10-Anthracenedione, 1,4-dimethyl-	1519-36-4	C16H12O2	1739380.0	86.3	
67.3540	Retene	483-65-8	C18H18	17272680.7	97.7	
70.0785	8-Isopropyl-1,3-dimethylphenanthrene	135886-06-5	C19H20	4120443.3	92.3	
70.2000	Pentadecane, 2,6,10-trimethyl-	3892-00-0	C18H38	863510.4	87.0	
70.2009	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	C20H42	877118.8	86.5	
70.9519	Methyl dehydroabietate	1235-74-1	C21H30O2	1530460.2	90.8	
73.6859	Dehydroabietic acid	1740-19-8	C20H28O2	9285071.9	94.2	
75.3809	n-Heptadecanol-1	1454-85-9	C17H36O	1252705.5	90.7	



-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2778218.2 79-09-4 C3H6O2 3.3936 Propanoic acid 97.0 Component RT: 3.3936 y x10² 0.9 74.0 0.8 0.7 29.0 0.6 0.5 45.0 0.4 57.0 0.3 0.2 0.1 42.1 15 20 35 40 55 70 10 25 45 50 65 80 Mass-to-Charge (m/z) Propanoic acid (NIST20.L) Square x10² 0.9 28.0 0.8 74.0 0.7 0.6 45.0 0.5 0.4 0.3 57.0 0.2 55.0 0.1 15.0 42.0 53.0 15 10 20 25 30 35 40 45 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.1143-3.4379 min, 55 scans) 14.D st x10² 0.9 0.8 29.1 0.7 45.0 0.6 0.5 0.4 0.3 57.0 0.2 0.1 60 20 40 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.3936 stuno x10⁵x10⁵-Component 74.0 74.0 29.0 0.9 3.5 ОН 0.8 73.0 73.0 3 0.7 45.0 2.5 29.0 0.6 57.0 2 45.0 0.5

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Acquisition Time (min)

3.4

57.0

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0.5

1

3.2

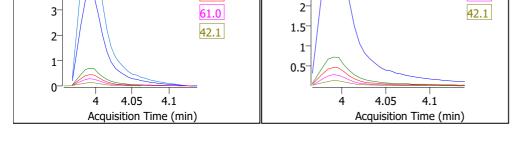
3.3

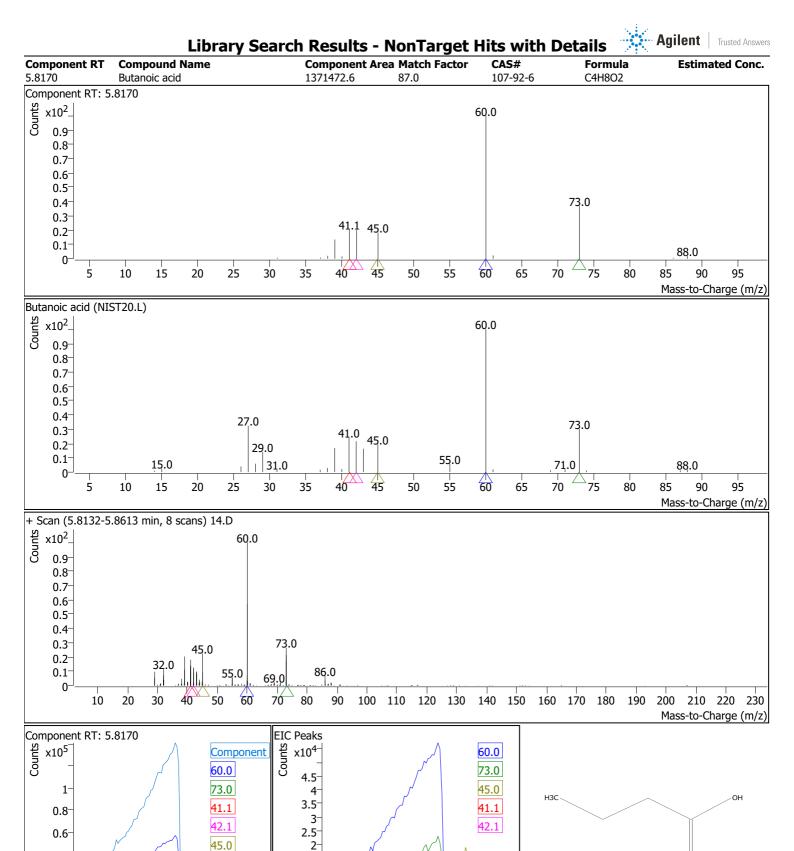
Acquisition Time (min)

3.4

CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1492931.4 57-55-6 3.9919 Propylene Glycol 93.6 C3H8O2 Component RT: 3.9919 y x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 31.0 61.0 0.1 29.0 39.0 15 25 30 70 75 5 10 20 35 40 50 55 60 65 80 Mass-to-Charge (m/z) Propylene Glycol (NIST20.L) Square x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 27.0 31.0 15.0 _{18.0} 0.1 41.0 33.0 76.0 40 75 5 10 20 25 30 35 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.9612-4.1395 min, 30 scans) 14.D st x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 61.0 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.9919 St x10⁵ St x10⁵ 45.0 Component 45.0 43.0 5 3 43.0 31.0 2.5 31.0 61.0





1.5⁻

5.5

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5.7

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Acquisition Time (min)

5.9

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0.2

5.5

5.6

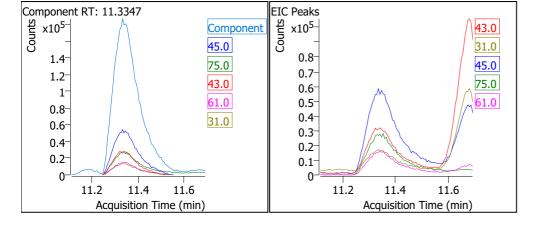
5.7

Acquisition Time (min)

5.8

5.9

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0

10

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50

60

70

80

90

100 110 120 130

140 150

160

170

180

190

200

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

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68.0

53.0

39.0

68.0

3

2.5

1.5

1

11.7

11.8

Acquisition Time (min)

11.9

1.2

1

0.8

0.6

0.4

0.2

11.7

11.8

Acquisition Time (min)

11.9

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12.3

12.4

Acquisition Time (min)

12.5

56.0

0.6

0.5⁻

0.3⁻ 0.2⁻ 29.0

56.0

12.2 12.3 12.4 12.5

Acquisition Time (min)

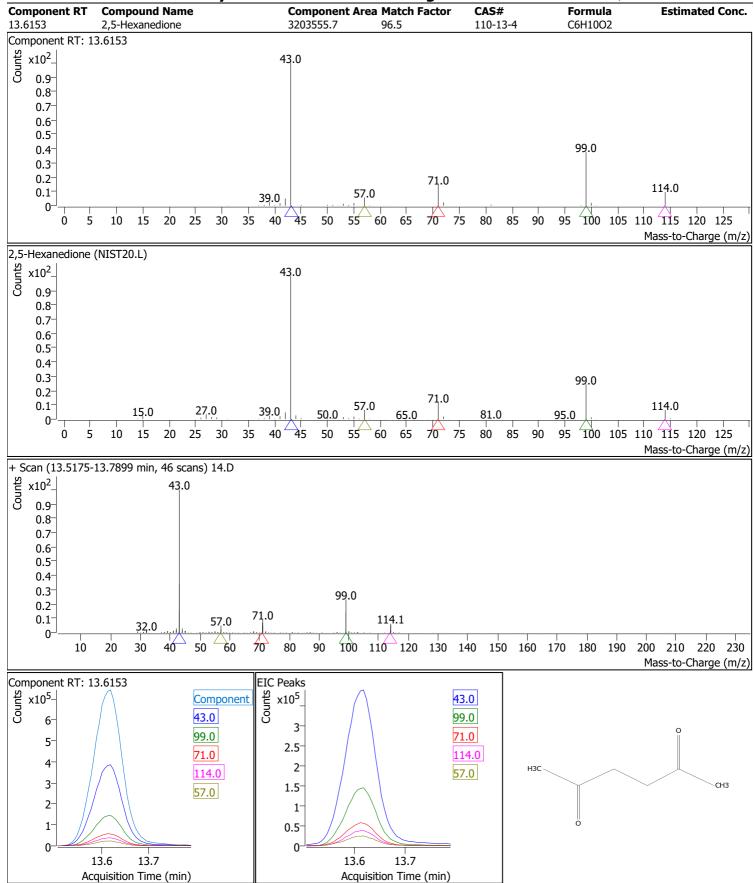
1.5

1

0.5







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16.1

Acquisition Time (min)

16.2

39.0

6

5

4

3

2-1

16.1

Acquisition Time (min)

16.2

53.0

81.0

39.0

1.25

0.75

0.5

0.25

16

1

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 17.8907 2-Cyclopenten-1-one, 3,4-dimethyl-997163.7 91.9 30434-64-1 C7H10O Component RT: 17.8907 v10² 0.9 95.0 0.8 0.7^{-} 0.6 67.0 110.0 0.5 0.4 0.3 39.0 0.2 41.1 65.0 53.0 82.0 0.1 65 95 110 20 25 30 35 40 50 55 60 80 85 90 100 105 115 120 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4-dimethyl- (NIST20.L) Counts x10²_ 0.9 95.0 0.8 110.0 67.0 0.7 0.6 0.5 39.0 0.4 0.3 0.2 82.0 53.0 65.0 0.1 31.0 77.0| 45.0 91.0 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (17.8406-17.9641 min, 21 scans) 14.D St x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 66.0 110.0 0.2 39.0 55.0 0.1 32.0 74.0 82.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 17.8907 **EIC Peaks** Counts Sounts x10⁵x10⁴ 95.0 Component 95.0 39.0 1.75 5 67.0 110.0 1.5 110.0 67.0 4 1.25

17.9

18 Acquisition Time (min)

41.1

НЗС

39.0

41.1

1

0.75

0.5

17.9

18

Acquisition Time (min)

0.25

3

2-

1

CH3

--- 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 17.9650 Phenol 4555984.7 97.2 C6H6O Component RT: 17.9650 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 50.0 495 25 10 15 20 30 35 40 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) Phenol (NIST20.L) S 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 74.0 79.0 95 10 15 20 25 30 35 40 45 50 55 60 65 70 75 85 90 100 105 Mass-to-Charge (m/z) + Scan (17.8927-18.2911 min, 68 scans) 14.D st x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 0.3 66.0 0.2 39.0 110.0 0.1 55.0 32.0 60 Ó 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 17.9650 Counts Counts x10⁵⁻ x10⁵ 94.0 Component 94.0 66.0 3 66.0 65.0 6 2.5 65.0 95.0 5 2-

18

18.1

18.2 Acquisition Time (min)

39.0

39.0

95.0

18.1 18.2

Acquisition Time (min)

1.5

1

0.5

4

3

2-

1

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 544-01-4 18.6617 Diisoamyl ether 2709097.1 87.4 C10H22O Component RT: 18.6617 v10² 0.9 70.0 43.0 0.8 0.7 0.6 0.5 0.4 0.3 41.0 55.0 0.2 39.0 0.1 53.0 85 95 20 25 30 35 40 50 55 60 65 75 90 100 105 110 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) Counts x10²_ 0.9 43.0 70.0 0.8 0.7 0.6 0.5 0.4 41.0 0.3 55.0 0.2 101.0 29.0 39.0 45.0 0.1 31.0 53.0 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (18.5706-18.7668 min, 34 scans) 14.D St x10² 57.0 103.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 29.0 0.2 0.1 131.0 Ó 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 18.6617 Counts St x10⁵ x10⁵ 70.0 Component 70.0 43.0 6 1.4 43.0 71.0 5 1.2



71.0

69.0

41.0

1

0.8

0.6

0.4

0.2

18.6

18.65

18.7

Acquisition Time (min)

4

3

2

1

0-

18.6

18.7

Acquisition Time (min)

69.0

41.0

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 30434-64-1 19.7612 2-Cyclopenten-1-one, 3,4-dimethyl-1072973.5 C7H10O Component RT: 19.7612 v10² 0.9 95.0 0.8 110.0 0.7 67.0 0.6 0.5 0.4 39.0 0.3 0.2 65.0 0.1 53.0 82.0 110 95 20 25 30 35 50 55 60 65 80 85 90 100 105 115 120 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4-dimethyl- (NIST20.L) Counts x10²_ 0.9 95.0 0.8 110.0 67.0 0.7 0.6 0.5 39.0 0.4 0.3 0.2 82.0 53.0 65.0 0.1 31.0 77.0| 91.0 110 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (19.6802-19.9025 min, 38 scans) 14.D St x10² 0.9 103.0 0.8 0.7 0.6 0.5 57.0 0.4^{-} 0.3 95.0 29.0 43.0 0.2 110.1 67.0 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: 19.7612 Counts x10⁵ x10⁴ 95.0 Component 95.0 110.0 1.8 1.6 110.0 67.0 1.4 67.0 39.0 1.2



19.8

Acquisition Time (min)

19.9

65.0

НЗС

3

2

1

19.7

39.0

65.0

1⁻ 0.8⁻

0.6⁻ 0.4⁻

0.2

19.7

19.8

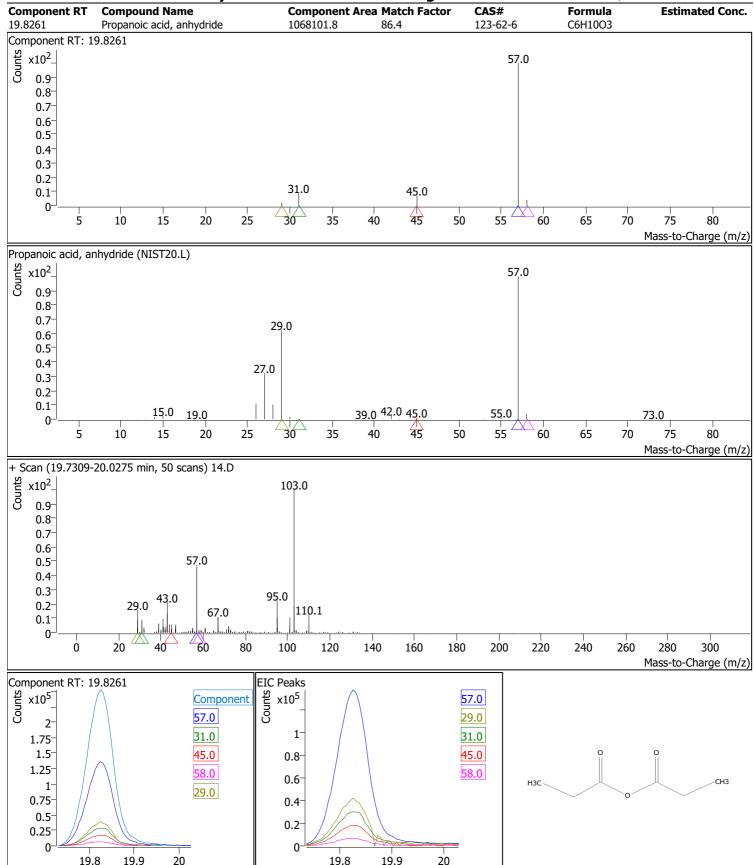
Acquisition Time (min)

19.9

CH3

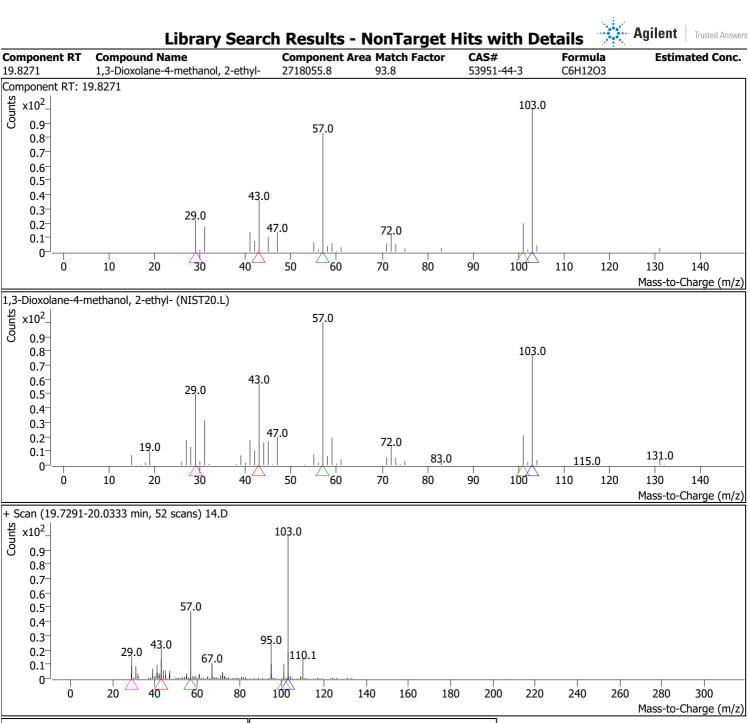
Library Search Results - NonTarget Hits with Details

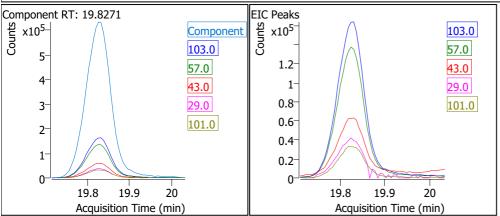




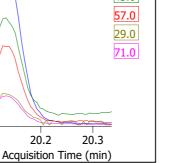
Acquisition Time (min)

Acquisition Time (min)





Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 1703-51-1 20.1347 3,6-Heptanedione 1327930.7 90.4 C7H12O2 Component RT: 20.1347 v10² 0.9 99.0 0.8 0.7^{-} 43.0 0.6 57.0 0.5 0.4 0.3 71.0 29.0 0.2 0.1 55.0 85.0 30 100 55 85 20 25 35 40 45 50 60 65 70 75 80 90 95 105 Mass-to-Charge (m/z) 3,6-Heptanedione (NIST20.L) S x10² 0.9 43.0 0.8 0.7 57.0 99.0 0.6 29.0 0.5 0.4 0.3 0.2 71.0 0.1 55.0 39.0 81.0 85.0 95.0 67.0 100 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 105 Mass-to-Charge (m/z) + Scan (20.0452-20.3365 min, 50 scans) 14.D st x10² 0.9 43.0 99.0 0.8 0.7 0.6 0.5 0.4 57.0 0.3 29.1 0.2 71.0 0.1 112.0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.1347 Counts Counts x10⁵ x10⁵ 99.0 Component 99.0 43.0 СНЗ 2.5 43.0 57.0 0.8 2 57.0



0.6

0.4

 0.2^{-}

20.1

71.0

29.0

1.5

0.5

1

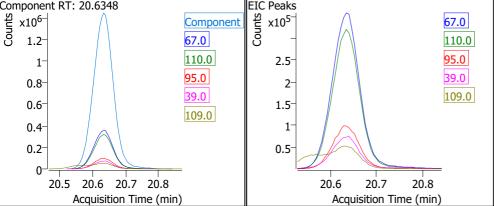
20.1

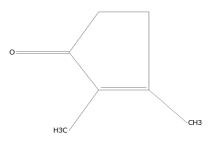
20.2

Acquisition Time (min)

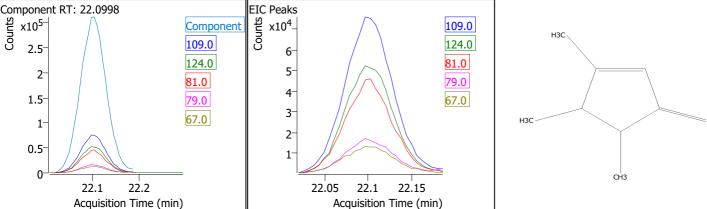
20.3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.6348 2-Cyclopenten-1-one, 2,3-dimethyl-6074252.1 96.0 1121-05-7 C7H10O Component RT: 20.6348 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 54.0 81.0 0.1 110 95 15 20 25 30 35 40 45 50 55 60 65 80 85 90 100 105 115 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 45 50 55 60 65 70 75 80 85 90 95 100 105 115 120 Mass-to-Charge (m/z) + Scan (20.5268-20.8420 min, 54 scans) 14.D St x10² 0.9 110.1 67.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 95.0 39.0 0.2 61.0 81.0 0.1 31.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.6348 Counts Str. x10⁶ x10⁵ 67.0 Component 67.0 110.0 110.0 95.0 2.5 1





--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 55683-21-1 22.0998 2-Cyclopenten-1-one, 3,4,5-trimethyl-1209804.7 C8H12O Component RT: 22.0998 $x10^{2}$ 109.0 0.9 0.8 124.0 0.7^{-} 81.0 0.6 0.5 0.4 0.3 79.0 67.0 0.2 39.0 96.0 53.0 0.1 30 35 40 45 50 55 65 70 75 80 85 90 95 100 105 110 115 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 109.0 0.8 0.7 0.6 124.0 0.5 81.0 0.4 0.3 0.2 41.0 53.0 79.0 67.0 0.1 96.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (22.0160-22.1858 min, 29 scans) 14.D st x10² 0.9 0.8 0.7^{-} 43.0 0.6 0.5 0.4^{-} 109.1 0.3 31.0 81.1 0.2 124.1 0.1 67.0 96.1 117.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z)



--- 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 22.2507 Phenol, 2-methyl-5293552.1 97.8 C7H8O Component RT: 22.2507 v10² 0.9 108.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 90.0 0.2 51.0 39.0 0.1 90 15 20 25 30 35 40 45 50 55 60 65 75 95 100 115 Mass-to-Charge (m/z) Phenol, 2-methyl- (NIST20.L) St x10²_ 0.9 108.0 0.8 0.7 0.6 0.5 0.4 79.0 0.3 90.0 0.2 39.0 51.0 27.0 0.1 63.0 43.0 74.0 29.0 68.0 86.0 90 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (22.1700-22.4593 min, 49 scans) 14.D st x10² 0.9 108.0 61.0 0.8 0.7 43.0 0.6 0.5 0.4^{-} 0.3 77.0 31.0 0.2 90.0 51.0 0.1 117.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 22.2507 **EIC Peaks** Counts Counts x10⁵-108.0 Component 108.0 107.0 2.5 1 107.0 79.0 0.8 2 77.0 77.0 НО



22.3

Acquisition Time (min)

22.4

90.0

79.0

90.0

0.6

0.4

0.2

22.2

22.3

Acquisition Time (min)

22.4

1.5

1

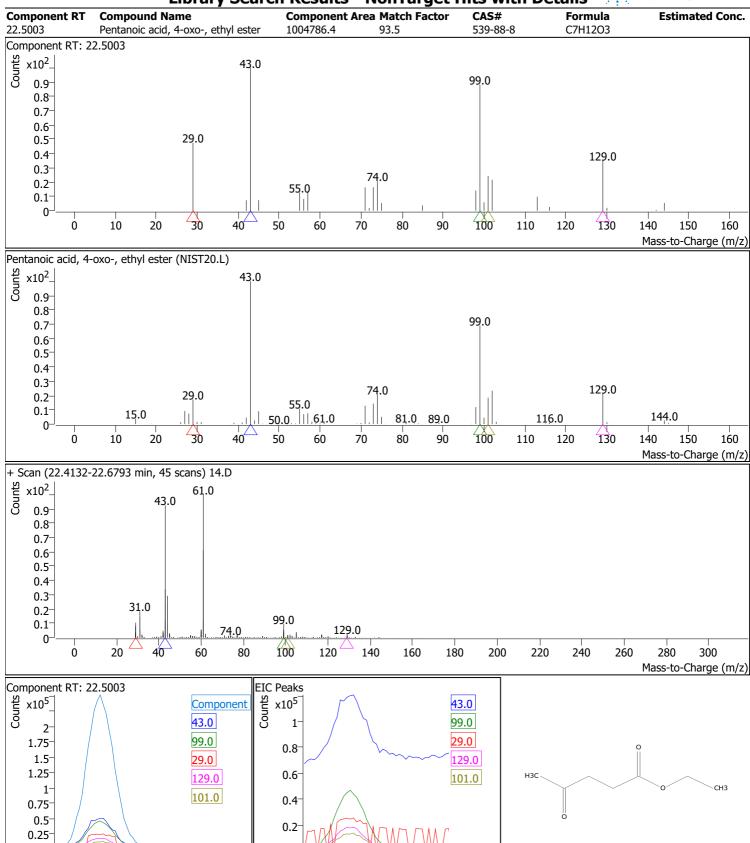
22.2

0.5

H3C







22.5

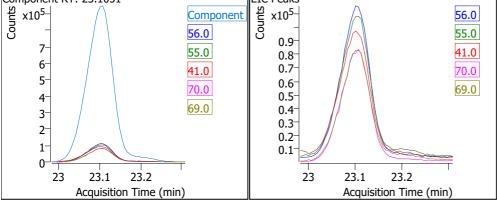
22.6 Acquisition Time (min)

22.5

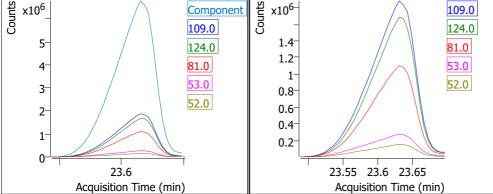
22.6

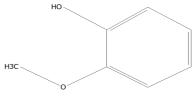
Acquisition Time (min)

--- **Agilent** Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.1051 1-Octanol 4330003.4 93.8 111-87-5 C8H18O Component RT: 23.1051 v10² 0.9 56.0 41.0 0.8 70.0 0.7^{-} 84.0 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 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 55 20 25 30 35 40 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9944-23.2439 min, 42 scans) 14.D st x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4^{-} 55.1 31.0 0.3 70.1 83.1 110.1 0.2 0.1 103.0 117.0 504 70 10 20 30 40 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 23.1051 EIC Peaks Counts x10⁵ Counts x10⁵-56.0 Component 56.0 55.0 0.9 55.0 41.0 0.8 6 0.7



--- 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 23.6315 Phenol, 2-methoxy-30767973.4 98.3 C7H8O2 Component RT: 23.6315 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 39.0 0.1 77.0 50 80 110 10 20 30 40 60 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 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4879-23.6961 min, 36 scans) 14.D st x10² 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4^{-} 0.3 61.0 0.2 53.0 0.1 31.0 39.0 77.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 23.6315 **EIC Peaks** Counts Counts x10⁶ x10⁶ 109.0 Component 109.0 124.0 1.4 5 124.0 81.0 1.2





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.7289 2-Cyclopenten-1-one, 2,3,4-trimethyl-2505961.1 90.5 28790-86-5 C8H12O Component RT: 23.7289 Counts $x10^{2}$ 109.0 0.9 81.0 124.0 0.8 0.7^{-} 96.0 0.6 0.5 0.4 67.0 0.3 79.0 29.0 0.2 53.0 39.0 0.1 0 30 35 40 45 50 55 65 70 75 80 95 100 105 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3,4-trimethyl- (NIST20.L) Counts x10²_ 0.9 109.0 0.8 0.7 0.6 81.0 0.5 124.0 0.4 0.3 0.2 79.0 96.0 67.0 0.1 41.0 45.0 53.0 91.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (23.6961-23.9514 min, 43 scans) 14.D Counts $x10^{2}$ 61.0 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 109.0 81.1 124.1 56.0 0.1

96.0

100

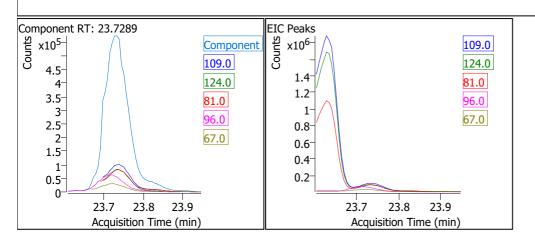
110

120 130

140 150 160

170 180

90



67.0

80

60

0

10

20

30

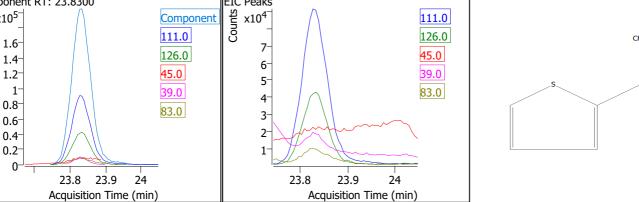
40

50

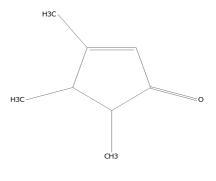
190

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

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 88-15-3 23.8300 Ethanone, 1-(2-thienyl)-776311.3 91.0 C6H6OS Component RT: 23.8300 v10² 0.9 111.0 0.8 0.7 0.6 126.0 0.5 0.4 0.3 0.2 39.0 45.0 83.0 0.1 57.0 35 55 75 80 100 105 110 115 Mass-to-Charge (m/z) Ethanone, 1-(2-thienyl)- (NIST20.L) st x10² 0.9 111.0 0.8 0.7 126.0 0.6 0.5 39.0 0.4 0.3 43.0 0.2 83.0 0.1 45.0 58.0 98.0 69.0 30 35 50 55 65 70 75 80 85 90 95 100 105 110 115 120 125 130 Mass-to-Charge (m/z) + Scan (23.7496-24.0469 min, 51 scans) 14.D st x10² 0.9 61.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 56.0 0.1 <u>7</u>3.0 81.1 111.0 10 20 30 40 50 60 70 90 100 110 120^{-/} 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 23.8300 **EIC Peaks** Counts x10⁵ x10⁴ 111.0 Component 111.0 126.0 СНЗ 1.6 7 126.0 45.0 1.4



- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 55683-21-1 24.3378 2-Cyclopenten-1-one, 3,4,5-trimethyl-1034472.6 86.4 C8H12O Component RT: 24.3378 v10² 0.9 124.0 81.0 0.8 0.7 0.6 109.0 0.5 67.0 0.4 79.0 0.3 53.0 41.1 0.2 0.1 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 120 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 109.0 0.8 0.7 0.6 124.0 0.5 81.0 0.4 0.3 0.2 41.0 53.0 79.0 67.0 0.1 96.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (24.2866-24.4061 min, 20 scans) 14.D St x10² 0.9 61.0 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 109.1 124.1 67.0 81.1 0.1 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 24.3378 Counts stuno x10⁵ 2.25 x10⁴ 124.0 Component НЗС 124.0 81.0 4.5 2.25 2 81.0 109.0 1.75 3.5 67.0 109.0



24.3

24.4 Acquisition Time (min)

79.0

3

2

1

2.5

1.5

0.5

67.0

79.0

1.5

1.25

0.75

0.25

0.5

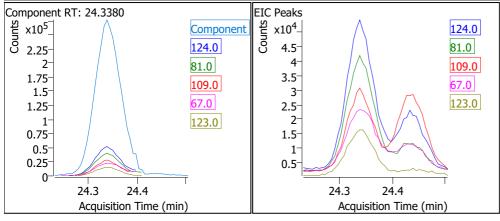
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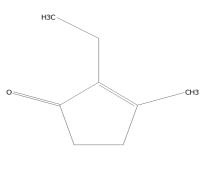
24.3

24.4

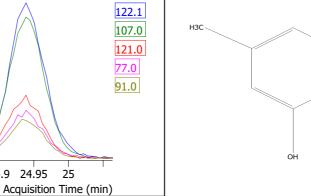
Acquisition Time (min)

- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1000423-46-8 24.3380 2-Ethyl-3-methylcyclopent-2-en-1-one 1047351.0 87.3 C8H12O Component RT: 24.3380 v10² 0.9 124.0 81.0 0.8 0.7 0.6 109.0 0.5 67.0 0.4 0.3 53.0 41.0 0.2 0.1 100 105 110 115 120 125 130 135 20 25 40 45 50 55 65 70 75 80 85 95 60 Mass-to-Charge (m/z) 2-Ethyl-3-methylcyclopent-2-en-1-one (NIST20.L) Counts x10²_ 0.9 81.0 0.8 0.7 124.0 67.0 0.6 39.0 0.5 109.0 27.0 53.0 0.4 0.3 0.2 95.0 0.1 32.0 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 (24.2866-24.4061 min, 20 scans) 14.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 0.3 31.0 0.2 109.1 124.1 0.1 67.0 81.1 0 80 Ó 20 40 60 100 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 24.3380 **EIC Peaks** x10⁴ 124.0 Component





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2.5

1.5

0.5

2

1

77.0

91.0

0.8

0.6

0.4

0.2

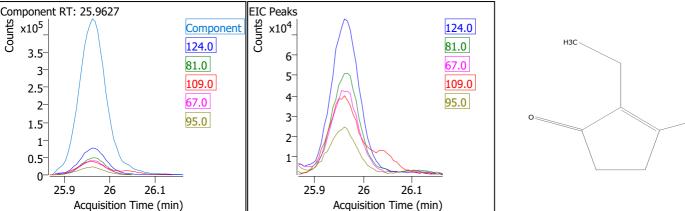
24.9

25

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.** 1000423-46-8 2-Ethyl-3-methylcyclopent-2-en-1-one 1912440.1 C8H12O Component RT: 25.9627 $x10^{2}$ 124.0 0.9 0.8 0.7^{-} 81.0 0.6 67.0 109.0 0.5 0.4 95.0 0.3 39.0 53.0 0.2 0.1 105 110 115 120 125 130 135 20 25 35 40 50 55 70 75 80 90 95 100 60 65 85 Mass-to-Charge (m/z) 2-Ethyl-3-methylcyclopent-2-en-1-one (NIST20.L) st x10²_ 0.9-81.0 0.8 0.7 124.0 67.0 0.6 39.0 0.5 109.0 27.0 53.0 0.4 0.3 0.2 95.0 0.1 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 (25.8664-26.1399 min, 47 scans) 14.D St x10² 0.9 43.0 124.1 81.1 0.8 0.7^{-} 0.6 0.5 67.0 109.1 0.4^{-} 0.3 61.0 95.0 53.0 0.2 103.0 74.0 29.0 91.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z)



-CH3

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-00-6 26.8468 Phenol, 2-ethyl-1071359.8 C8H10O Component RT: 26.8468 v10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 122.0 0.4 77.0 0.3 0.2 0.1 103.0 75 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) Phenol, 2-ethyl- (NIST20.L) Counts x10²_ 0.9 107.0 0.8 0.7 0.6 0.5 122.0 0.4 77.0 0.3 0.2 51.0 0.1 91.0 27.0 65.0 103.0 15.0 74.0 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 (26.7753-27.0258 min, 43 scans) 14.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 122.1 0.3 138.1 77.0 0.2 95.1 117.1 151.0 67.0 0.1 166.0 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: 26.8468 EIC Peaks 00 x10⁵ Counts x10⁵ 107.0 Component 107.0 122.0 0.9 2.25 0.8 122.0 77.0 0.7 1.75 77.0 79.0

26.9

Acquisition Time (min)

91.0

27

0.6

 0.5°

 0.4^{-}

0.3

0.2

26.8

79.0

91.0

27

1.5

1.25

0.75

0.5 0.25

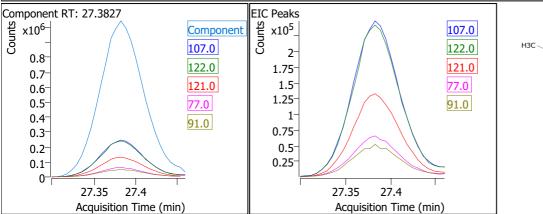
26.8

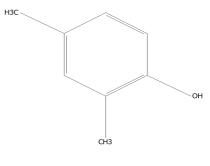
26.9

Acquisition Time (min)

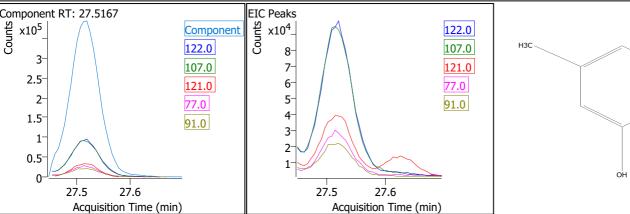
1

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Phenol, 2,4-dimethyl-27.3827 3882447.9 98.8 105-67-9 C8H10O Component RT: 27.3827 y x10² 0.9 107.0 122.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 77.0 91.0 0.2 0.1 35 50 55 70 80 85 95 100 105 110 115 120 125 130 135 75 Mass-to-Charge (m/z) Phenol, 2,4-dimethyl- (NIST20.L) Counts x10²_ 0.9 122.0 107.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 0.2 91.0 0.1 103.0 74.0 10 15 20 25 30 35 40 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (27.3045-27.4599 min, 27 scans) 14.D St x10²_ 0.9 122.1 0.8 0.7^{-} 107.0 0.6 0.5 0.4^{-} 0.3 77.0 0.2 91.0 0.1 151.0 65.0 166.0 100 110 10 20 30 40 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 27.3827 Counts Counts x10⁵ 107.0 Component 107.0 122.0 2-0.8 122.0 121.0 1.75 0.7^{-1}

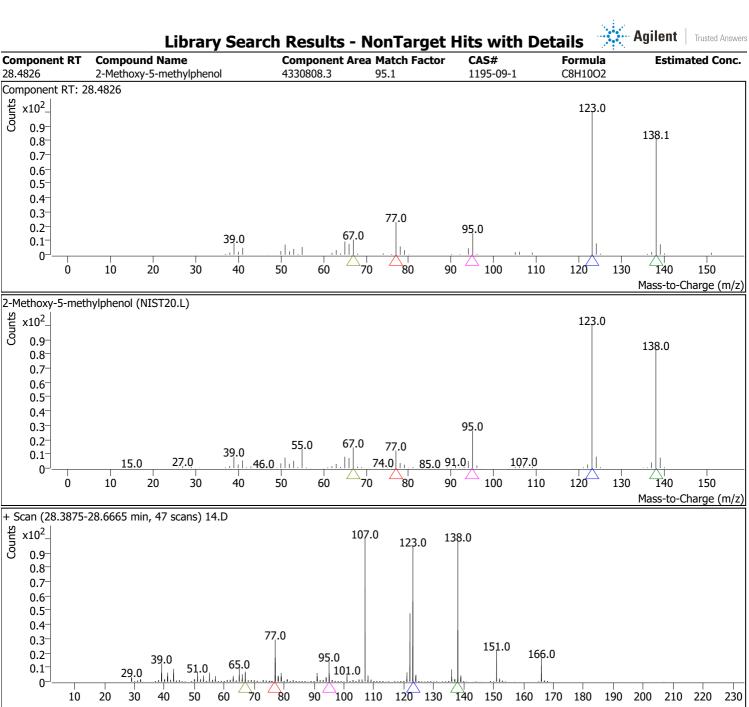


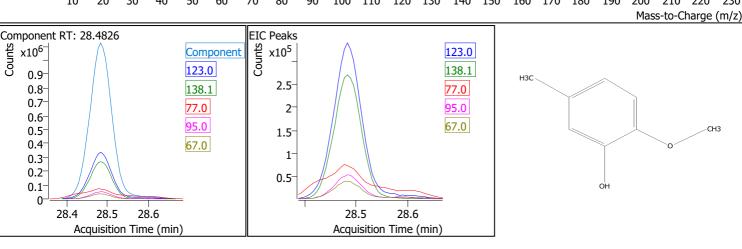


Library Search Results - NonTarget Hits with Details ··· Agilent | Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 95-87-4 27.5167 Phenol, 2,5-dimethyl-1543933.7 97.5 C8H10O Component RT: 27.5167 v10² 0.9 122.0 107.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 91.0 0.2 0.1 35 50 55 70 75 08 85 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) Phenol, 2,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 107.0 122.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 91.0 0.2 39.0 65.0 0.1 27.0 74.0 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 (27.4599-27.5788 min, 21 scans) 14.D st x10² 0.9 122.1 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 77.0 91.0 151.0 0.2 166.0 39.0 65.0 51.0 0.1 136.0 100 110 10 20 30 40 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 27.5167 Counts Counts x10⁴ 122.0 Component 122.0 107.0 8

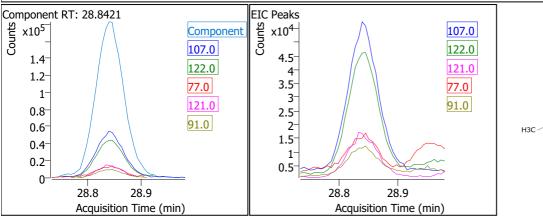


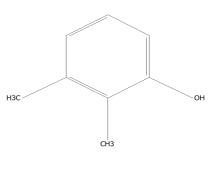
CH3

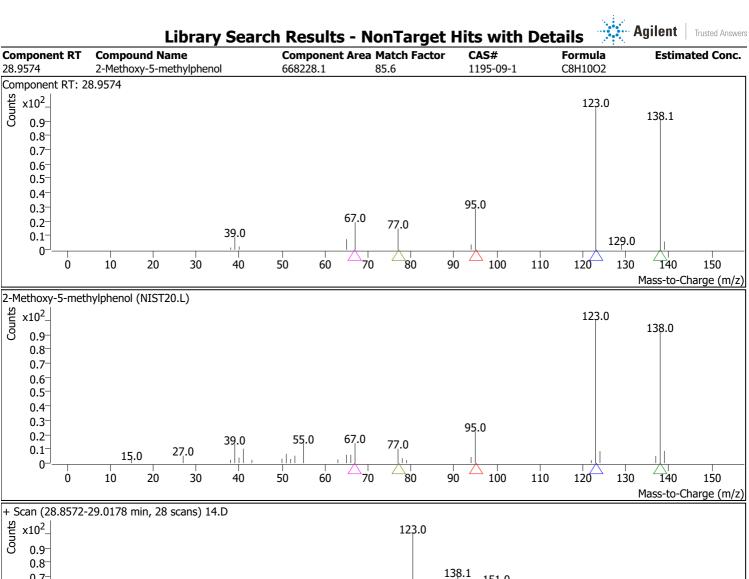


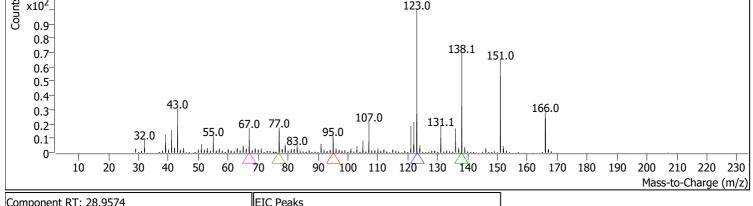


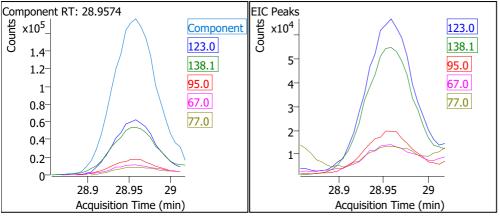
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 28.8421 Phenol, 2,3-dimethyl-682887.8 526-75-0 C8H10O Component RT: 28.8421 y x10² 0.9 107.0 122.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 77.0 91.0 0.2 79.0 103.0 39.0 0.1 100 105 110 115 120 125 130 135 75 Mass-to-Charge (m/z) Phenol, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 122.0 0.8 107.0 0.7 0.6 0.5 0.4 0.3 77.0 0.2 0.1 89.0 93.0 98.0 103.0 74.0 90 95 100 105 110 115 120 125 130 135 20 25 30 35 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (28.7839-28.8984 min, 19 scans) 14.D St x10²_ 0.9 107.0 122.1 0.8 151.0 0.7^{-} 0.6 0.5 0.4^{-} 166.0 0.3 128.0 77.0 0.2 0.1 100 110 10 20 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 28.8421 Counts Counts x10⁴ 107.0 Component 107.0 122.0 4.5 1.4 122.0 121.0

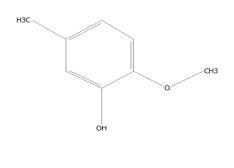


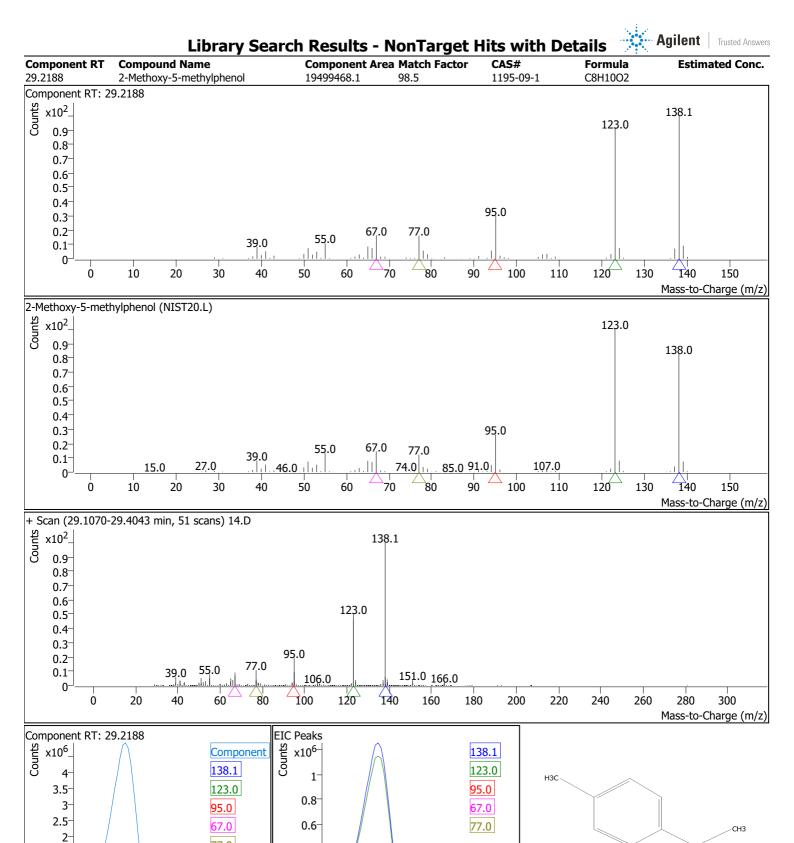












29.2

29.3

Acquisition Time (min)

77.0

1.5⁻

0.5

29.2

29.3

Acquisition Time (min)

0.4

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 124-07-2 29.4972 Octanoic acid 2222956.8 C8H16O2 Component RT: 29.4972 v10² 0.9 60.0 73.0 0.8 0.7^{-} 0.6 0.5 0.4 101.0 43.0 0.3 85.0 55.0 0.2 0.1 40 100 10 20 30 50 60 80 90 110 120 130 140 150 160 Mass-to-Charge (m/z) Octanoic acid (NIST20.L) st x10²_ 0.9-60.0 73.0 0.8 0.7 0.6 0.5 0.4 43.0 101.0 55.0 0.3 85.0 0.2 115.0 69.0 29.0 0.1 97.0 144.0 127.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (29.2072-29.5648 min, 61 scans) 14.D st x10² 0.9 138.1 0.8 0.7 0.6 123.0 0.5 0.4 0.3 95.0 0.2 55.0 67.0 39.0 0.1 151.0 166.0 106.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 29.4972 Counts Counts x10⁵ x10⁴ Component 41.1 60.0 60.0 6 2.5 73.0 73.0 5 2 101.0 43.0 4

43.0

41.1

3

2

29.3

29.4

Acquisition Time (min)

29.5

1.5

0.5

29.3

29.4

Acquisition Time (min)

29.5

1

Library Search Results - NonTarget Hits with Details --- Agilent Trusted Answers **Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 29.7328 Phenol, 3,4-dimethyl-951301.7 95-65-8 C8H10O Component RT: 29.7328 v10² 0.9 107.0 0.8 122.1 0.7^{-} 0.6 0.5 0.4 0.3 77.0 0.2 91.0 0.1 39.0 65 100 105 ¹110 115 75 Mass-to-Charge (m/z) Phenol, 3,4-dimethyl- (NIST20.L) Counts x10²_ 0.9 122.0 107.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 89.093.0 98.0 103.0 90 95 100 105 110 115 120 125 130 135 20 25 30 35 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (29.6622-29.8205 min, 27 scans) 14.D Sounds x10² 0.9 107.0 0.8 151.0 0.7^{-} 0.6 122.1 0.5° 0.4^{-} 166.0 0.3 136.0 0.2 91.0 43.0 55.0 67.0 0.1 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 50 60 10 20 Mass-to-Charge (m/z) EIC Peaks Component RT: 29.7328 Counts x10⁵ Counts x10⁴ 107.0 Component 107.0 122.1 5 1.75 122.1 121.0 1.5

29.8

Acquisition Time (min)

77.0

91.0

НЗС

121.0

77.0

91.0

3

2-

29.7

1.25

0.75

0.5⁻ 0.25⁻

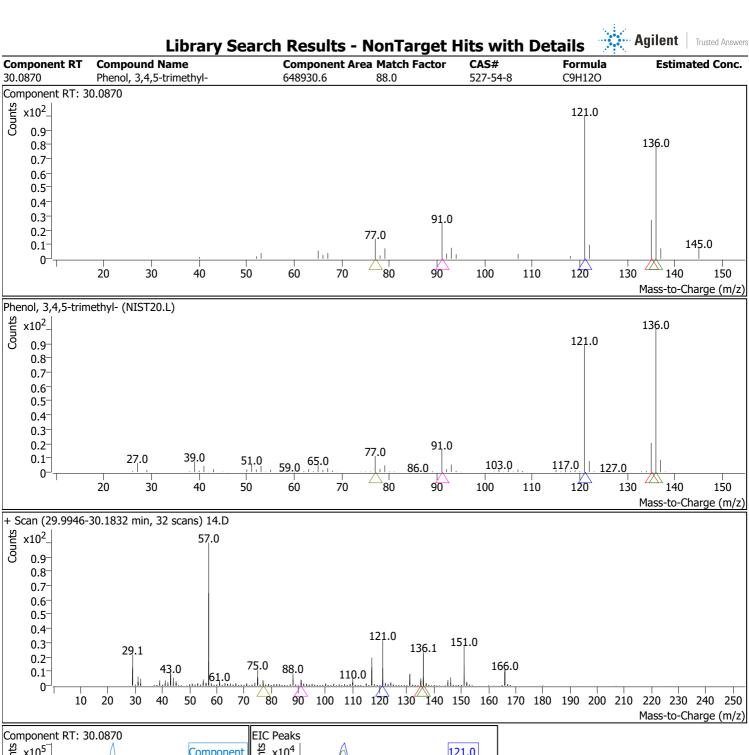
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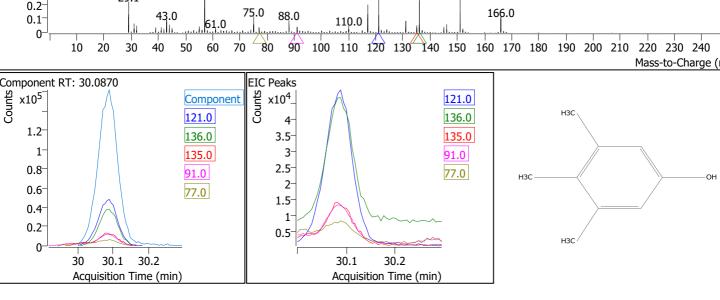
29.8

Acquisition Time (min)

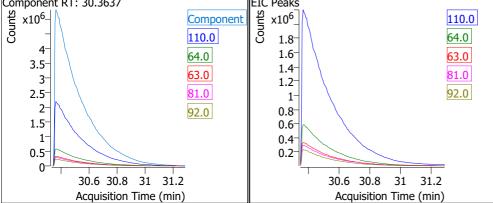
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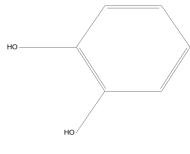
CH3





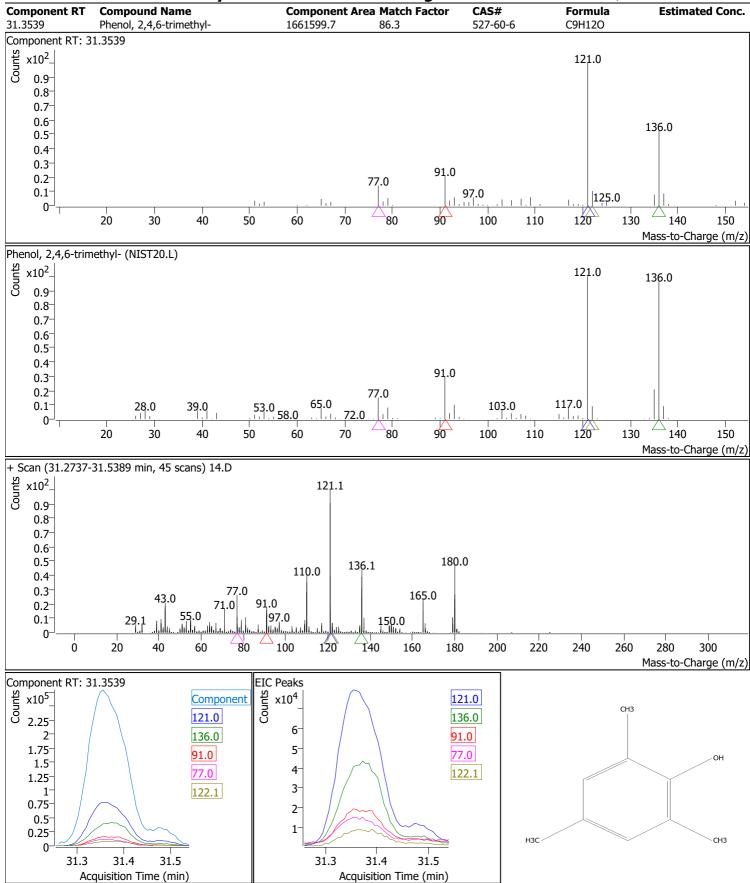
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.3637 Catechol 65503490.7 98.7 C6H6O2 Component RT: 30.3637 v10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 10 15 35 50 55 60 65 75 80 85 90 95 100 105 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 81.0 92.0 0.1 69.0 74.0 79.0 95.0 65 10 15 20 30 35 40 45 50 55 60 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.3381-31.2945 min, 160 scans) 14.D st x10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 64.0 0.4^{-} 0.3 81.0 92.0 0.2 53.0 0.1 39.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.3637 **EIC Peaks** Counts Counts x10⁶x10⁶ 110.0 Component 110.0 64.0 1.8 1.6 64.0 63.0 3.5 1.4

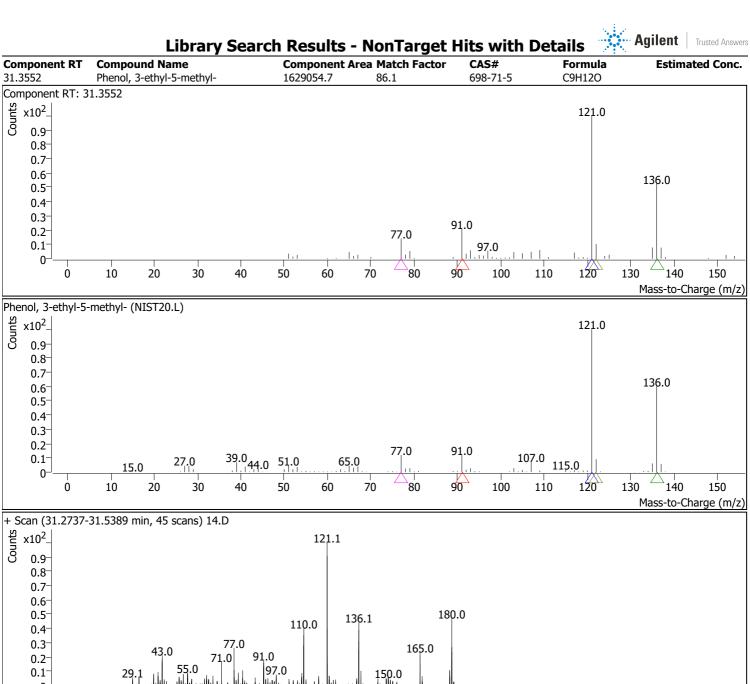


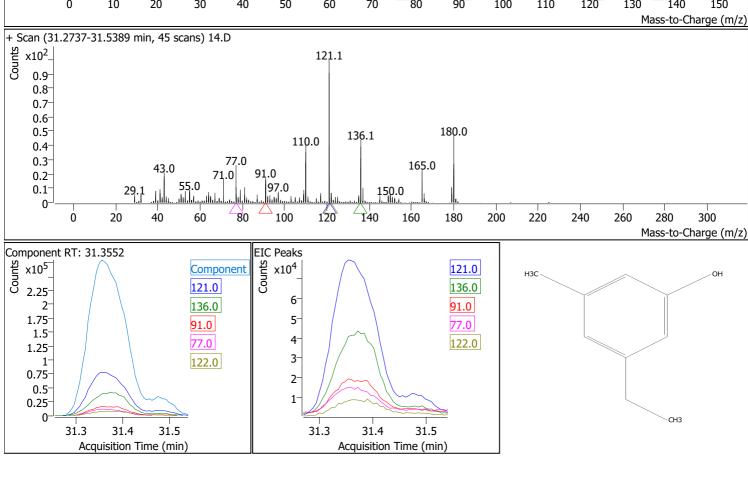












-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 886403.4 150-19-6 31.5858 m-Guaiacol 86.8 C7H8O2 Component RT: 31.5858 $x10^{2}$ 124.0 0.9 0.8 0.7^{-} 0.6 0.5 94.0 0.4 81.0 0.3 0.2 109.0 53.0 66.0 137.0 39.0 0.1 0 110 Ó 10 20 30 40 50 60 80 90 100 130 140 Mass-to-Charge (m/z) m-Guaiacol (NIST20.L) Square value 124.0 0.8 0.7 0.6 94.0 0.5 0.4 81.0 0.3 53.0 0.2 66.0 39.0 0.1 69.0 27.0 77.0 109.0 15.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (31.5271-31.6638 min, 23 scans) 14.D st x10² 0.9 124.0 0.8 0.7 0.6 165.0 180.0 0.5 95.0 0.4 81.0 0.3 110.0 136.1 0.2 152.1 0.1 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 31.5858 **EIC Peaks** Counts x10⁵ x10⁴ 124.0 Component ОН 124.0 94.0 1.4 4.5 94.0 81.0 1.2 95.0 3.5 95.0 1

31.6

31.7

Acquisition Time (min)

31.8

109.0

H3C-

3

2⁻ 1.5⁻

1

0.5

2.5

81.0

109.0

0.8

0.6

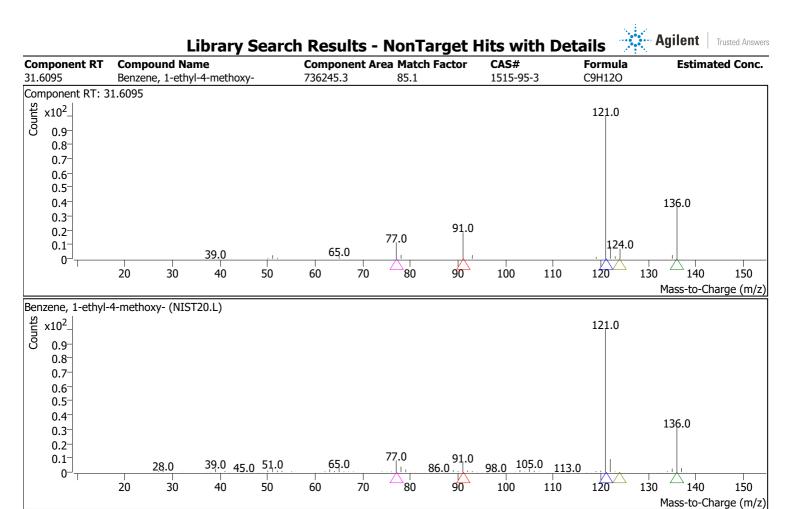
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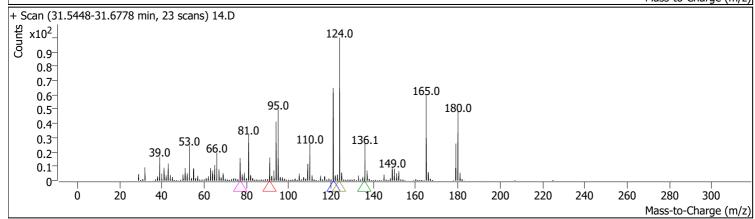
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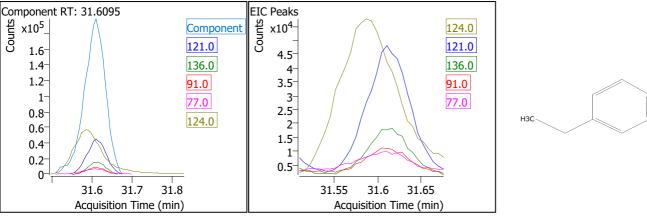
31.6

31.7

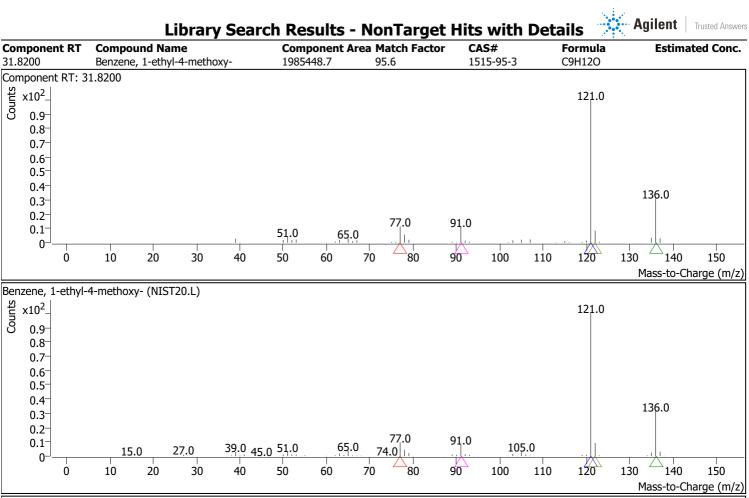
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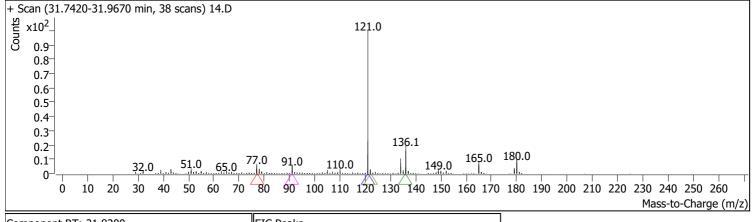


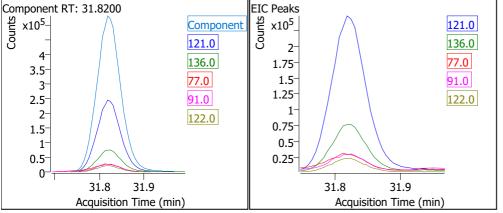


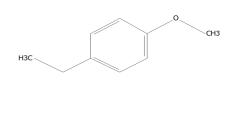


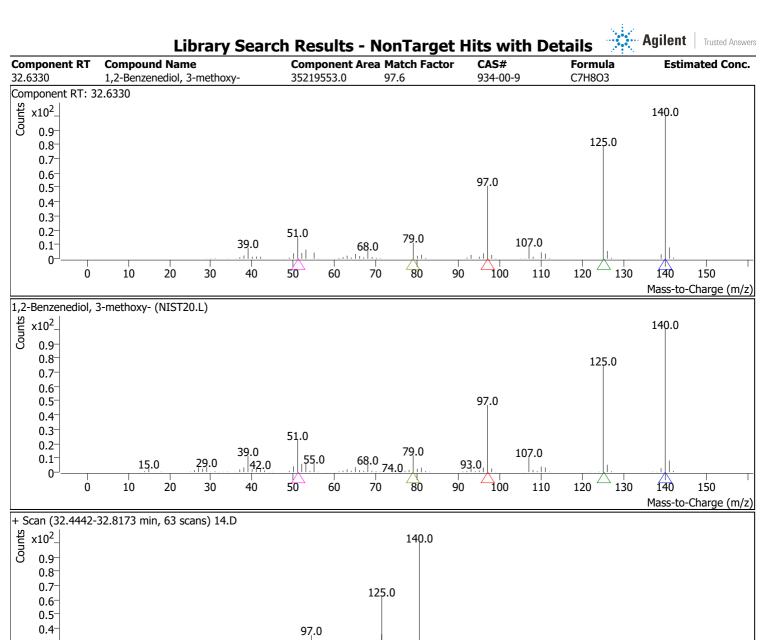
CH3

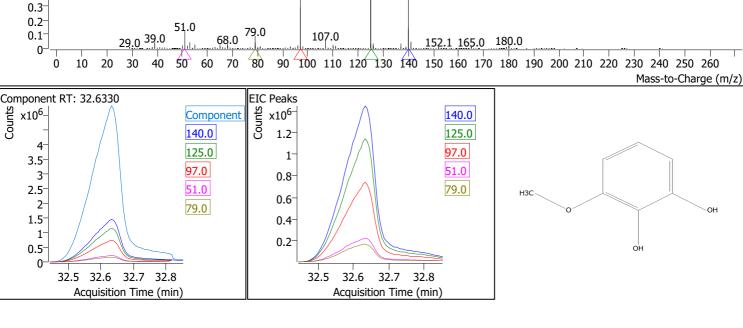




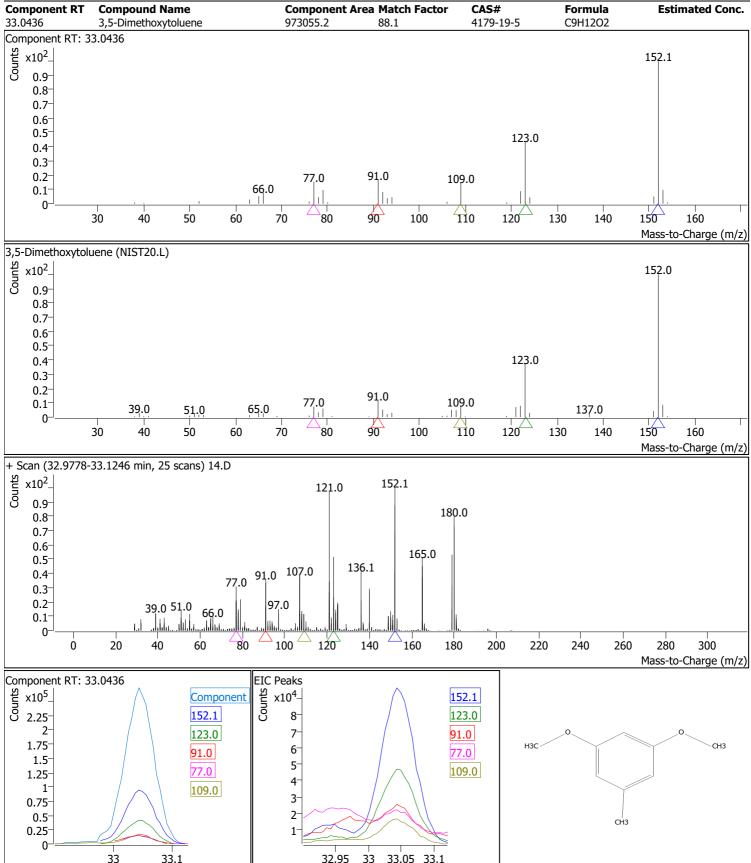






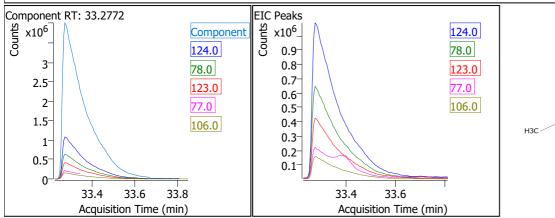


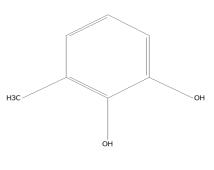




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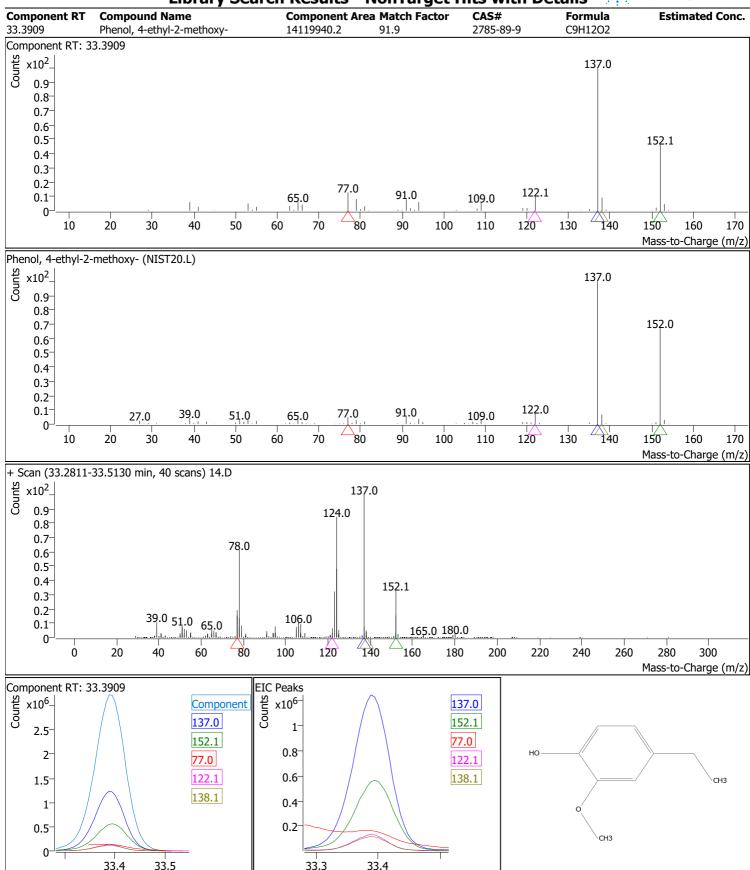
-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 29487251.2 488-17-5 33.2772 1,2-Benzenediol, 3-methyl-96.3 C7H8O2 Component RT: 33.2772 v10² 0.9 124.0 0.8 0.7 78.0 0.6 0.5 0.4 0.3 0.2 106.0 39.0 51.0 0.1 10 20 30 40 50 60 70 90 100 110 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 3-methyl- (NIST20.L) Counts x10²_ 0.9 124.0 0.8 0.7 0.6 0.5 0.4 78.0 0.3 0.2 106.0 39.0 51.0 0.1 62.0 67.0 27.0 18.0 80 10 20 30 40 50 60 70 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (33.2276-33.6676 min, 75 scans) 14.D st x10² 0.9 124.0 0.8 78.0 0.7 0.6 0.5 0.4 152.1 0.3 0.2 39.0 51.0 65.0 106.0 0.1 165.0 180.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 33.2772 EIC Peaks Counts x10⁶ x10⁶_ 124.0 Component 124.0 78.0 0.9 3 0.8 78.0 123.0 0.7 2.5





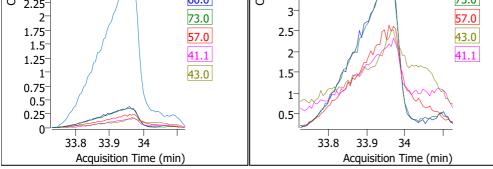


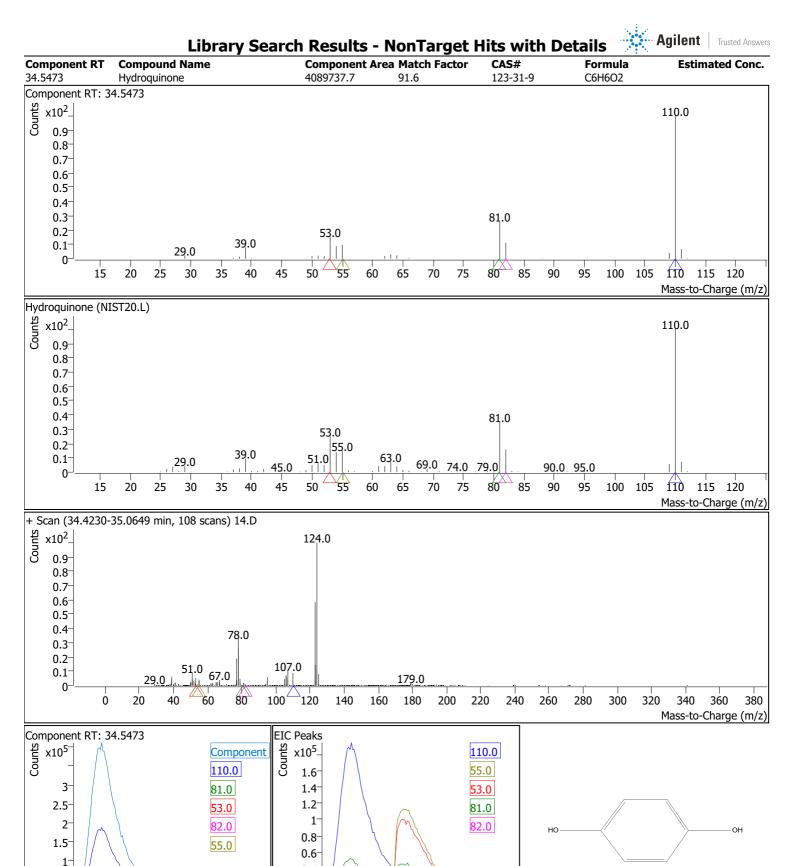




Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 112-05-0 33.9590 Nonanoic acid 2233804.3 88.5 C9H18O2 Component RT: 33.9590 v10² 0.9 60.0 73.0 0.8 0.7^{-} 57.0 0.6 0.5 41.1 0.4 115.0 129.0 0.3 0.2 29.0 0.1 0 40 10 20 30 50 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Nonanoic acid (NIST20.L) st x10² 0.9 60.0 0.8 73.0 0.7 0.6 57.0 0.5 41.0 0.4 0.3 29.0 115.0 0.2 129.0 69.0 98.0 87.0 0.1 158.0 14.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (33.7506-34.1254 min, 64 scans) 14.D St x10² 0.9 180.0 0.8 71.0 0.7 60.0 41.0 165.0 0.6 0.5 124.0 0.4^{-} 115.1 0.3 194.1 29.1 149.0 0.2 91.0 0.1 0 ^{_}80 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 33.9590 Counts st x10⁵ x10⁴ 60.0 Component 60.0 73.0 2.25 3 2 73.0 57.0 2.5







0.4

 0.2^{-}

34.6

34.8

Acquisition Time (min)

35

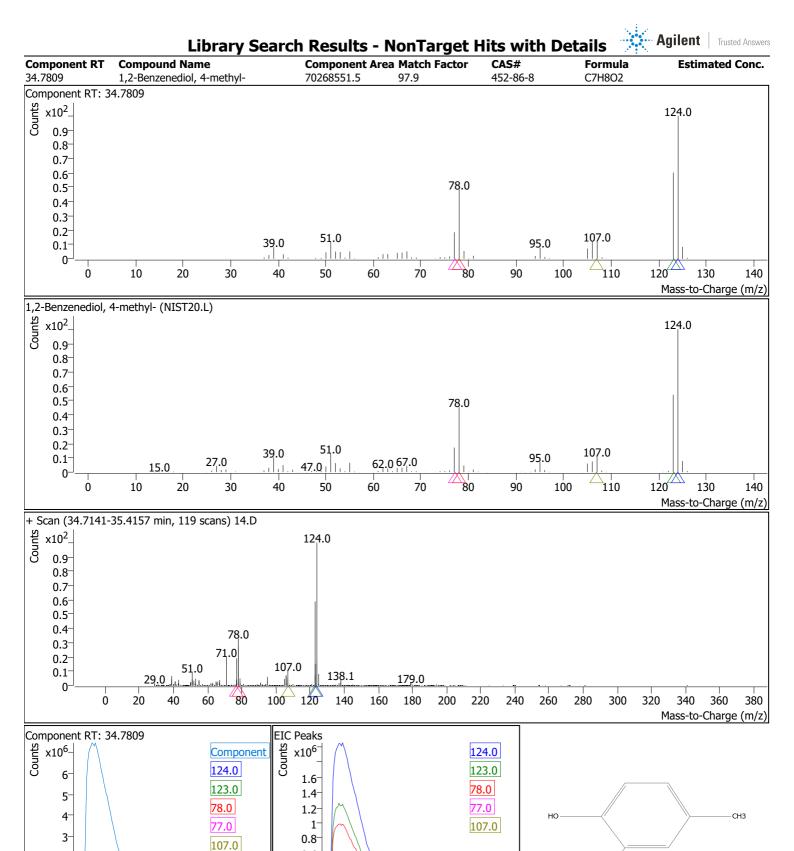
0.5

34.6

34.8

Acquisition Time (min)

35





0.6

0.4

0.2

34.8

35

35.2

Acquisition Time (min)

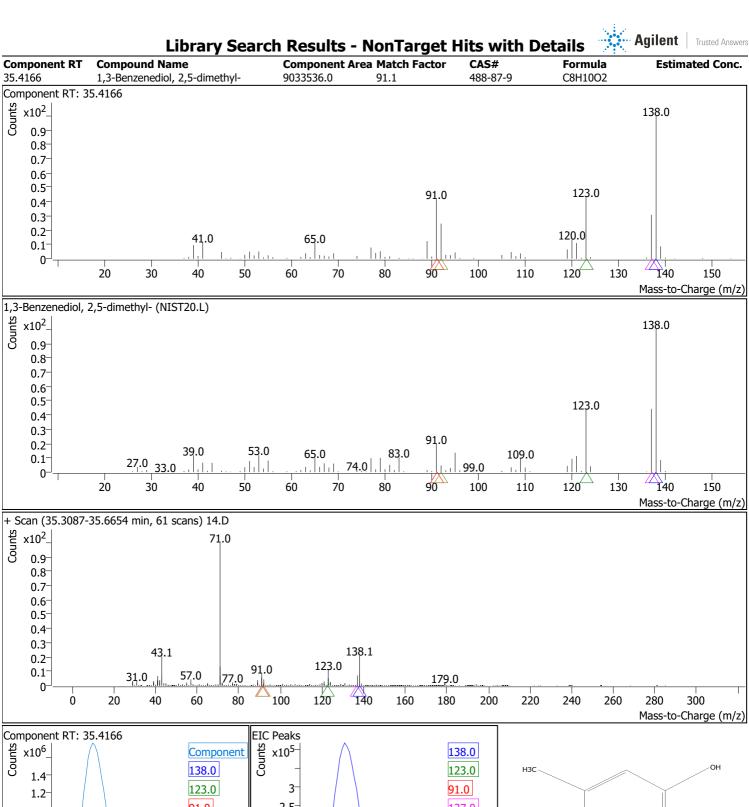
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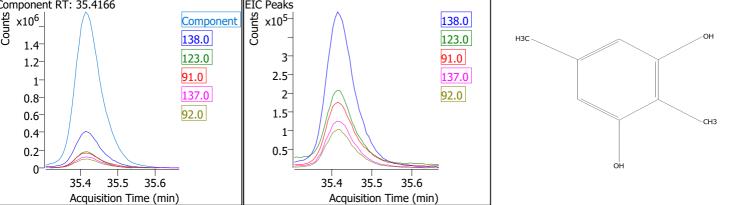
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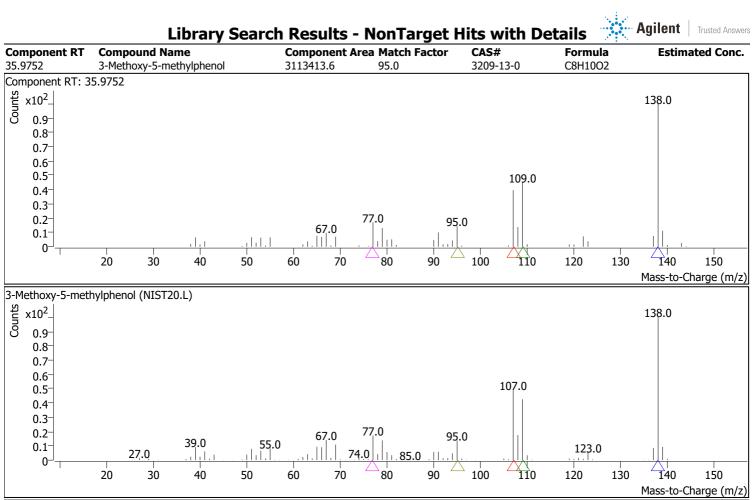
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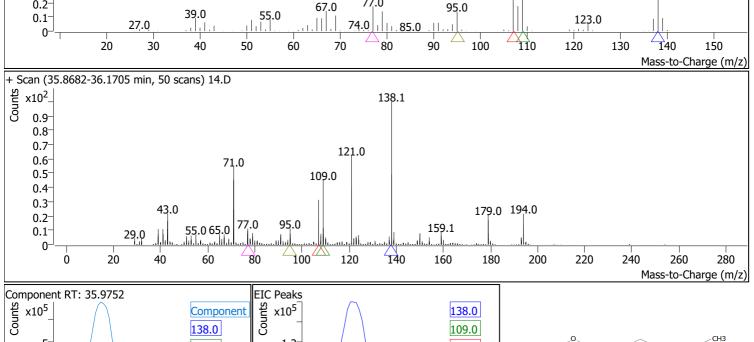
35

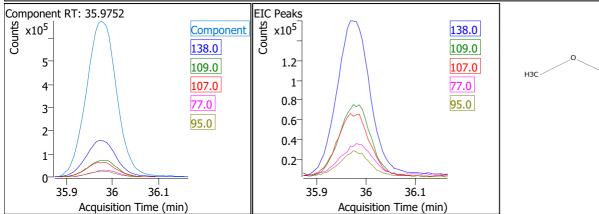
35.2

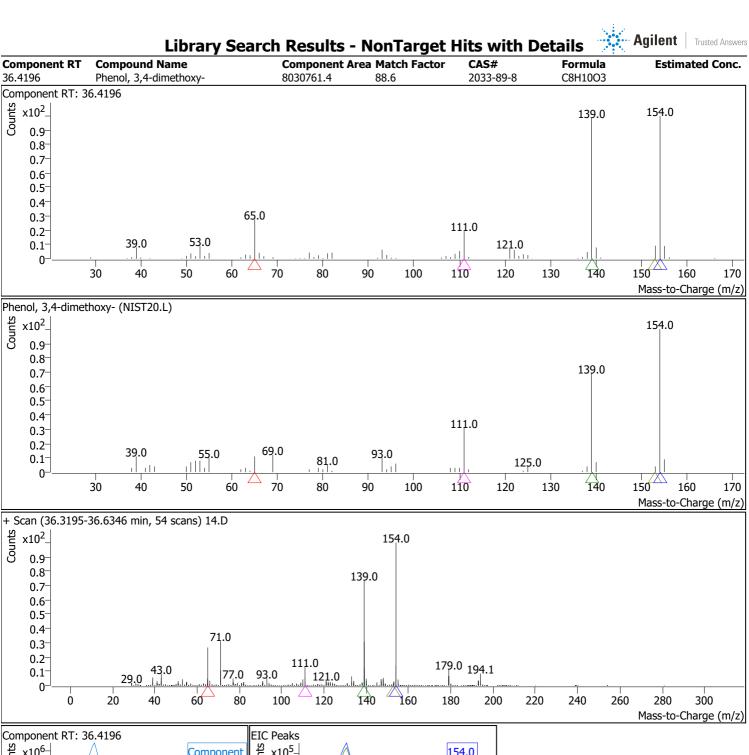


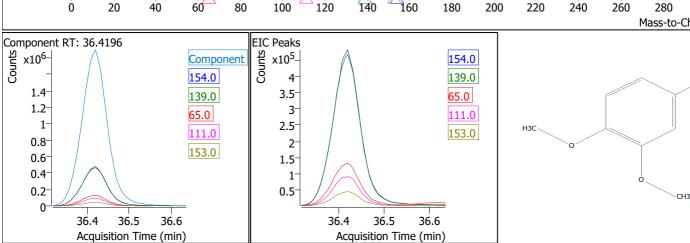


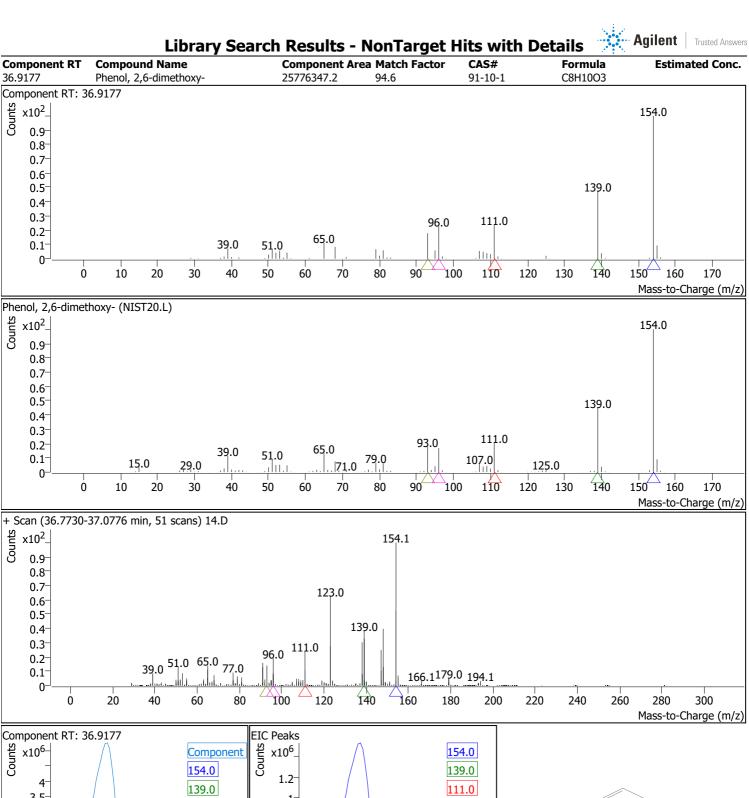


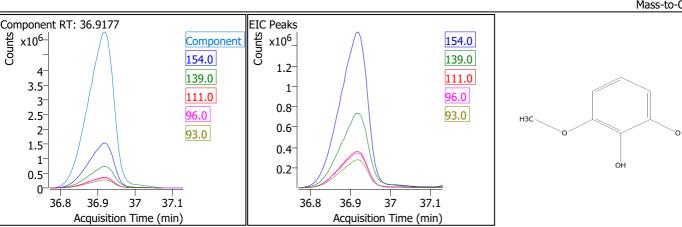












--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 703-23-1 37.1290 Ethanone, 1-(2-hydroxy-6-928707.8 85.1 C9H10O3 methoxyphenyl)-Component RT: 37.1290 x10²_ 151.0 0.9 8.0 0.7 0.6 0.5 166.0 0.4 0.3 0.2^{-} 136.0 0.1 108.0 0-110 150 170 30 40 50 60 70 80 90 100 120 130 140 160 180 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 0 110 150 30 40 50 60 70 80 90 100 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (37.0390-37.2828 min, 42 scans) 14.D st x10² 139.0 154.0 0.8 0.7 0.6 0.5 0.4 111.0 0.3 65.0 0.2 39.0 91.0 53.0 71.0 123.0 166.1^{179.0} 194.1 0.1 0 Ó 160 200 260 20 40 60 80 100 120 140 180 220 240 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 37.1290 Counts Counts x10⁵ x10⁵ 151.0 Component 151.0 166.0 2 1.2 СНЗ 166.0 152.0 1.75 1-152.0 136.0 1.5 0.8 1.25 136.0 108.0 CH3

37.2

Acquisition Time (min)

0.6

0.4

0.2

37.1

108.0

1

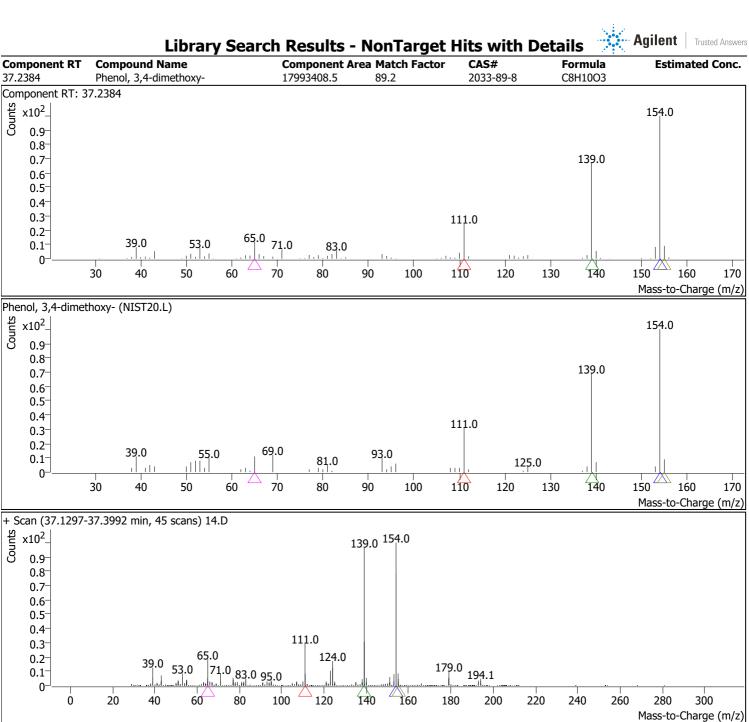
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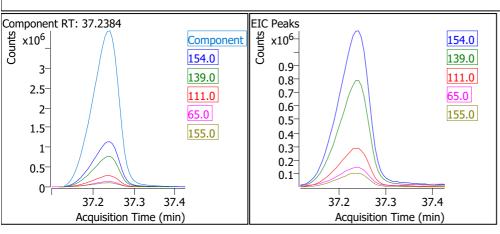
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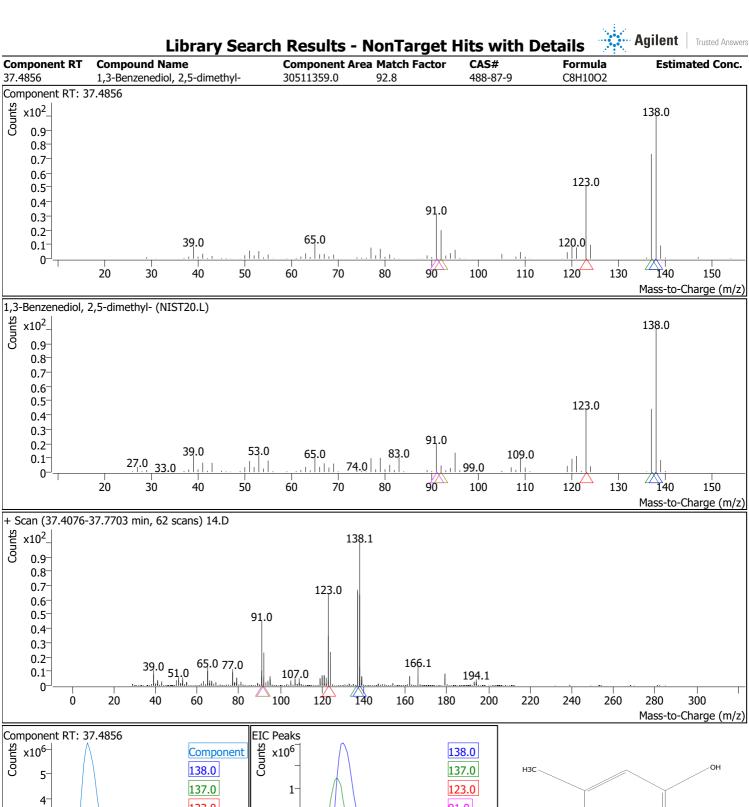
0.25

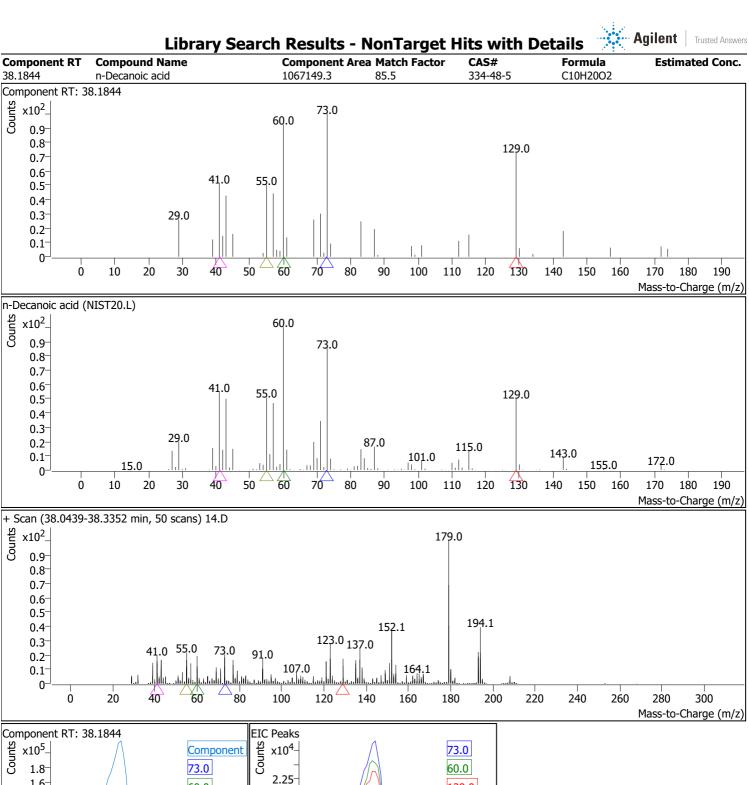
37.1

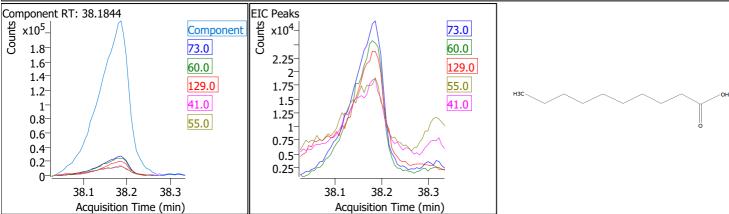
37.2



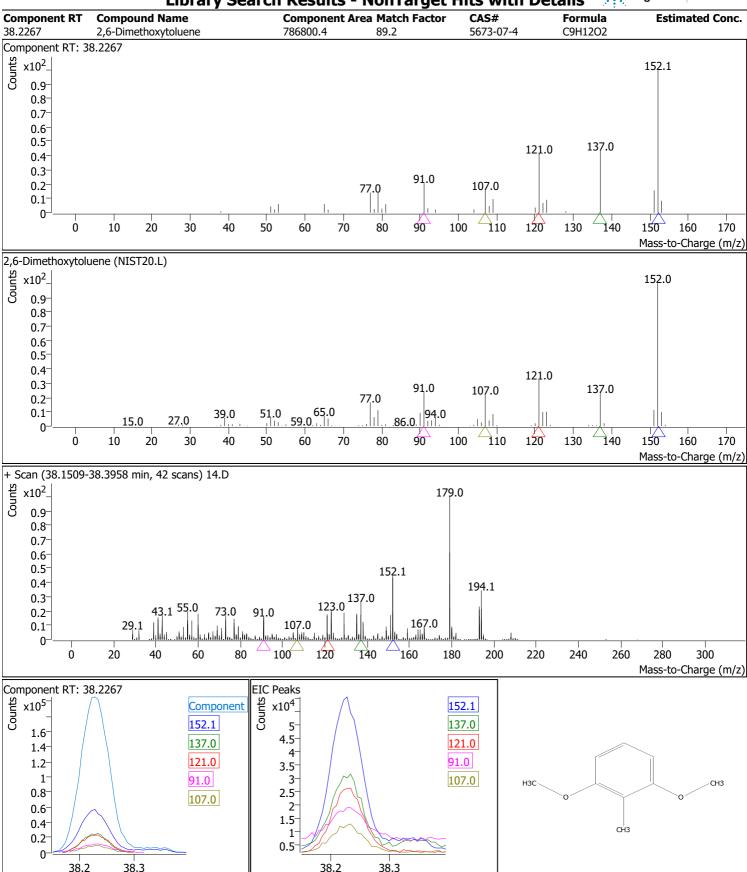












Acquisition Time (min)

- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 527-55-9 38.7326 1,3-Benzenediol, 4,5-dimethyl-9228419.3 91.2 C8H10O2 Component RT: 38.7326 v10² 0.9 138.0 0.8 123.0 0.7 0.6 0.5 0.4 91.0 0.3 0.2 65.0 77.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) 1,3-Benzenediol, 4,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 123.0 138.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 91.0 109.0 69.0 79.0 0.1 53.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (38.6325-38.8168 min, 32 scans) 14.D st x10² 0.9 138.1 123.0 0.8 0.7 0.6 0.5 0.4 91.0 0.3 152.1 0.2 179.0 1<u>93.1</u> 39.0 51.0 65.0 77.0 0.1 107.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) EIC Peaks Component RT: 38.7326 Counts Counts x10⁵-Component 137.0 НЗС 138.0 138.0 4.5 1.4 123.0 123.0 1.2 91.0 3.5 91.0



38.7

38.75

Acquisition Time (min)

38.8

92.0

H3C

3

2

2.5

1.5

0.5

137.0

92.0

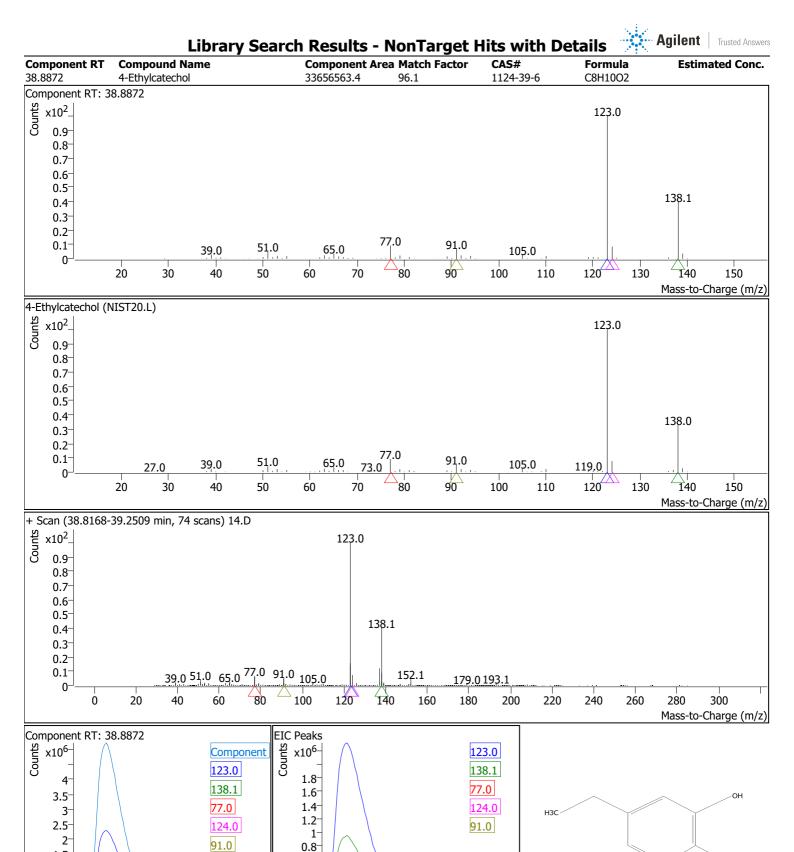
38.7 38.75 38.8

Acquisition Time (min)

1

0.8

0.6





0.6

0.4

38.9

39

39.1 39.2

Acquisition Time (min)

1.5

0.5

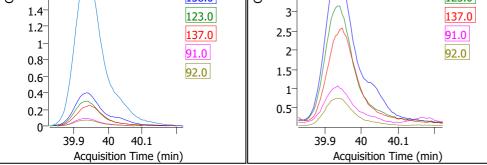
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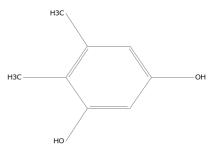
39

Acquisition Time (min)

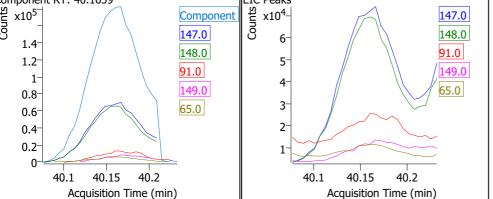
39.1 39.2

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 527-55-9 39.9391 1,3-Benzenediol, 4,5-dimethyl-11120641.6 89.8 C8H10O2 Component RT: 39.9391 v10² 0.9 138.0 0.8 123.0 0.7^{-} 0.6 0.5 0.4 0.3 91.0 0.2 39.0 65.0 77.0 109.0 0.1 110 120 140 10 20 30 40 50 60 70 80 100 130 150 Mass-to-Charge (m/z) 1,3-Benzenediol, 4,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 138.0 123.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 109.0 0.1 39.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (39.8396-40.2201 min, 65 scans) 14.D st x10² 0.9 123.0 138.0 153.0 0.8 0.7 0.6 0.5 0.4 91.0 0.3 193.0 168.1 0.2 39.0 51.0 65.0 77.0 208.1 0.1 109.1 179.0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 39.9391 EIC Peaks Counts Counts x10⁵ 138.0 Component НЗС 138.0 123.0 1.4 3 123.0 137.0 1.2



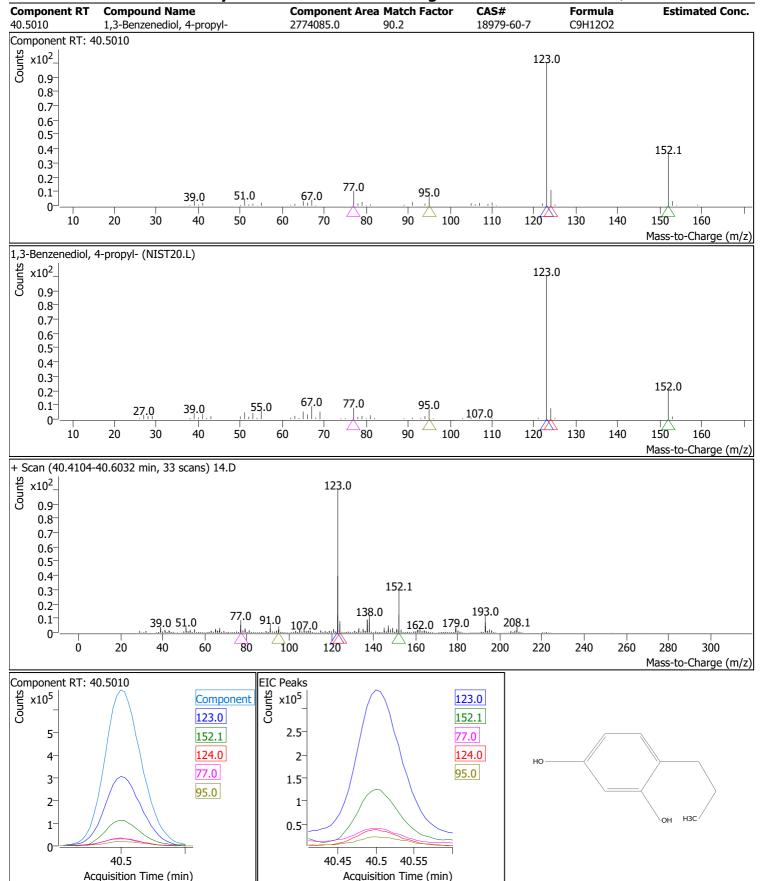


--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 40.1639 4-Formyl-3,5-dimethyl-1H-pyrrole-2-757262.7 1000296-05-3 C8H8N2O carbonitrile Component RT: 40.1639 Counts x10²_ 147.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 91.0 0.2^{-} 0.1 94.0 119.0 150 30 40 90 100 110 120 130 140 160 Mass-to-Charge (m/z) 4-Formyl-3,5-dimethyl-1H-pyrrole-2-carbonitrile (NIST20.L) Counts x10²_ 147.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 119.0 0.1 39.0 53.0 78.083.0 92.0 105.0 133.0 0 90 80 150 30 40 50 100 110 120 130 140 160 Mass-to-Charge (m/z) + Scan (40.0774-40.2082 min, 23 scans) 14.D st x10² 0.9 148.0 193.0 0.8 0.7 165.1 0.6 123.0 137.0 0.5 91.0 0.4 0.3 208.1 43.0 53.0 65.0 77.0 0.2 179.0 105.0 0.1 40 60 80 100 120 Ó 20 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 40.1639 Counts Counts x10⁴x10⁵ 147.0 Component 147.0 148.0 6 1.4 148.0 91.0 1.2 5

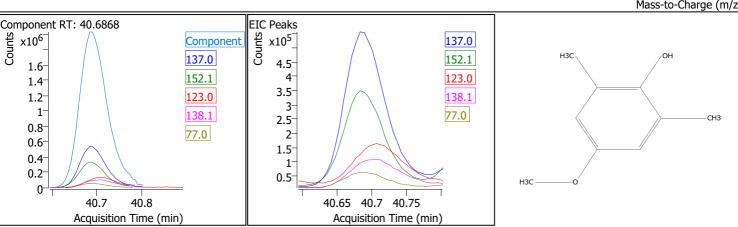


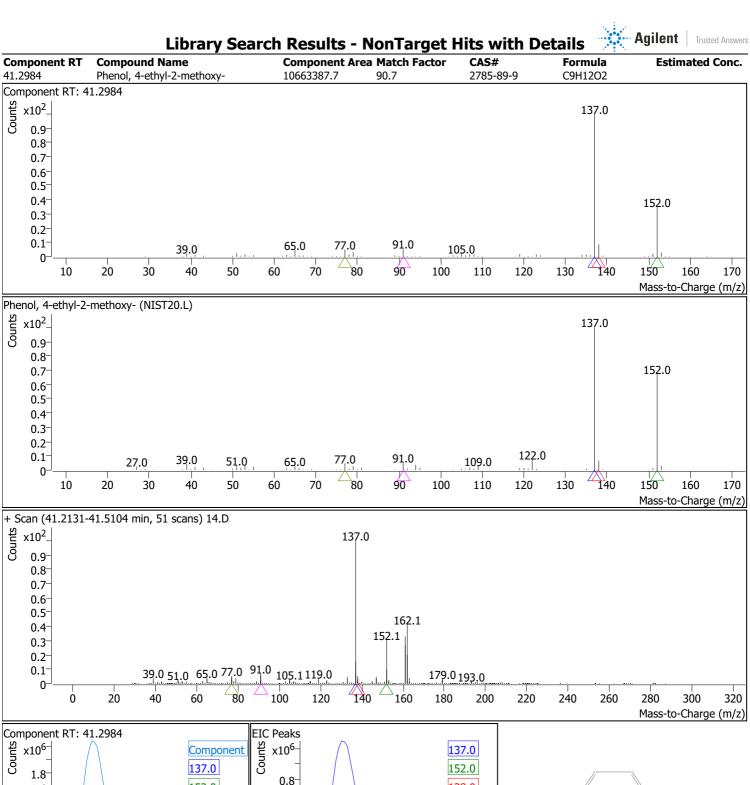


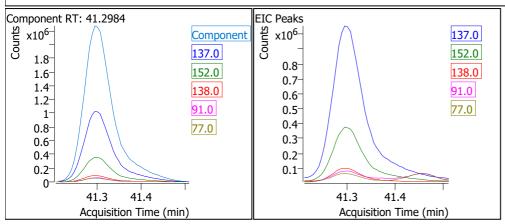


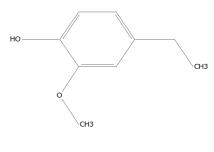


- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2431-91-6 40.6868 4-Methoxy-2,6-dimethylphenol 8794778.3 86.4 C9H12O2 Component RT: 40.6868 v10² 0.9 137.0 0.8 0.7 152.1 0.6 0.5 0.4 0.3 123.0 0.2 91.0 109.0 65.0 0.1 150 10 20 30 40 50 60 70 90 100 110 120 130 160 170 Mass-to-Charge (m/z) 4-Methoxy-2,6-dimethylphenol (NIST20.L) st x10²_ 0.9-137.0 152.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 81.0 91.0 109.0 39.0 53.0 67.0 0.1 123.0 0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (40.6080-40.7850 min, 30 scans) 14.D st x10² 0.9 137.0 0.8 0.7 0.6 152.1 0.5 0.4 0.3 123.0 0.2 39.0 51.0 65.0 77.0 91.0 0.1 109.0 179.0 193.0 208.1 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 40.6868 x10⁵ 137.0 Component









--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 7044-92-0 41.4560 1,4-Benzenedicarboxaldehyde, 2,5-10145575.8 85.2 C10H10O2 dimethyl-Component RT: 41.4560 x10²_ 162.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 147.0 119.0 133.0 0.1 105.0 0-150 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) 1,4-Benzenedicarboxaldehyde, 2,5-dimethyl- (NIST20.L) $x10^{2}$ 162.0 0.9 0.8 0.7 0.6 0.5 133.0 0.4 105.0 77.0 0.3 51.0 39.0 0.2 27.0 91.0 63.0 0.1 74.0 118.0 15.0 98.0 147.0 0 150 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (41.3558-41.6412 min, 49 scans) 14.D st x10² 162.1 0.8 0.7 0.6 0.5 0.4 137.0 0.3 0.2 39.0 51.0 65.0 ^{77.0} ^{91.0} _{105.1} 123.0 179.0 0.1 193.0 0 40 80 100 260 280 Ó 20 60 120 140 160 180 200 220 240 300 Mass-to-Charge (m/z) Component RT: 41.4560 EIC Peaks Counts Counts x10⁶ x10⁵ 162.1 Component 161.0 162.1 1.8 5 161.0 147.0 1.6 1.4 147.0 163.0 1.2

41.5

Acquisition Time (min)

41.6

77.0

163.0

77.0

0.8

0.6⁻ 0.4⁻ 0.2⁻

41.5

Acquisition Time (min)

41.6

3-

2-

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 14007415.2 18979-60-7 42.6896 1,3-Benzenediol, 4-propyl-86.5 C9H12O2 Component RT: 42.6896 v10² 0.9 123.0 0.8 0.7^{-} 0.6 0.5 0.4 152.1 0.3 0.2 0.1 51.0 39.0 105.0 50 40 150 10 20 30 90 100 110 120 130 140 160 Mass-to-Charge (m/z) 1,3-Benzenediol, 4-propyl- (NIST20.L) Counts x10²_ 0.9 123.0 0.8 0.7 0.6 0.5 0.4 0.3 152.0 0.2 67.0 95.0 0.1 55.0 39.0 27.0 107.0 50 10 20 30 40 60 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (42.5985-42.9791 min, 65 scans) 14.D st x10² 0.9 123.0 0.8 0.7 0.6 0.5 0.4 0.3 152.1 0.2 0.1 39.0 51.0 140.0 166.1 65.0 193.1207.1 20 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) EIC Peaks Component RT: 42.6896 Counts x10⁶ x10⁶-123.0 Component 123.0 152.1 1.2 152.1 77.0 2 1-

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3770 Dodecanoic acid, methyl ester 7644054.6 93.2 111-82-0 C13H26O2 Component RT: 44.3770 v10² 0.9 74.0 0.8 0.7^{-} 87.0 0.6 0.5 0.4 0.3 43.0 55.0 143.1 0.2 171.1 183.1 69.1 0.1 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) Dodecanoic acid, methyl ester (NIST20.L) Counts x10²_ 0.9 74.0 0.8 0.7 87.0 0.6 0.5 0.4 0.3 0.2 55.0 29.0 69.0 214.0 0.1 83.0 101.0 115.0 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 (44.2872-44.5390 min, 43 scans) 14.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 161.0 176.1 87.0 0.3 144.0 0.2 115.0 43.0 55.0 0.1 101.0 205.1 20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 44.3770 **EIC Peaks** Counts Counts x10⁶ x10⁵ 74.0 Component 74.0 87.0 1.6 87.0 43.0 3.5



44.4

Acquisition Time (min)

55.0

41.1

44.5

1.4

1.2

0.6

0.4

0.2 0-

44.4

Acquisition Time (min)

1 0.8 43.0

55.0

41.1

44.5

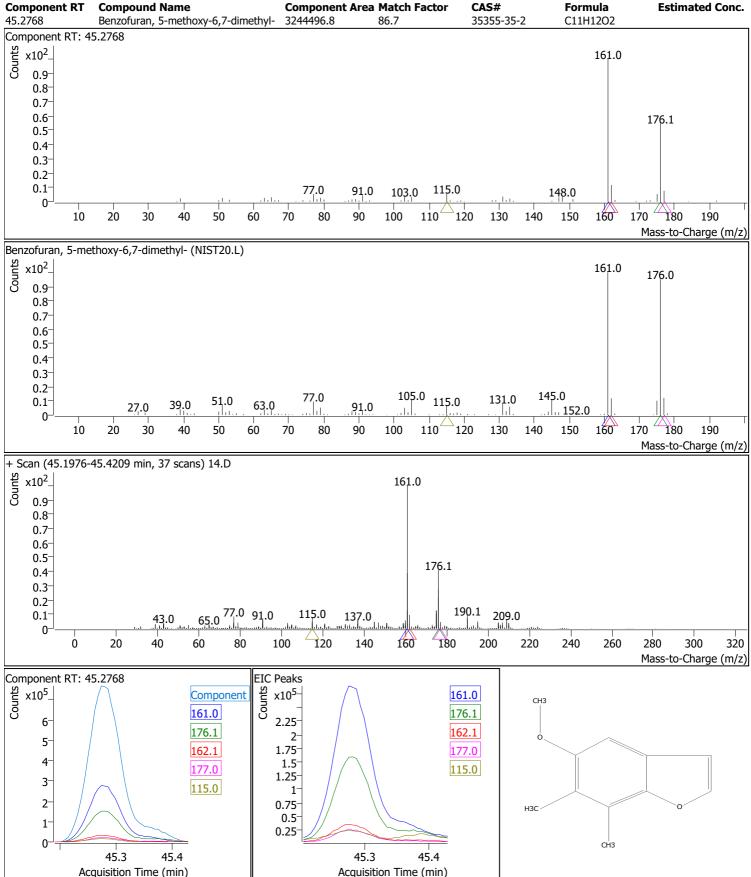
3-

2

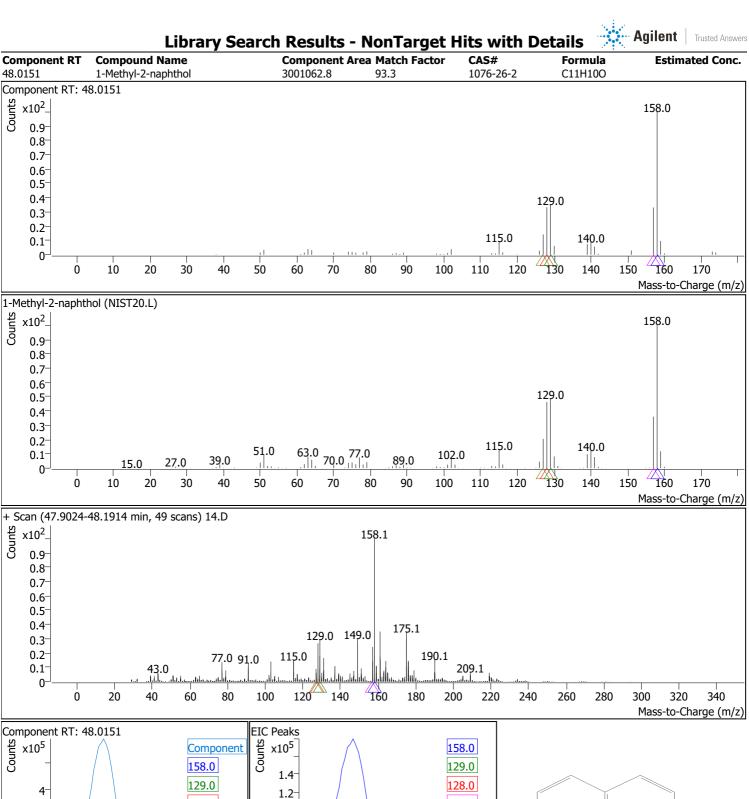
1 0.5

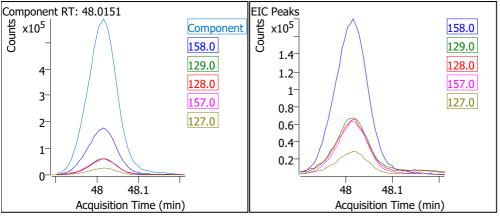
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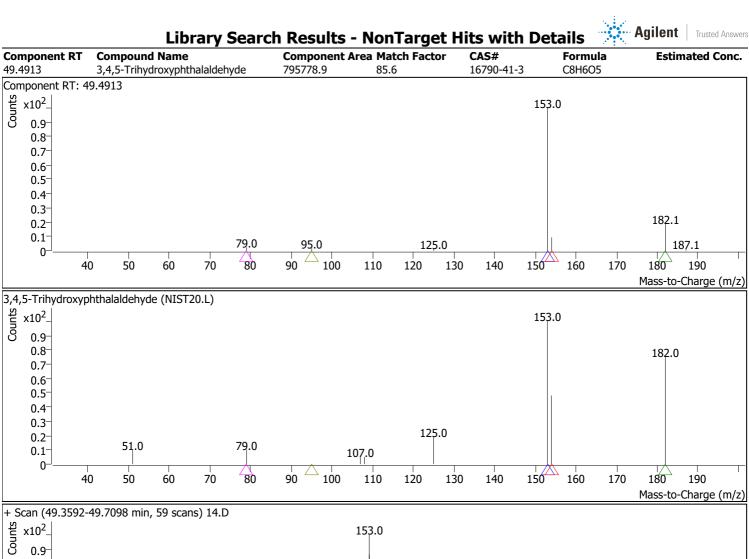


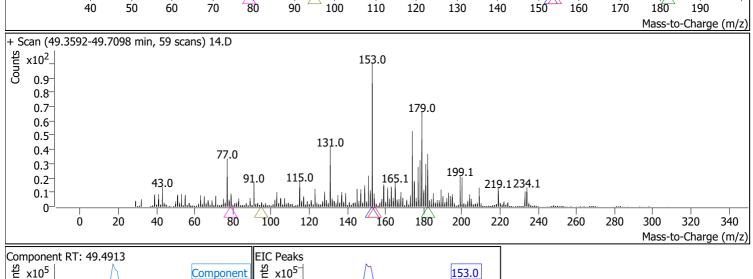


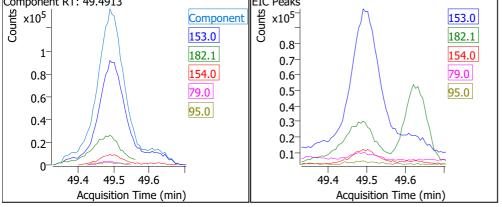
- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 45.2768 2,2'-Isopropylidenedifuran 3222981.3 85.8 17920-88-6 C11H12O2 Component RT: 45.2768 y x10² 0.9 161.0 0.8 0.7 0.6 176.0 0.5 0.4 0.3 0.2 0.1 103.0 115.0 77.0 91.0 148.0 0 150 10 20 30 40 50 70 100 110 120 130 140 160 180 190 Mass-to-Charge (m/z) 2,2'-Isopropylidenedifuran (NIST20.L) Counts x10²_ 0.9 161.0 0.8 0.7 0.6 0.5 0.4 0.3 176.0 0.2 0.1 131.0 147.0 170 180 160 10 20 50 60 70 80 90 100 110 120 130 140 150 190 Mass-to-Charge (m/z) + Scan (45.1975-45.4214 min, 37 scans) 14.D St x10²_ 0.9 161.0 0.8 0.7 0.6^{-} 0.5 176.1 0.4^{-} 0.3 0.2 190.1 209.0 115.0 137.0 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 45.2768 EIC Peaks Counts x10⁵ Counts 161.0 Component 161.0 176.0 6 2.25 176.0 175.0 2 5 1.75

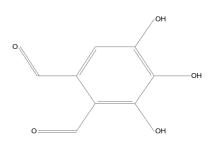


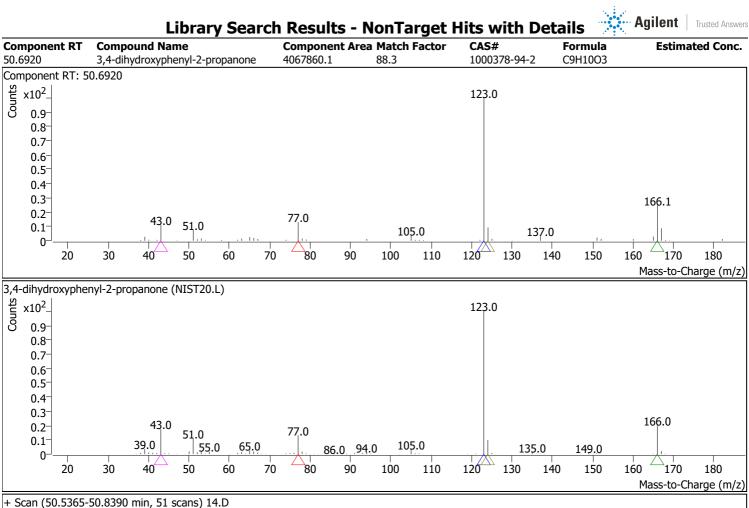


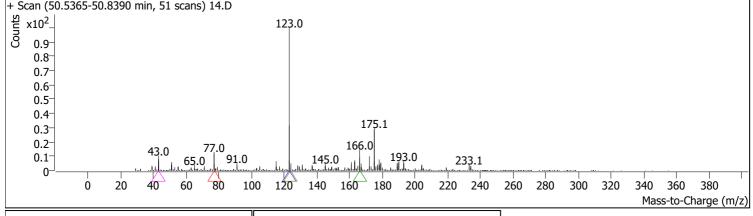


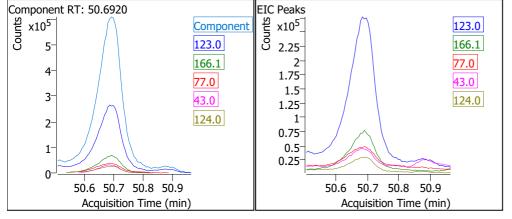


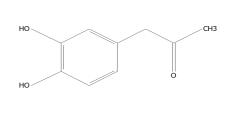






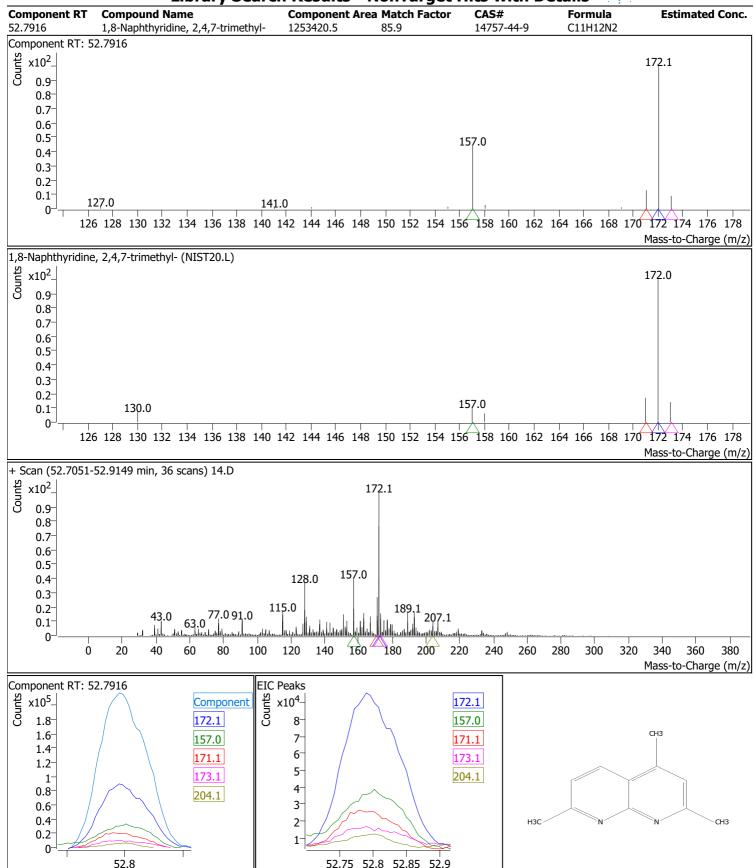






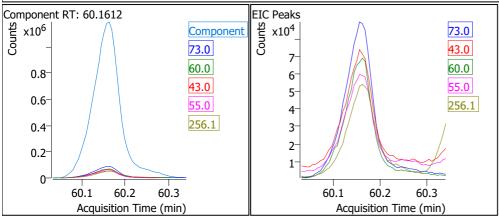


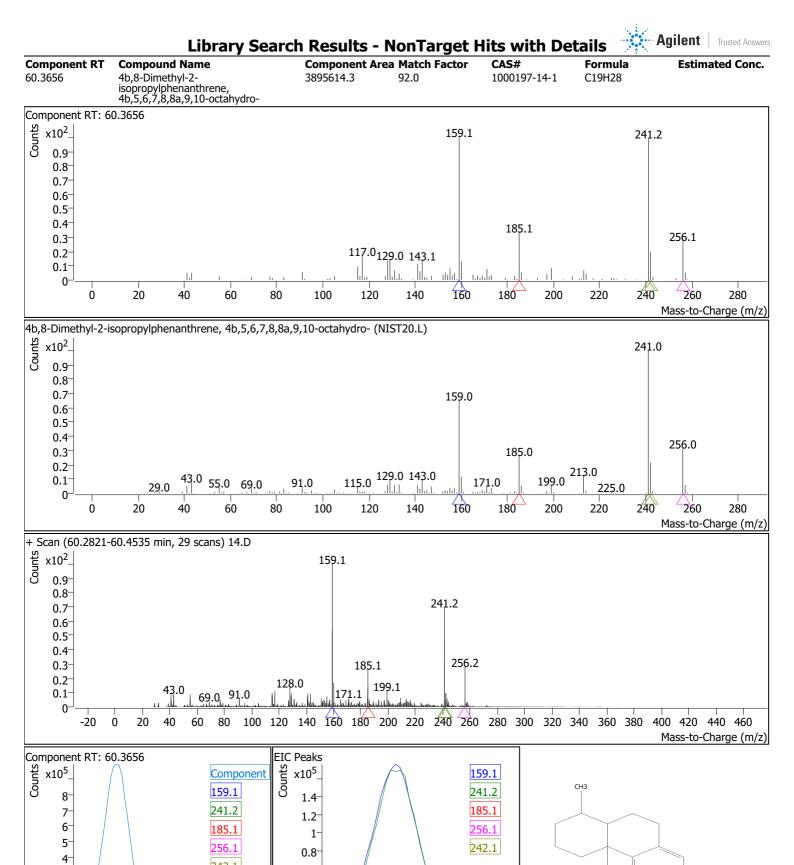




Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 57-10-3 60.1612 n-Hexadecanoic acid 5177133.8 90.8 C16H32O2 Component RT: 60.1612 v10² 0.9 73.0 60.0 0.8 43.0 0.7^{-} 55.0 256.1 129.0 0.6 0.5 0.4 0.3 0.2 0.1 0 260 20 40 100 120 140 160 180 200 220 240 280 Mass-to-Charge (m/z) n-Hexadecanoic acid (NIST20.L) st x10²_ 0.9-73.0 0.8 60.0 0.7 43.0 129.0 256.0 0.6 0.5 213.0 0.4 83.0 0.3 97.0 115.0 157.0 171.0 185.0 0.2 29.0 227.0 143.0 199.0 0.1 220.0 239.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) + Scan (60.0561-60.3356 min, 48 scans) 14.D St x10² 73.0 0.8 129.1 0.7 0.6 159.1 0.5 213.2 241.2 115.0 0.4^{-} 185.1 83.1 143.1 0.3 29.1 97.1 0.2 229.1 0.1 20 40 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 -20 Mass-to-Charge (m/z) EIC Peaks Component RT: 60.1612 x10⁴ 73.0 Component





60.35

60.4

Acquisition Time (min)

242.1

3

2

60.3

60.4

Acquisition Time (min)

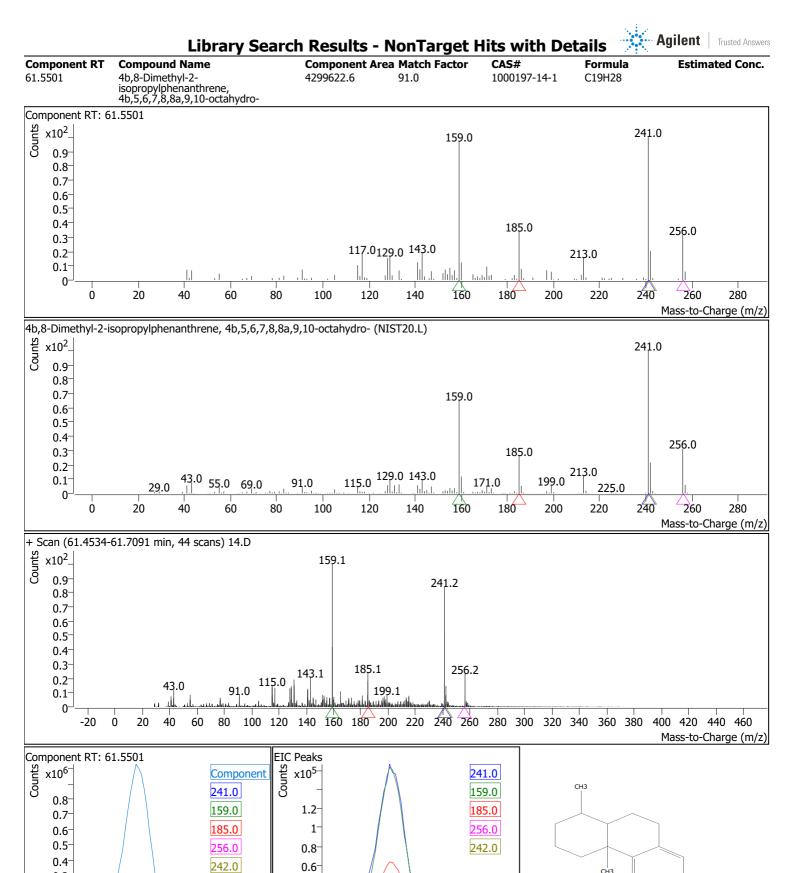
60.5

0.6

0.4

СНЗ

СНЗ



0.4

0.2

0.3

0.2

0.1

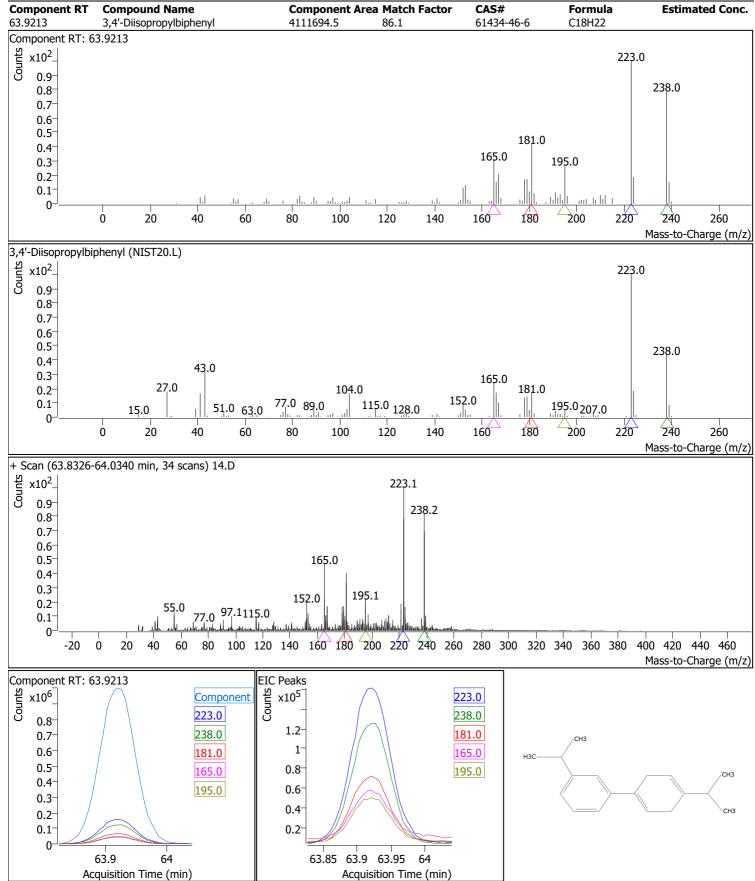
61.5

61.6 Acquisition Time (min) СНЗ

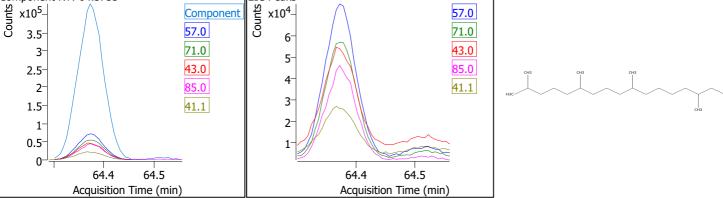
СНЗ





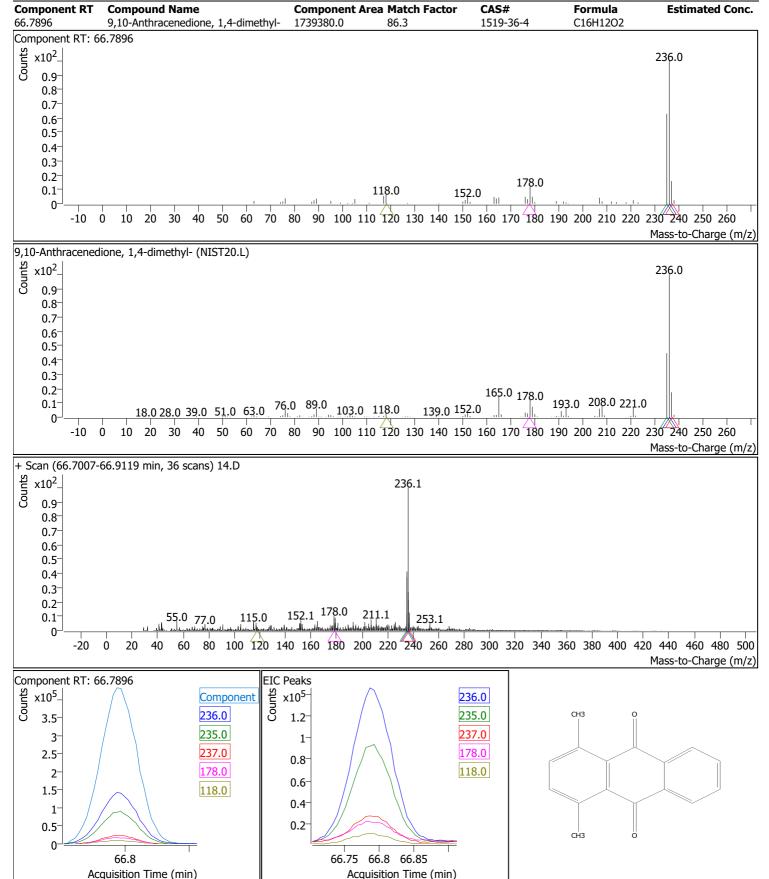


Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 54833-48-6 64.3733 Heptadecane, 2,6,10,15-tetramethyl-1599453.9 87.0 C21H44 Component RT: 64.3733 y x10² 0.9 57.0 71.0 0.8 0.7^{-} 43.0 85.0 0.6 0.5 0.4 0.3 99.0 29.0 0.2 0.1 0 20 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Heptadecane, 2,6,10,15-tetramethyl- (NIST20.L) Counts x10²_ 0.9 57.0 0.8 71.0 0.7 43.0 0.6 0.5 85.0 0.4 0.3 0.2 $99.0 \ 113.0 \ 127.0141.0 \ 155.0169.0183.0197.0211.0225.0239.0253.0267.0281.0296.0$ 0.1 0-40 60 200 260 280 20 80 100 120 140 160 180 220 240 300 320 Mass-to-Charge (m/z) + Scan (64.2957-64.4562 min, 27 scans) 14.D St x10² 0.9 0.8 197.1 0.7^{-} 71.1 254.2 0.6 0.5 85.1 0.4^{-} 212.1 239.1 0.3 0.2 29.1 128.0 0.1 -20 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: 64.3733 $x10^{4}$ 57.0 Component



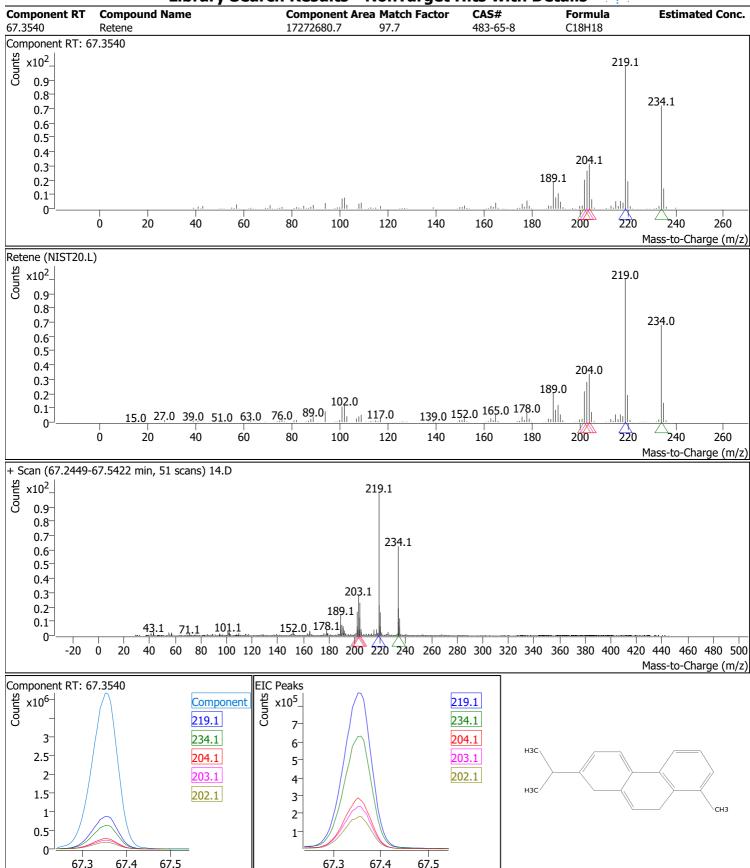




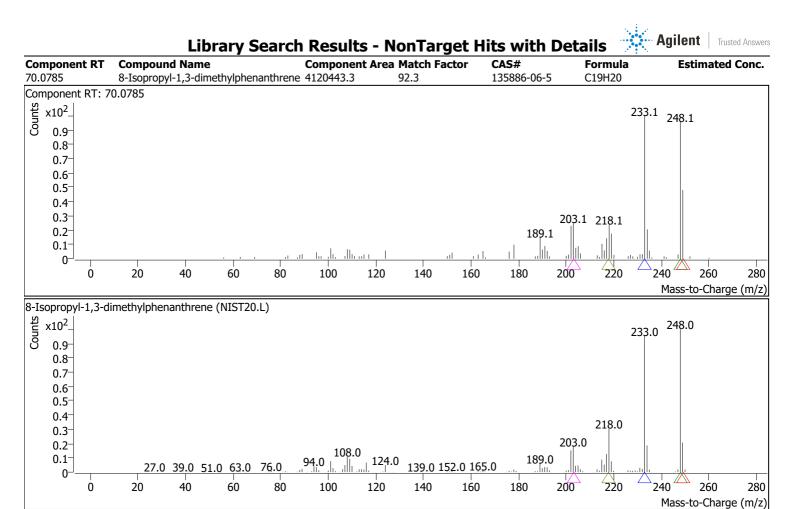


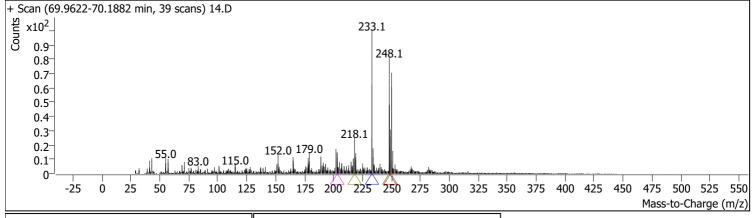


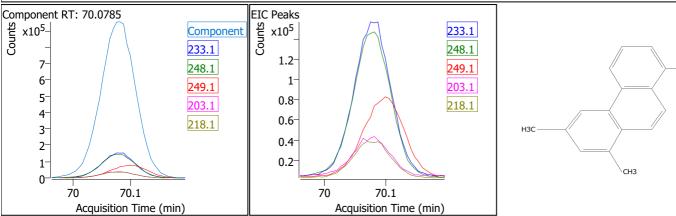




Acquisition Time (min)

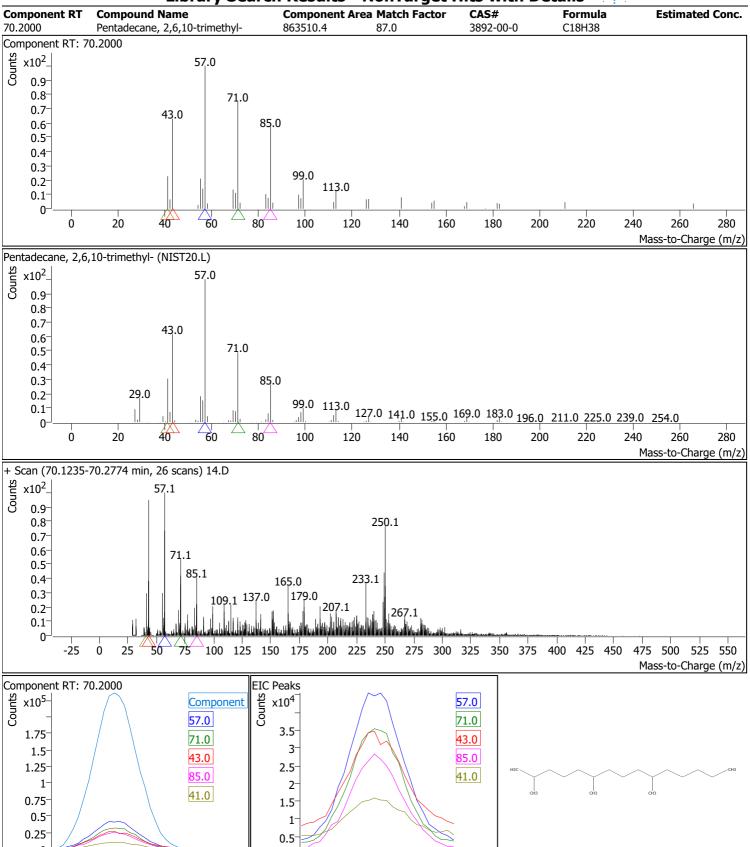






СНЗ





70.2

Acquisition Time (min)

70.25

70.15

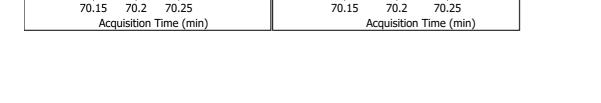
70.15

70.2

Acquisition Time (min)

70.25

-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 638-36-8 70.2009 Hexadecane, 2,6,10,14-tetramethyl-877118.8 86.5 C20H42 Component RT: 70.2009 y x10² 0.9 57.0 0.8 71.0 0.7 43.0 85.0 0.6 0.5 0.4 0.3 99.0 0.2 113.0 0.1 0 200 20 100 120 140 160 180 220 240 260 280 300 Mass-to-Charge (m/z) Hexadecane, 2,6,10,14-tetramethyl- (NIST20.L) st x10²_ 0.9-57.0 0.8 71.0 0.7 43.0 0.6 0.5 0.4 85.0 0.3 29.0 0.2 99.0 113.0 127.0 0.1 $141.0\,155.0\,169.0\,{}^{183.0\,197.0}_{\,211.0\,225.0\,239.0\,253.0\,267.0\,\,282.0}$ 260 20 40 80 100 120 140 160 200 220 240 280 300 Mass-to-Charge (m/z) + Scan (70.1235-70.2774 min, 26 scans) 14.D St x10² 0.9 0.8 250.1 0.7^{-} 0.6 71.1 0.5 85.1 0.4^{-} 233.1 165.0 0.3 109.1 137.0 179.0 207.1 0.2 0.1 -25 25 50 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 Mass-to-Charge (m/z) EIC Peaks Component RT: 70.2009 Counts x10⁵ Counts 57.0 Component 71.0 57.0



3.5

2.5

1.5

1

0.5

3

2-

71.0

43.0

85.0

41.1

1.75

1.5

1.25

0.75

0.5

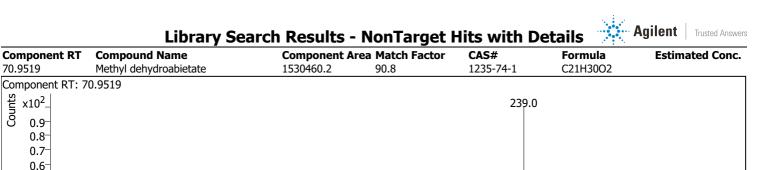
0.25

1

43.0

85.0

41.1



197.0

220

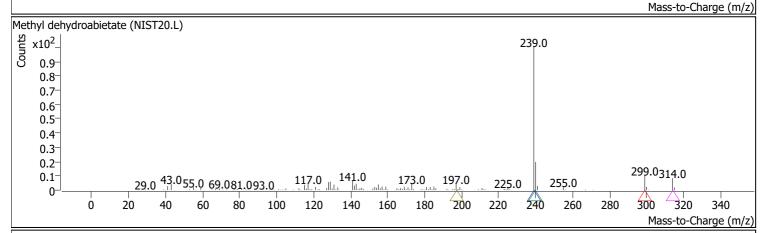
260

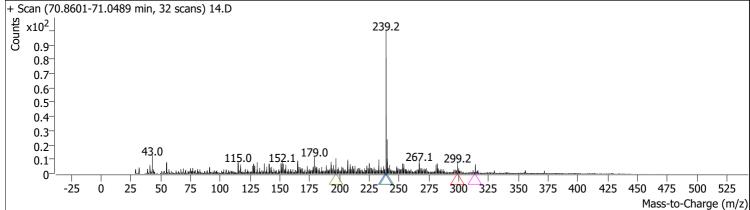
280

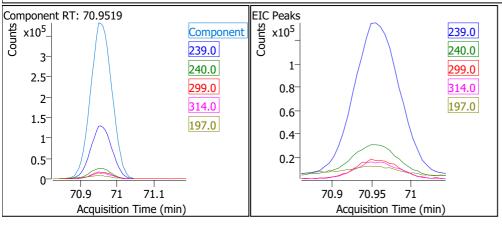
173.0

180

160







70.9519

y x10² 0.9

0.8 0.7 0.6 0.5 0.4 0.3 0.2

0.1

0

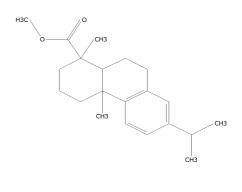
20

40

60

100

120



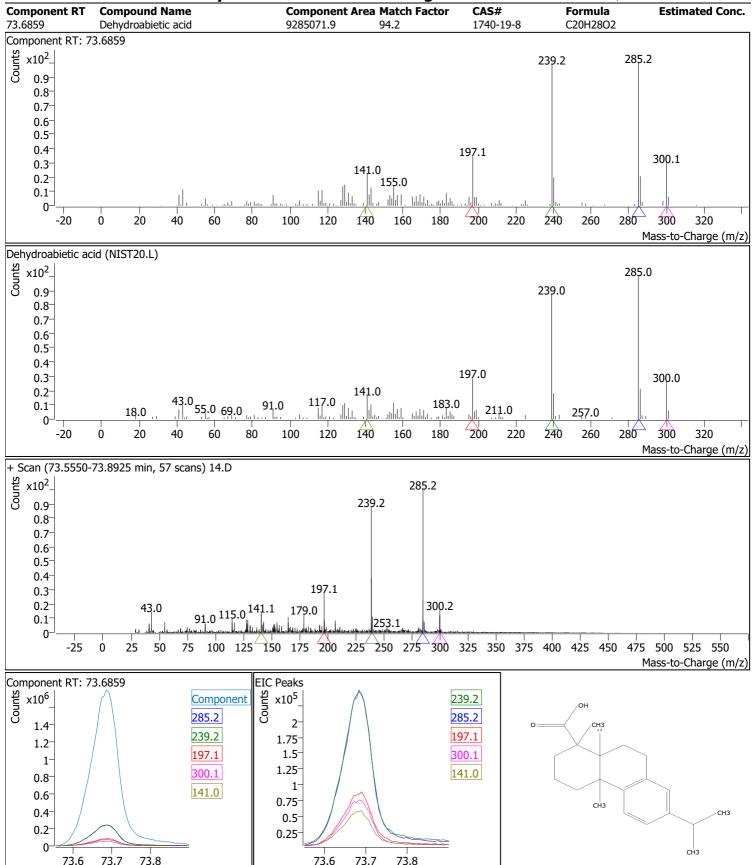
299.0314.0

320

340







Acquisition Time (min)

