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** 13.D **Path Name Sample Name Sample Type** 13 Sample Acq. Method Path Acq. Operator Acq. Method File 240501 scan D:\MassHunter\GCMS\1\methods\RBEL\

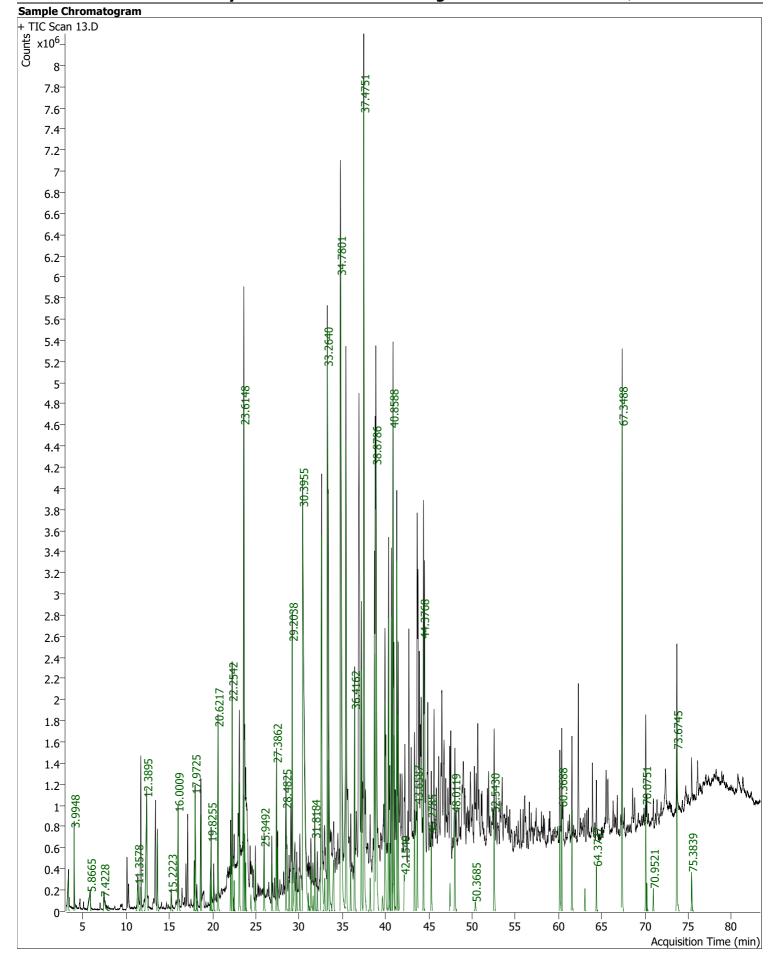
Acq. Date-Time 5/2/2024 6:15:53 AM **Instrument Name** GCMSD Dil. 1

Instrument Na	ime GCMSD	DII.	1			
Component R1	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
3.3520	Propanoic acid	79-09-4	C3H6O2	2214167.5	96.6	
3.9948	Propylene Glycol	57-55-6	C3H8O2	1841187.5	93.6	
5.8665	Butanoic acid	107-92-6	C4H8O2	2041109.9	90.3	
7.4228	1,3-Propanediol	504-63-2	C3H8O2	1539331.7	86.3	
11.3578	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	2046203.8	87.2	
11.7273	2-Cyclopenten-1-one, 2-methyl-	1120-73-6	C6H8O	1221748.2	93.2	
12.3895	Butyrolactone	96-48-0	C4H6O2	8424393.6	97.7	
13.6131	2,5-Hexanedione	110-13-4	C6H10O2	3002329.7	96.1	
15.2223	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	C5H8O2	789157.8	94.5	
16.0009	2-Cyclopenten-1-one, 3-methyl-	2758-18-1	C6H8O	4537925.2	97.7	
17.8795	2-Cyclopenten-1-one, 3-4-dimethyl-	30434-64-1	C7H10O	1604291.5	95.1	
17.9725	Phenol	108-95-2	C6H6O		98.1	
			C7H10O	5541228.9 625968.4		
18.1835	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7			91.1	
18.6651	Diisoamyl ether	544-01-4	C10H22O	3388163.8	87.3	
19.7442	2-Cyclopenten-1-one, 3,4-dimethyl-	30434-64-1	C7H10O	1133086.9	91.4	
19.8255	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2781298.9	93.4	
20.1288	3,6-Heptanedione	1703-51-1	C7H12O2	1289071.6	89.0	
20.6217	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	7360343.1	95.6	
22.0874	2-Cyclopenten-1-one, 3,4,5-trimethyl-	55683-21-1	C8H12O	2016960.9	93.0	
22.2542	Phenol, 2-methyl-	95-48-7	C7H8O	8300321.4	98.4	
22.4172	Acetophenone	98-86-2	C8H8O	542756.9	91.6	
22.4939	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	1114128.9	93.5	
23.0965	1-Octanol	111-87-5	C8H18O	5300991.4	96.0	
23.5745	p-Cresol	106-44-5	C7H8O	4084851.2	85.3	
23.6148	Mequinol	150-76-5	C7H8O2	19633263.2	96.8	
23.7224	2-Cyclopenten-1-one, 2,3,4-trimethyl-	28790-86-5	C8H12O	3246750.2	87.0	
23.7246	Mequinol	150-76-5	C7H8O2	2421167.4	86.7	
23.8259	Ethanone, 1-(2-thienyl)-	88-15-3	C6H6OS	1771486.3	90.3	
24.4261	5-Ethyl-2-furaldehyde	23074-10-4	C7H8O2	568966.7	86.1	
24.9444	Phenol, 2,6-dimethyl-	576-26-1	C8H10O	1689235.8	97.9	
25.9492	2-Ethyl-3-methylcyclopent-2-en-1-one	1000423-46-8	C8H12O	2619665.5	88.7	
26.8501	Phenol, 2-ethyl-	90-00-6	C8H10O	1842418.3	94.9	
27.3862	Phenol, 2,4-dimethyl-	105-67-9	C8H10O	5299381.8	99.1	
27.5169	Phenol, 2,5-dimethyl-	95-87-4	C8H10O	2446879.7	98.1	
28.4825	Phenol, 4-methoxy-3-methyl-	14786-82-4	C8H10O2	3796783.9	93.9	
28.8404	Phenol, 2,3-dimethyl-	526-75-0	C8H10O	1102017.8	96.2	
29.2038	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	9782401.8	98.7	
29.5255	Octanoic acid	124-07-2	C8H16O2	3539630.2	92.9	
29.7331	Phenol, 3,4-dimethyl-	95-65-8	C8H10O	1376652.3	94.9	
30.0836	Phenol, 3,4,5-trimethyl-	527-54-8	C9H12O	1282704.1	93.1	
30.3955	Catechol	120-80-9	C6H6O2	46924505.4	97.9	
31.0752	Phenol, 2-propyl-	644-35-9	C9H12O	619043.3	89.8	
31.3739	Phenol, 2-ethyl-4-methyl-	3855-26-3	C9H12O	2397343.8	93.2	
31.6138	Benzene, 1-ethyl-4-methoxy-	1515-95-3	C9H12O	488574.7	85.3	
31.8184	Benzene, 1-ethyl-4-methoxy-	1515-95-3	C9H12O	2677050.6	95.9	
32.0999	Phenol, 2-(1-methylethyl)-	88-69-7	C9H12O	906542.2	87.6	
32.6017	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	21891711.4	96.7	
	• • • • • • • • • • • • • • • • • • • •				85.6	
32.9676	Benzene, 1-ethyl-4-methoxy-	1515-95-3	C9H12O	1565635.8		
33.2640	1,2-Benzenediol, 3-methyl-	488-17-5	C7H8O2	38503347.8	96.9	
33.3784	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	6502882.8	85.5	
34.0012	Nonanoic acid	112-05-0	C9H18O2	3864001.9	88.9	
34.7801	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	50782596.9	92.3	
35.4100	1,3-Benzenediol, 2,5-dimethyl-	488-87-9	C8H10O2	22235668.2	93.5	
35.9620	3-Methoxy-5-methylphenol	3209-13-0	C8H10O2	1712998.0	92.6	
36.4162	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	7962698.4	87.7	
37.2107	3,4-Dimethoxyphenol, 2-methylpropionate	1000447-30-5	C12H16O4	10174951.8	89.2	
37.4751	1,3-Benzenediol, 4,5-dimethyl-	527-55-9	C8H10O2	37475302.6	93.9	
38.2168	2,6-Dimethoxytoluene	5673-07-4	C9H12O2	1323689.5	86.9	
38.7203	4-Ethylcatechol	1124-39-6	C8H10O2	12750652.6	85.8	
38.8786	4-Ethylcatechol	1124-39-6	C8H10O2	26567306.4	94.0	
39.6422	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	868109.4	86.6	
39.9257	1,3-Benzenediol, 4,5-dimethyl-	527-55-9	C8H10O2	11298478.4	91.0	
40.3432	5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-,	62732-46-1	C10H14N2	11326319.3	86.2	
40.4967	hydrate 1,3-Benzenediol, 4-propyl-	18979-60-7	C9H12O2	2888350.8	85.7	
TU.TJU/	1,5-benzeneuloi, T-propyi-	Page 1 of 94	CFITIZUZ		enerated at 11:34 A	M on 5/2/2024

Library Search Results - NonTarget Hits with Details

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Component	RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
40.6807	4-Methoxy-2,6-dimethylphenol	2431-91-6	C9H12O2	11509289.2	88.7	
40.8588	1,4-Benzenediol, 2,3,5-trimethyl-	700-13-0	C9H12O2	22747764.7	87.2	
40.9610	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	10587575.0	88.2	
41.2953	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	15126812.2	91.9	
41.4486	5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-, hydrate	62732-46-1	C10H14N2	8539314.1	86.7	
42.1540	Resorcinol, 2-acetyl-	699-83-2	C8H8O3	1228531.2	85.6	
43.3361	Resorcinol, 2-acetyl-	699-83-2	C8H8O3	4162547.1	87.1	
43.6587	2-Acetyl-7-hydroxybenzofuran	40020-87-9	C10H8O3	4339587.2	85.1	
44.3768	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	8849443.4	93.8	
45.2785	Benzofuran, 5-methoxy-6,7-dimethyl-	35355-35-2	C11H12O2	3066275.4	87.6	
47.4453	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	1048188.3	89.1	
48.0119	1-Methyl-2-naphthol	1076-26-2	C11H10O	4603513.9	96.2	
50.3685	3,4-Dihydroxybenzaldehyde, diacetate	67727-64-4	C11H10O5	479762.8	86.7	
52.5430	1-Naphthol, 6,7-dimethyl-	31776-14-4	C12H12O	4343396.2	90.5	
60.1443	n-Hexadecanoic acid	57-10-3	C16H32O2	3405167.5	87.4	
60.3688	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	3932372.4	91.8	
61.5449	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	3889092.5	91.5	
63.0434	Anthracene, 9-(1-methylethyl)-	1498-80-2	C17H16	854595.7	86.5	
64.3737	Heneicosane	629-94-7	C21H44	1587679.9	88.6	
67.3488	Retene	483-65-8	C18H18	19297850.8	97.8	
70.0751	8-Isopropyl-1,3-dimethylphenanthrene	135886-06-5	C19H20	4357126.2	92.5	
70.1961	Pentadecane, 2,6,10-trimethyl-	3892-00-0	C18H38	971960.2	88.8	
70.1962	Tetracosane	646-31-1	C24H50	979093.7	89.4	
70.9521	Methyl dehydroabietate	1235-74-1	C21H30O2	850764.8	88.6	
73.6745	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	7845639.3	94.2	
75.3839	1-Octadecanol	112-92-5	C18H38O	1645129.4	90.9	
75.3841	5-Eicosene, (E)-	74685-30-6	C20H40	1572685.1	89.4	



Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 79-09-4 C3H6O2 3.3520 Propanoic acid 2214167.5 96.6 Component RT: 3.3520 v10² 0.9 74.0 0.8 29.0 0.7 45.0 0.6 0.5 0.4 57.0 0.3 55.0 0.2 42.1 0.1 15 20 25 35 55 70 10 40 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 30 10 15 20 25 35 40 45 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.1276-3.4321 min, 52 scans) 13.D st x10² 0.9 74.0 0.8 29.1 0.7 0.6 45.0 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 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.3520 Counts Counts x10⁴ 74.0 Component 74.0 29.0 ОН 2.5 29.0 6 73.0 5 45.0 73.0 2 4 57.0

3.3

Acquisition Time (min)

3.4

45.0

57.0

3-

2

1

3.2

1.5

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0.5

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.** 3.9948 Propylene Glycol 1841187.5 93.6 57-55-6 C3H8O2 Component RT: 3.9948 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 39.0 15 25 30 45 70 75 5 10 20 35 40 50 55 60 65 80 Mass-to-Charge (m/z) Propylene Glycol (NIST20.L) St 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 75 5 10 20 25 30 35 40 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.9614-4.0980 min, 23 scans) 13.D st x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 29.0 0.1 61.0 10 20 30 40 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.9948 Counts Counts x10⁵ 45.0 Component 45.0 43.0 6 3.5 43.0 29.0 5 3-31.0 31.0 2.5

4.05

Acquisition Time (min)

61.0

4

3-

2

1

4.05

Acquisition Time (min)

4.1

61.0

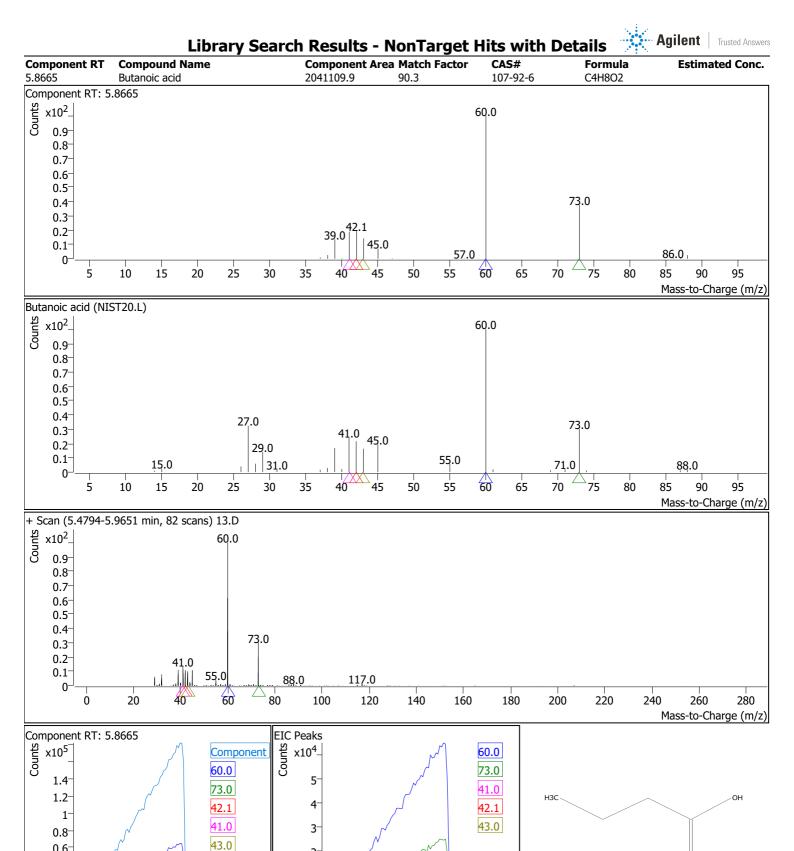
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1.5

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5.7

5.6

5.8

Acquisition Time (min)

5.9

2

1

0.6

0.4

0.2

5.7

5.8 5.9

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.** 504-63-2 7.4228 1,3-Propanediol 1539331.7 86.3 C3H8O2 Component RT: 7.4228 v10² 0.9 57.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 45.0 0.2 42.1 0.1 5 15 25 30 55 70 75 80 10 20 35 40 45 50 85 Mass-to-Charge (m/z) 1,3-Propanediol (NIST20.L) Counts x10²_ 0.9 28.0 58.0 0.8 31.0 0.7 0.6 0.5 0.4 0.3 45.0 0.2 0.1 15.0 18.0 41.0 49.0 55.0 68.0 73.0 30 5 10 15 20 25 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (7.3267-8.1057 min, 132 scans) 13.D st x10² 0.9 57.0 0.8 0.7 31.0 0.6 0.5 0.4^{-} 0.3 43.0 0.2 0.1 20 40 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 7.4228 EIC Peaks Counts Counts x10⁵ x10⁴_ 57.0 Component 57.0 58.0 3 1 58.0 31.0 2.5 0.8 45.0 31.0 2-

45.0

30.0

1.5

0.5

1

7.4

7.6

7.8

Acquisition Time (min)

0.6

0.4

0.2

7.4

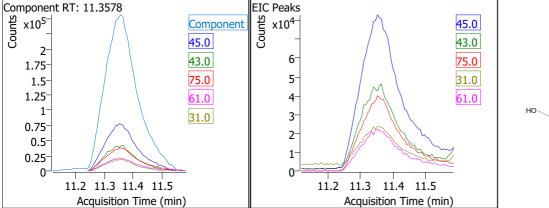
7.6

7.8

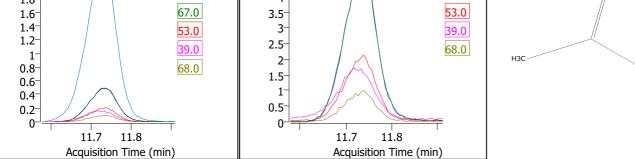
Acquisition Time (min)

30.0

--- **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 11.3578 1,2-Propanediol, 3-methoxy-2046203.8 87.2 C4H10O3 Component RT: 11.3578 v10² 0.9 45.0 0.8 0.7 0.6 43.0 75.0 0.5 0.4 61.0 0.3 31.0 0.2 33.0 0.1 88.0 10 15 20 25 30 35 40 55 60 65 75 80 85 100 105 110 115 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Counts x10²_ 0.9 45.0 0.8 0.7 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 15.0 0.2 33.0 18.0 0.1 88.0 63.0 103.0 71.0 10 15 20 25 30 35 40 45 50 55 60 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (11.2406-11.5484 min, 52 scans) 13.D St x10² 0.9 45.0 0.8 0.7 0.6 75.0 0.5 0.4^{-} 0.3 31.0 61.0 0.2 0.1 88.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z)



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12.2 12.3 12.4

Acquisition Time (min)

56.0

12.5

0.6

0.5 0.4

0.3 0.2-

0.1

29.0

56.0

12.2 12.3 12.4 12.5

Acquisition Time (min)

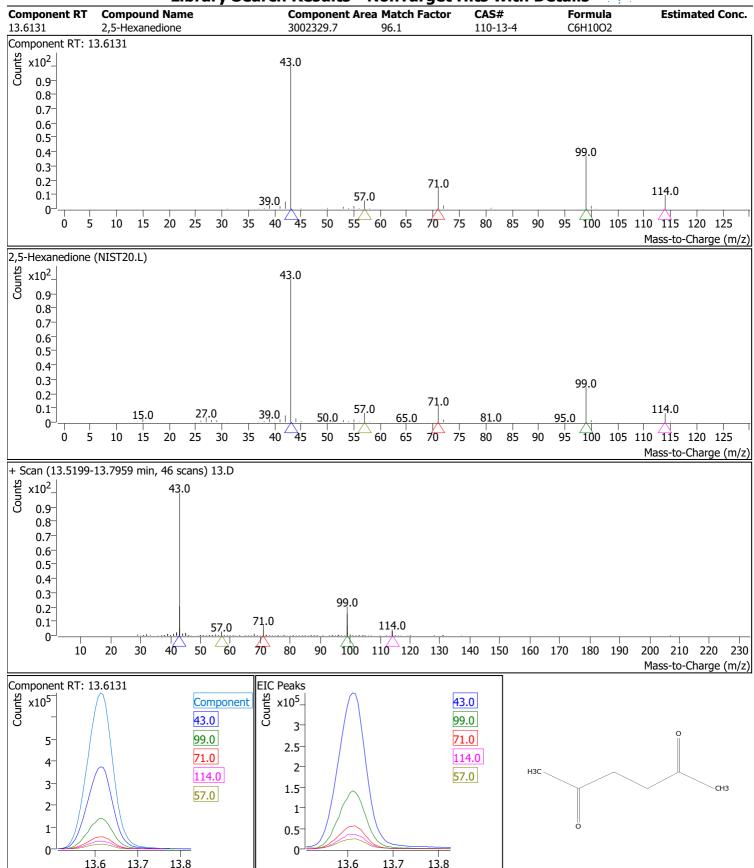
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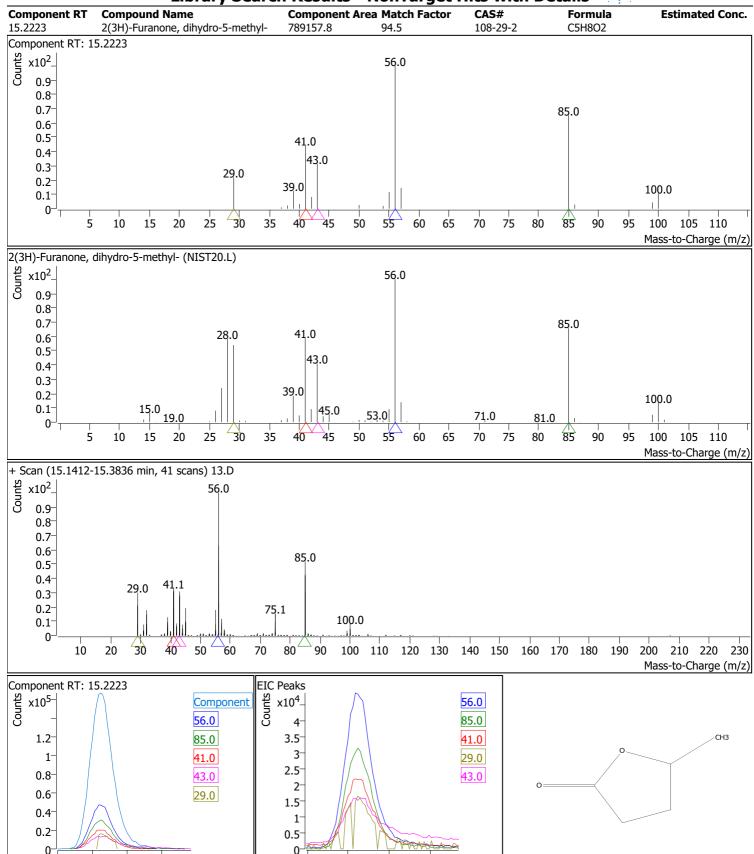


Acquisition Time (min)

Acquisition Time (min)







15.2

15.3

Acquisition Time (min)

15.4

15.2

15.3

Acquisition Time (min)

15.4

--- 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 16.0009 2-Cyclopenten-1-one, 3-methyl-4537925.2 97.7 C6H8O Component RT: 16.0009 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 51.0 0.1 10 15 20 25 30 35 45 50 55 60 65 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 (15.9107-16.2517 min, 58 scans) 13.D st x10² 0.9 96.0 0.8 0.7 0.6 67.0 0.5 0.4^{-} 53.0 0.3 81.0 39.0 0.2 0.1 117.0 32.0 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: 16.0009 **EIC Peaks** Counts Counts x10⁵ 96.0 Component 96.0 67.0 1.8 67.0 1.6 53.0 CH3 6 1.4 81.0 53.0



39.0

1.2

0.8

0.6

0.4

16

16.1

16.2 Acquisition Time (min)

1

81.0

39.0

5

4

3

2-

16

16.1

Acquisition Time (min)

16.2

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 17.8795 2-Cyclopenten-1-one, 3,4-dimethyl-1604291.5 95.1 30434-64-1 C7H10O Component RT: 17.8795 v10² 0.9 95.0 0.8 110.0 0.7^{-} 67.0 0.6 0.5 0.4 0.3 39.0 0.2 41.0 53.0 82.0 0.1 65.0 110 95 20 25 30 35 40 50 55 60 65 75 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 91.0 110 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 (17.7980-17.9404 min, 24 scans) 13.D St x10² 0.9 95.0 0.8 0.7 0.6 110.1 0.5 67.0 0.4^{-} 0.3 39.0 0.2 53.0 0.1 82.0 32.0 103.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 17.8795 EIC Peaks Counts Counts x10⁵-95.0 Component 95.0 39.0 0.9 3 0.8 110.0 110.0 0.7^{-1} 2.5 67.0 67.0 0.6

17.9

18

Acquisition Time (min)

41.0

НЗС

2

1.5

1

17.9

18

Acquisition Time (min)

0.5

39.0

41.0

0.5

0.4

0.3

0.2

0.1

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 17.9725 Phenol 5541228.9 98.1 C6H6O Component RT: 17.9725 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 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 (17.9117-18.3329 min, 71 scans) 13.D St x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 39.0 0.2 0.1 110.1 50.0 32.0 0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 17.9725 EIC Peaks Counts Counts x10⁶ x10⁵ 94.0 Component 94.0 66.0 0.9 3.5 0.8 66.0 65.0 0.7 3-39.0 65.0 0.6 2.5 39.0 95.0

18.1

18.2

Acquisition Time (min)

18.3

2

1

18

1.5

0.5

95.0

0.5

 0.4^{-}

0.3

0.2

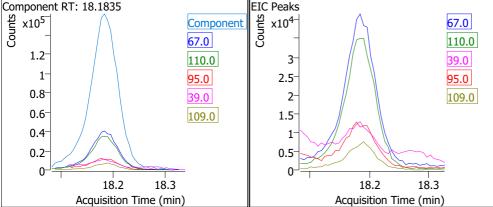
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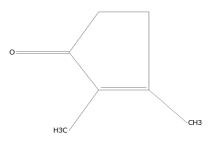
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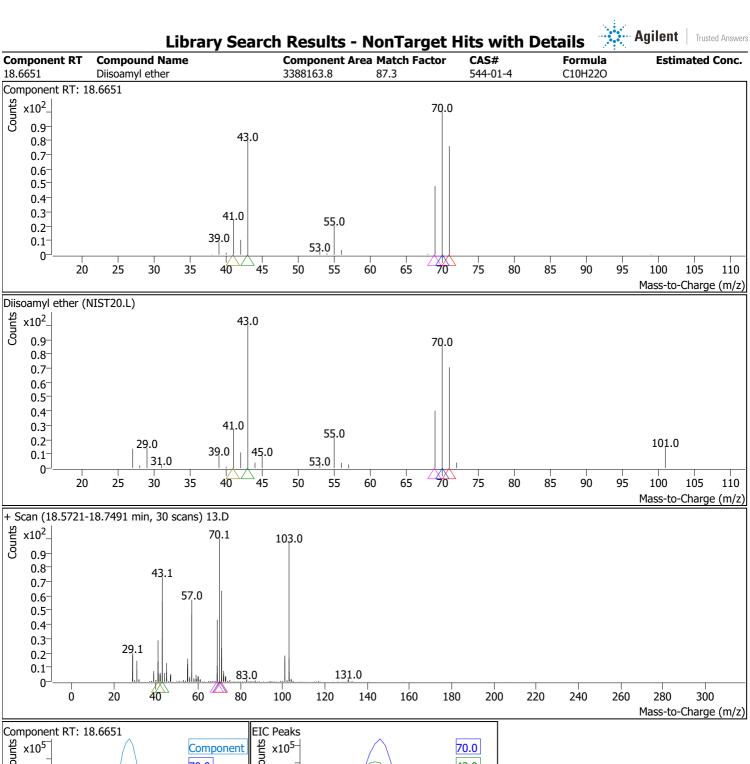
18.1 18.2 18.3

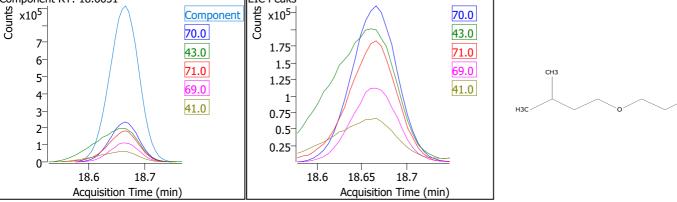
Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 18.1835 2-Cyclopenten-1-one, 2,3-dimethyl-625968.4 91.1 1121-05-7 C7H10O Component RT: 18.1835 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 39.0 0.3 53.0 0.2 41.0 81.0 0.1 110 15 20 30 35 40 45 50 55 60 80 85 100 105 115 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) st 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 (18.0891-18.3321 min, 41 scans) 13.D St x10² 0.9 94.0 67.0 110.1 0.8 0.7 0.6 39.0 0.5 0.4^{-} 32.0 0.3 55.0 0.2 81.0 60.0 0.1 0 10 20 30 40 50 60 70 80 904 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 18.1835 Counts Counts x10⁴ 67.0 Component 67.0 110.0 1.2 110.0 3 39.0









··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 19.7442 2-Cyclopenten-1-one, 3,4-dimethyl-1133086.9 30434-64-1 C7H10O Component RT: 19.7442 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 82.0 110 95 20 25 30 35 45 50 55 60 65 75 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 91.0 110 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 (19.6708-19.8428 min, 28 scans) 13.D St x10² 0.9 103.0 57.0 0.8 0.7 110.1 0.6 43.0 0.5 95.0 0.4^{-} 67.0 0.3 29.1 39.0 47.0 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 19.7442 **EIC Peaks** Counts Counts x10⁴ 95.0 Component 95.0 110.0 2 110.0 5 67.0 1.75 1.5 67.0 39.0

19.8

Acquisition Time (min)

65.0

НЗС

1.25

0.75

0.5 0.25

19.7

19.8

Acquisition Time (min)

1

39.0

65.0

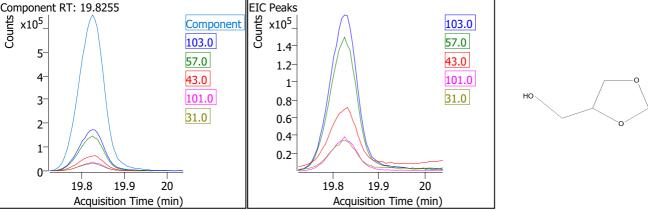
3

2-

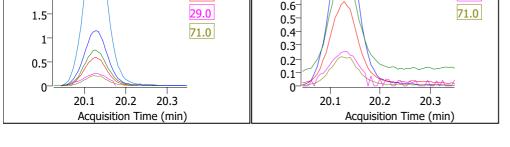
19.7

CH3

--- 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 19.8255 1,3-Dioxolane-4-methanol, 2-ethyl-2781298.9 93.4 C6H12O3 Component RT: 19.8255 v10² 0.9 103.0 57.0 0.8 0.7^{-} 0.6 0.5 43.0 0.4 0.3 31.0 0.2 47.0 72.0 0.1 40 30 100 120 130 Ó 10 20 50 70 80 90 110 140 Mass-to-Charge (m/z) 1,3-Dioxolane-4-methanol, 2-ethyl- (NIST20.L) Counts x10²_ 0.9 57.0 103.0 0.8 0.7 43.0 0.6 29.0 0.5 0.4 0.3 47.0 0.2 72.0 19.0 0.1 131.0 83.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (19.7185-20.0394 min, 54 scans) 13.D St x10² 0.9 57.0 103.0 0.8 0.7 43.0 0.6 0.5 0.4 110.1 0.3 95.0 29.1 0.2 67.0 0.1 81.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 19.8255

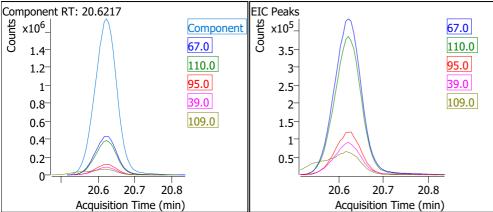


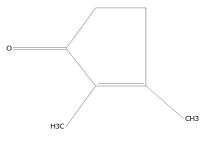
-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1703-51-1 1289071.6 20.1288 3,6-Heptanedione 89.0 C7H12O2 Component RT: 20.1288 v10² 0.9 99.0 0.8 0.7^{-} 43.0 0.6 57.0 0.5 0.4 0.3 29.0 71.0 0.2 0.1 81.0 85.0 100 50 55 65 70 85 20 25 30 35 40 45 60 75 80 90 95 105 Mass-to-Charge (m/z) 3,6-Heptanedione (NIST20.L) Counts 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 (20.0397-20.3486 min, 52 scans) 13.D st x10² 0.9 99.0 0.8 43.0 0.7 0.6 0.5 0.4 0.3 57.0 29.1 0.2 71.0 112.0 0.1 81.0 0 20 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.1288 Counts Counts x10⁵ 99.0 Component 99.0 43.0 0.9 2.5 43.0 57.0 0.8 2 29.0 0.7^{-} 57.0



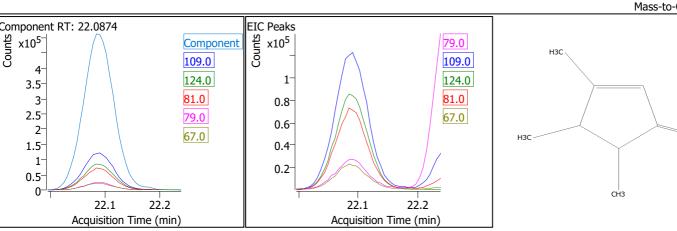
Page 20 of 94

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.6217 2-Cyclopenten-1-one, 2,3-dimethyl-7360343.1 95.6 1121-05-7 C7H10O Component RT: 20.6217 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 95 110 15 20 25 30 35 40 45 50 55 60 65 80 85 90 100 105 115 75 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 (20.5151-20.8361 min, 55 scans) 13.D St x10² 0.9 67.0 110.1 0.8 0.7 0.6 0.5 0.4^{-} 0.3 95.0 0.2 61.0 39.0 81.0 0.1 124.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 20.6217 **EIC Peaks** x10⁶ Counts x10⁵-67.0 Component 67.0 110.0 1.4 3.5 110.0 95.0 1.2 3

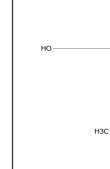




--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 55683-21-1 22.0874 2-Cyclopenten-1-one, 3,4,5-trimethyl-2016960.9 93.0 C8H12O Component RT: 22.0874 $x10^{2}$ 109.0 0.9 0.8 124.0 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 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 (21.9956-22.1859 min, 33 scans) 13.D St x10² 0.9 61.0 0.8 0.7^{-} 0.6 109.0 0.5 0.4^{-} 81.1 0.3 124.1 31.0 0.2 0.1 53.0 67.1 96.1 117.0 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: 22.0874 x10⁵ 79.0 Component НЗС



... 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 22.2542 Phenol, 2-methyl-8300321.4 98.4 C7H8O Component RT: 22.2542 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 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 74.0 43.0 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 (22.1681-22.4773 min, 53 scans) 13.D st x10² 0.9 108.0 0.8 61.0 0.7 43.0 0.6 0.5 0.4^{-} 77.0 0.3 0.2 31.0 90.0 51.0 0.1 39.0 99.0 0 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) EIC Peaks Component RT: 22.2542 Counts x10⁶ x10⁵ 108.0 Component 108.0 107.0 1.6 4 1.4 107.0 3.5 77.0 1.2 3 77.0 79.0



90.0

22.3

22.4

Acquisition Time (min)

2.5

1.5

2

1.5 0.5

22.2

79.0

90.0

1

0.8

0.6

0.4

0.2

22.2

22.3

22.4

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.** 98-86-2 22.4172 Acetophenone 542756.9 91.6 **C8H8O** Component RT: 22.4172 y x10² 0.9 105.0 0.8 77.0 0.7 0.6 0.5 0.4 120.0 0.3 51.0 0.2 0.1 58.0 100 105 110 115 120 125 130 135 35 50 55 60 65 70 75 98 85 90 95 Mass-to-Charge (m/z) Acetophenone (NIST20.L) \$\frac{\psi}{0.9} \tag{0.9} 105.0 0.8 77.0 0.7 0.6 0.5 0.4 0.3 120.0 51.0 0.2 43.0 0.1 15.0 39.0 74.0 63.0 56.0 15 20 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 (22.3286-22.5902 min, 45 scans) 13.D St x10²_ 0.9 43.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 31.0 0.2 99.0 0.1 77.0 55.0 117.0 129.0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 22.4172 EIC Peaks Counts St x10⁴-105.0 Component 105.0 77.0 3.5 77.0 120.0 3 0.8

51.0

50.0

нзс

120.0

51.0

50.0

0.6

0.4

0.2

22.4

22.5

Acquisition Time (min)

2.5

1.5

0.5

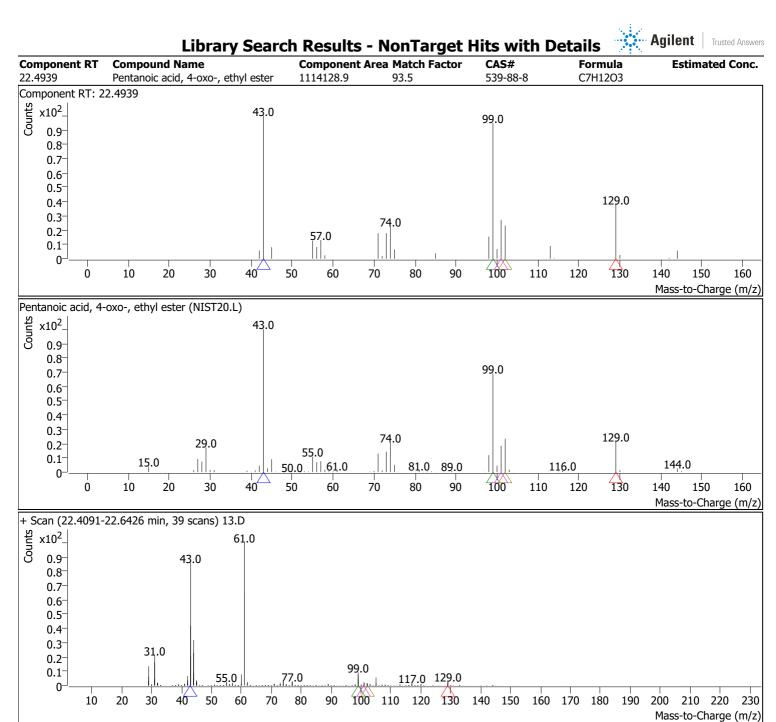
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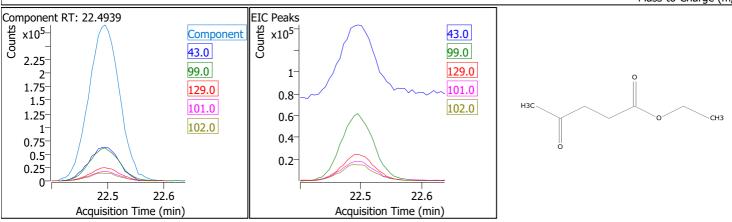
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22.4

22.5

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.** 23.0965 1-Octanol 5300991.4 96.0 111-87-5 C8H18O Component RT: 23.0965 v10² 0.9 56.0 41.0 0.8 69.1 0.7^{-} 84.1 0.6 29.0 0.5 0.4 0.3 0.2 0.1 100 105 110 115 120 125 130 135 140 45 50 65 70 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10²_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 55 20 25 30 35 40 45 50 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9886-23.2443 min, 44 scans) 13.D St x10²_ 0.9 0.8 0.7 43.0 0.6 0.5 0.4^{-} 31.0 0.3 56.1 69.1 84.1 0.2^{-} 110.1 0.1 0 50 10 20 30 40 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 60 Mass-to-Charge (m/z) Component RT: 23.0965 **EIC Peaks** Counts x10⁶ Counts x10⁵-56.0 Component 56.0 55.0 1 1.2 55.0 41.0 1-0.8 41.0 69.1 0.8

23.1

23.2 Acquisition Time (min)

70.1

0.6

0.4

0.2

0

23.1

23.2

Acquisition Time (min)

69.1

70.1

0.6

0.4

0.2

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.5745 p-Cresol 4084851.2 85.3 106-44-5 C7H8O Component RT: 23.5745 y x10² 0.9 107.0 0.8 0.7 0.6 0.5 0.4 0.3 79.0 0.2 90.0 0.1 55.0 61.0 55 60 90 110 15 20 25 30 35 40 45 50 65 70 75 85 95 100 105 115 Mass-to-Charge (m/z) p-Cresol (NIST20.L) st x10²_ 0.9-107.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 0.2 90.0 0.1 90 15 20 25 30 35 40 50 55 60 70 75 80 85 95 100 105 110 115 120 Mass-to-Charge (m/z) + Scan (23.5012-23.6189 min, 20 scans) 13.D St x10²_ 0.9 124.0 109.0 0.8 0.7 81.0 0.6 0.5 0.4^{-} 61.0 0.3 43.0 53.0 0.2 77.0 31.0 39.0 0.1 71.0 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) EIC Peaks Component RT: 23.5745 Counts x10⁶ 0.9 Counts x10⁵ 107.0 Component 107.0 108.0 3 8.0 108.0 77.0 2.5 0.7^{-1} 79.0 79.0 2-0.6

23.55

77.0

90.0

1.5

1-

0.5

0.5

0.4

0.3

0.2

0.1

23.6

23.7

Acquisition Time (min)

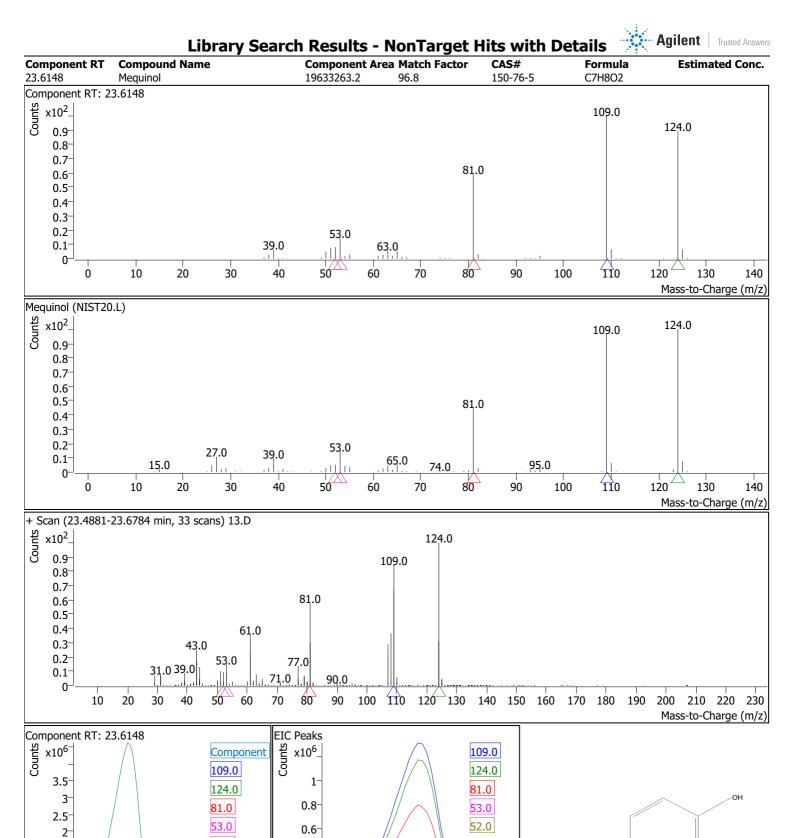
23.8

90.0

23.6

Acquisition Time (min)

Н3С



23.55

23.6

Acquisition Time (min)

23.65

52.0

0.4

0.2

1.5

0.5

1

23.6

23.7

Acquisition Time (min)

нзс-

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 28790-86-5 23.7224 2-Cyclopenten-1-one, 2,3,4-trimethyl-3246750.2 87.0 C8H12O Component RT: 23.7224 v10² 0.9 109.0 124.0 81.0 0.8 0.7^{-} 0.6 96.0 0.5 0.4 0.3 67.0 39.0 0.2 53.0

80

85

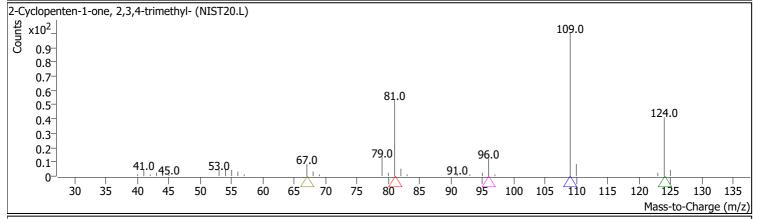
95

100

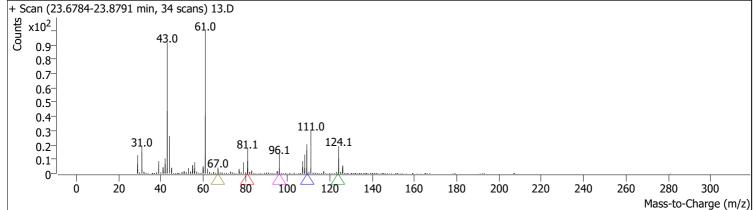
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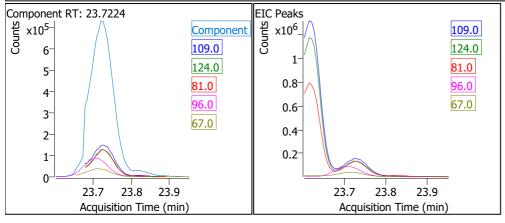
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0 125 130 135 Mass-to-Charge (m/z)



75





0.1

30

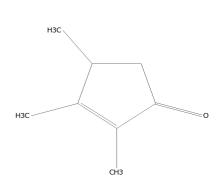
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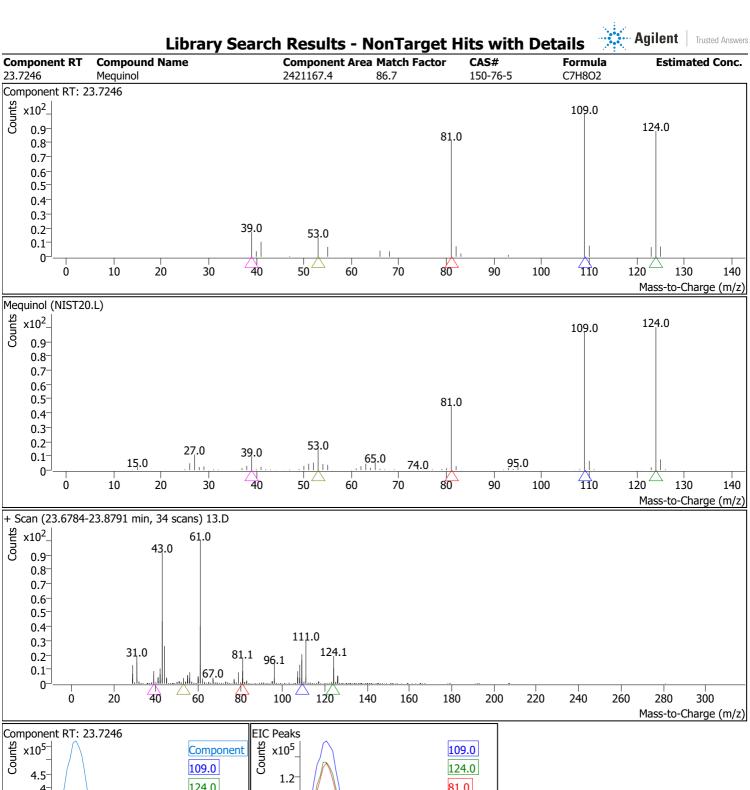
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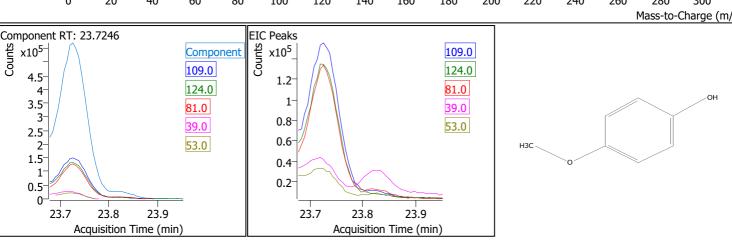
50

55

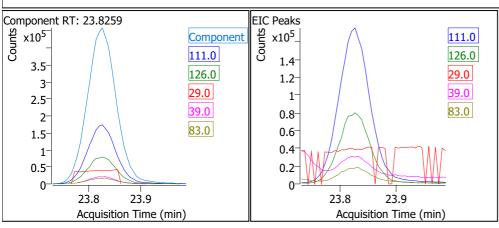
65

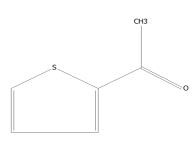




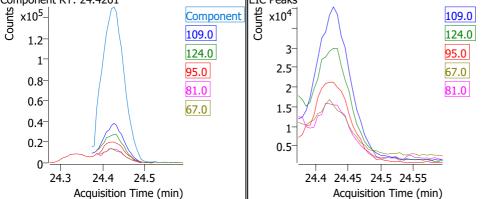


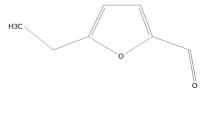
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 88-15-3 23.8259 Ethanone, 1-(2-thienyl)-1771486.3 90.3 C6H6OS Component RT: 23.8259 v10² 0.9 111.0 0.8 0.7 0.6 0.5 126.0 0.4 29.0 0.3 0.2 83.0 45.0 55.0 0.1 0 30 804 110 10 20 50 60 70 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 15.0 50.0 27.032.0 97.0 30 110 10 20 40 50 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.7319-23.9928 min, 44 scans) 13.D st x10² 0.9 43.0 0.8 0.7 0.6 0.5 0.4 0.3 31.0 111.0 0.2 0.1 124.1 81.1 96.1 80 20 60 100 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 23.8259 **EIC Peaks** Counts x10⁵ 111.0 Component 111.0 126.0 СНЗ



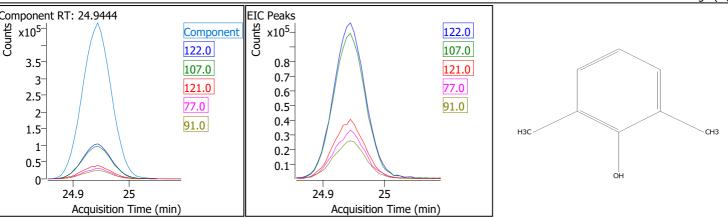


··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23074-10-4 24.4261 5-Ethyl-2-furaldehyde 568966.7 86.1 C7H8O2 Component RT: 24.4261 $x10^{2}$ 109.0 0.9 0.8 124.0 0.7^{-} 95.0 0.6 0.5 67.0 0.4 81.0 0.3 53.0 0.2 39.0 0.1 110 10 20 30 40 50 60 80 90 100 130 140 Mass-to-Charge (m/z) 5-Ethyl-2-furaldehyde (NIST20.L) Counts x10²_ 0.9 124.0 109.0 0.8 0.7 0.6 0.5 0.4 95.0 0.3 53.0 67.0 39.0 81.0 0.2 27.0 0.1 15.0 105.0 74.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (24.3740-24.5276 min, 26 scans) 13.D St x10² 0.9 60.0 0.8 73.0 0.7 109.1 0.6 0.5 0.4^{-} 124.1 95.0 0.3 55.0 81.0 0.2 29.0 67.0 0.1 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 70 Mass-to-Charge (m/z) Component RT: 24.4261 EIC Peaks Counts x10⁵x10⁴ 109.0 Component 109.0 124.0 1.2 3 124.0 95.0 1

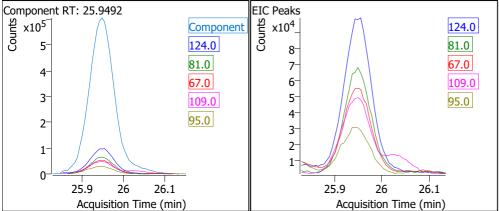


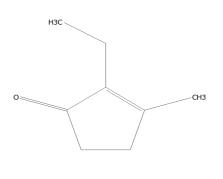


··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Phenol, 2,6-dimethyl-24.9444 1689235.8 97.9 576-26-1 C8H10O Component RT: 24.9444 v10² 0.9 122.0 107.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 91.0 0.2 39.0 103.0 51.0 0.1 30 35 50 55 08 85 90 95 100 105 110 115 120 125 130 135 15 75 Mass-to-Charge (m/z) Phenol, 2,6-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 0.2 103.0 39.0 51.0 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 (24.8868-25.0026 min, 19 scans) 13.D st x10² 0.9 122.1 0.8 107.0 0.7^{-} 0.6 0.5 0.4^{-} 0.3 77.0 91.0 0.2 61.0 43.0 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 24.9444 **EIC Peaks** x10⁵_ 122.0 Component



··· 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 2619665.5 88.7 C8H12O Component RT: 25.9492 $x10^{2}$ 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 20 25 35 40 50 55 65 80 85 90 95 100 105 110 115 120 125 130 135 60 70 75 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 (25.8665-26.0664 min, 34 scans) 13.D st x10² 0.9 124.1 43.0 0.8 0.7^{-} 0.6 81.1 0.5 67.0 0.4^{-} 109.1 0.3 95.0 39.0 0.2 53.0 61.0 91.0 103.0 0.1 29.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 190 200 210 220 230 160 Mass-to-Charge (m/z) Component RT: 25.9492 **EIC Peaks**





--- 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 26.8501 Phenol, 2-ethyl-1842418.3 C8H10O Component RT: 26.8501 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 39.0 91.0 51.0 65.0 35 50 55 60 65 75 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) Phenol, 2-ethyl- (NIST20.L) St x10²_ 0.9 107.0 0.8 0.7 0.6 0.5 122.0 0.4 0.3 77.0 0.2 39.0 51.0 0.1 91.0 27.0 103.0 65.0 15.0 15 20 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 (26.7770-27.0022 min, 38 scans) 13.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 122.1 0.3 77.0 0.2 138.1 95.1 39.0 51.0 67.0 0.1 117.1 151.0 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) EIC Peaks Component RT: 26.8501 Counts x10⁵ Counts x10⁵ 107.0 Component 107.0 122.0 4 1.4 3.5 122.0 77.0 1.2 3 77.0 79.0

26.9

Acquisition Time (min)

108.0

1

0.8

0.6

0.4

0.2

26.8

79.0

108.0

27

2.5

1.5

2

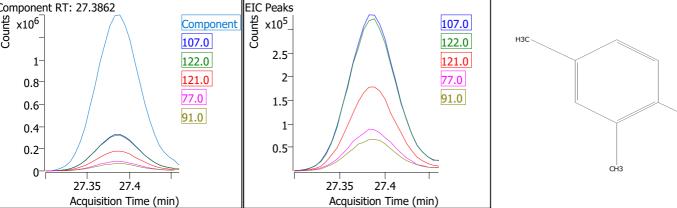
1⁻ 0.5⁻

26.8

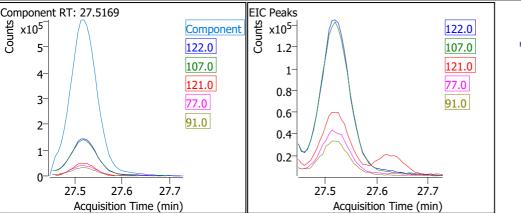
26.9

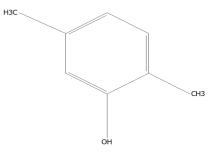
Acquisition Time (min)

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Phenol, 2,4-dimethyl-27.3862 5299381.8 105-67-9 C8H10O Component RT: 27.3862 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 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 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (27.3006-27.4600 min, 27 scans) 13.D St x10²_ 0.9 122.1 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 0.1 136.0 100 110 120 130 10 20 50 60 70 80 90 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 27.3862 Counts Counts x10⁵ 107.0 Component 107.0 122.0 2.5 1 122.0 121.0



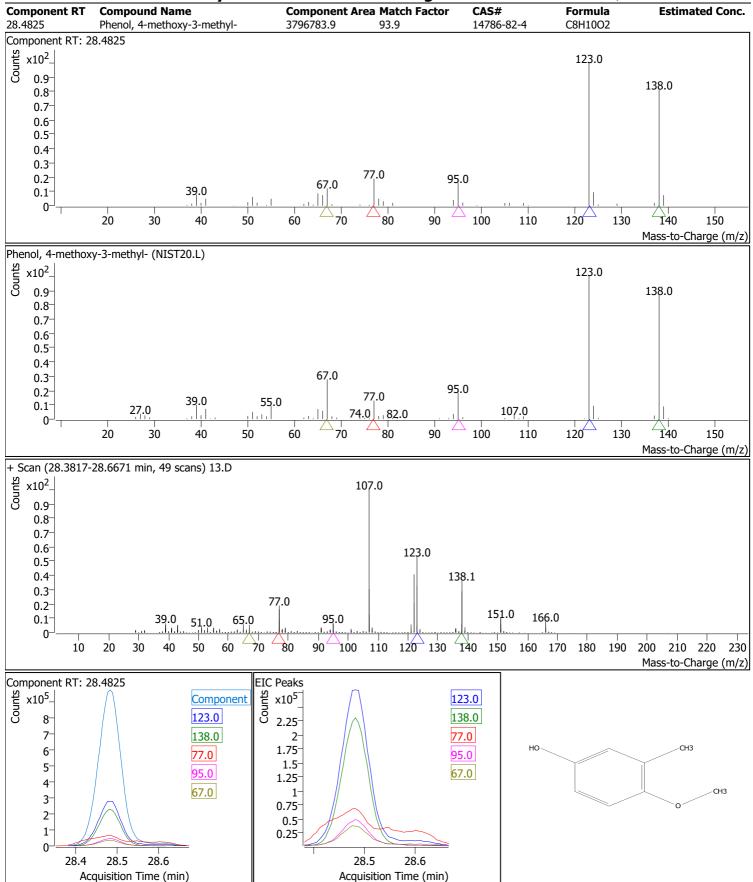
--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Phenol, 2,5-dimethyl-95-87-4 27.5169 2446879.7 98.1 C8H10O Component RT: 27.5169 v10² 0.9 122.0 107.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 91.0 0.2 39.0 0.1 35 40 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 (27.4600-27.5849 min, 22 scans) 13.D St x10²_ 0.9 122.1 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 77.0 0.2 91.0 151.0 39.0 166.0 51.0 0.1 65.0 136.0 100 110 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) Component RT: 27.5169 EIC Peaks x10⁵ 122.0 Component



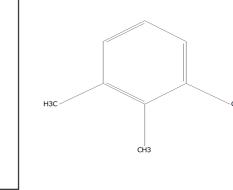








··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 28.8404 Phenol, 2,3-dimethyl-1102017.8 96.2 526-75-0 C8H10O Component RT: 28.8404 v10² 0.9 107.0 122.0 0.8 0.7 0.6 0.5 0.4 0.3 77.0 91.0 0.2 103.0 0.1 39.0 55 75 80 85 90 100 105 110 115 65 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 91.0 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 (28.7630-28.9347 min, 29 scans) 13.D St x10²_ 0.9 107.0 122.1 0.8 0.7^{-} 151.0 0.6 0.5 0.4^{-} 128.0 166.0 0.3 77.0 91.0 0.2 136.0 55.0 39.0 67.0 0.1 بنياباني بالمسابل والمسابل وال 10 20 30 40 50 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 28.8404 **EIC Peaks** x10⁵ Counts x10⁴ 107.0 Component 107.0 122.0 2.25 6 122.0 121.0 5 1.75 121.0 77.0



91.0

28.8

28.9 Acquisition Time (min)

4

3-

2

77.0

91.0

1.5

1.25

0.75

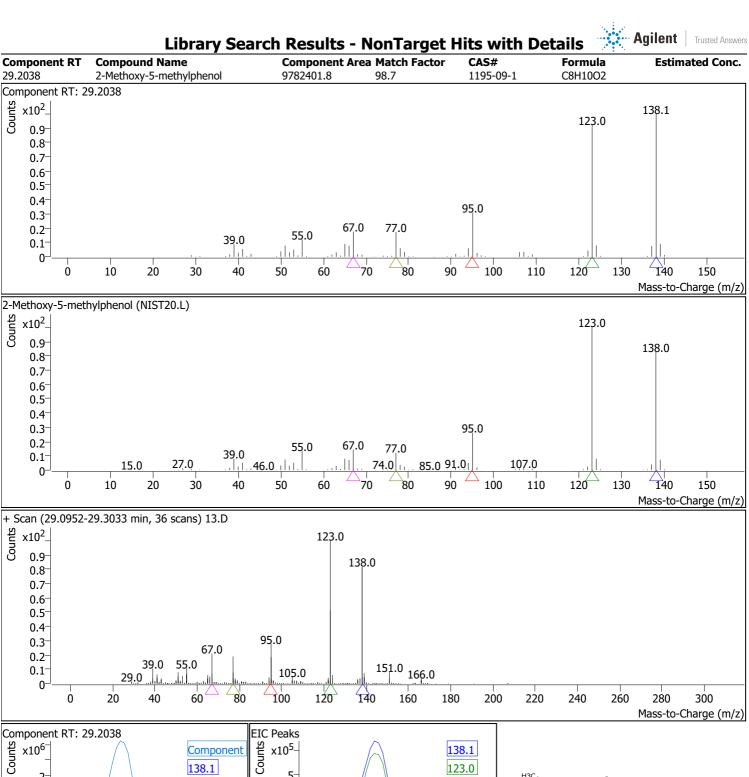
0.5 0.25

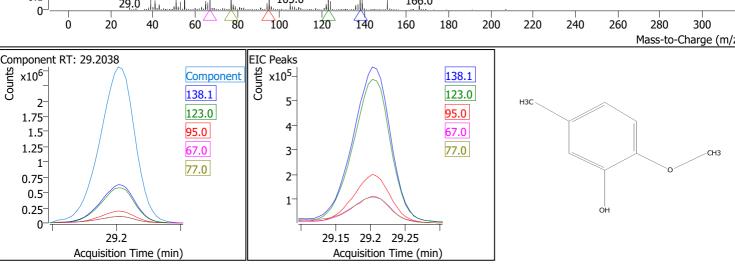
28.8

28.9

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.** 124-07-2 29.5255 Octanoic acid 3539630.2 92.9 C8H16O2 Component RT: 29.5255 $x10^{2}$ 60.0 0.9 73.0 0.8 0.7^{-} 0.6 0.5 0.4 43.0 101.0 55.0 0.3 85.0 29.0 0.2 0.1 0 40 60 10 20 30 50 70 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) Octanoic acid (NIST20.L) st x10²_ 0.9-60.0 0.8 0.7 73.0 0.6 0.5 43.0 55.0 0.4 0.3 101.0 85.0 0.2 29.0 69.0 115.0 0.1 91.0 97.0 127.0 144.0 40 60 10 20 30 50 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (29.2201-29.5938 min, 63 scans) 13.D st x10² 0.9 138.1 123.0 0.8 0.7 60.0 0.6 0.5 0.4^{-} 73.0 151.0 43.0 0.3 55.0 67.0 0.2 166.0 7.085.1 115.0 0.1 20 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 10 Mass-to-Charge (m/z) EIC Peaks Component RT: 29.5255 X10⁵ Counts x10⁴ 60.0 Component 60.0 73.0 3.5 6 73.0 43.0 3 5 43.0 41.0 2.5



29.3 29.4 29.5 29.6 Acquisition Time (min)

101.0

101.0

41.0

29.6

3

2

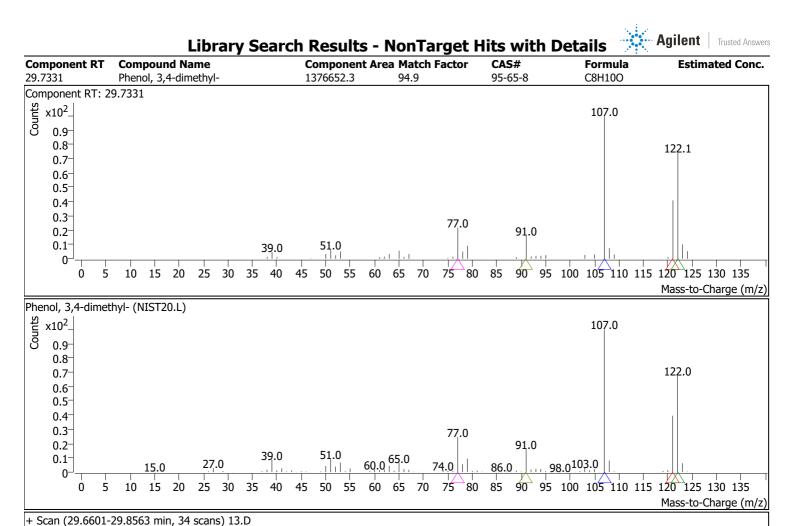
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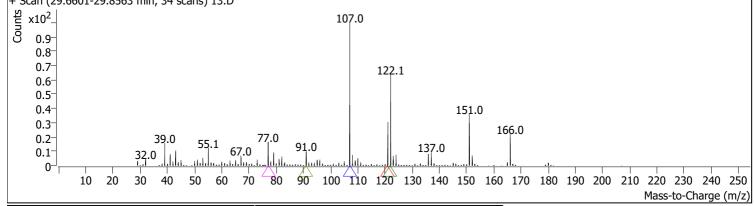
1.5

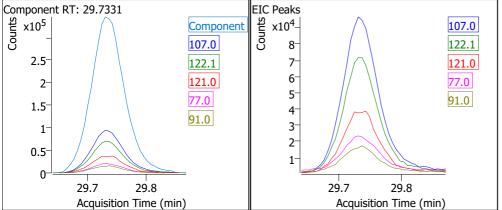
1⁻ 0.5

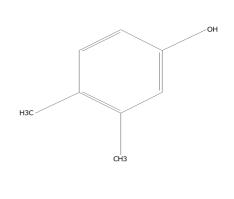
29.4

Acquisition Time (min)

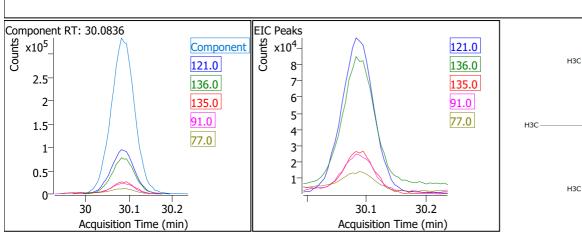




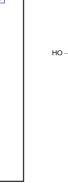




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 527-54-8 30.0836 Phenol, 3,4,5-trimethyl-1282704.1 93.1 C9H12O Component RT: 30.0836 v10² 0.9 121.0 136.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 91.0 0.2 77.0 39.0 65.0 0.1 ___80 120 20 30 40 50 60 70 90 100 110 130 140 150 Mass-to-Charge (m/z) Phenol, 3,4,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 136.0 121.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 91.0 77.0 39.0 0.1 27.0 51.0 65.0 103.0 117.0 59.0 120 20 30 40 50 60 70 80 90 100 110 130 140 150 Mass-to-Charge (m/z) + Scan (29.9931-30.1952 min, 35 scans) 13.D St x10²_ 0.9 57.0 0.8 0.7 121.0 0.6 0.5 136.1 0.4^{-} 0.3 151.0 29.1 0.2 166.0 43.0 67.1 ^{75.0} 91.0 146.0 0.1 110.0 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: 30.0836 $x10^{4}$ 121.0 Component



--- 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 30.3955 Catechol 46924505.4 97.9 C6H6O2 Component RT: 30.3955 y x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 ² 95 10 15 35 45 50 55 75 80 85 90 100 105 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 ∠65 10 15 25 30 35 40 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.3558-31.3250 min, 164 scans) 13.D st x10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 81.092.0 53.0 0.1 39.0 180.0 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.3955 EIC Peaks Counts Counts x10⁶ x10⁶ 110.0 Component 110.0 64.0 3 1.2 64.0 63.0 2.5 1 63.0 81.0



92.0

31.2

30.6 30.8 31

Acquisition Time (min)

0.8

0.6

 0.4°

0.2

81.0

92.0

2

1

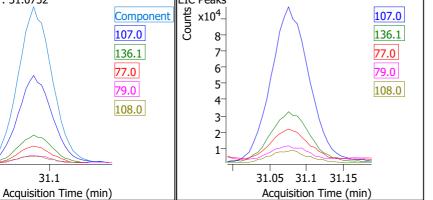
30.5 30.75

31

Acquisition Time (min)

1.5

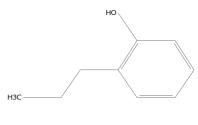
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 644-35-9 31.0752 Phenol, 2-propyl-619043.3 89.8 C9H12O Component RT: 31.0752 v10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4 136.1 0.3 77.0 0.2 79.0 0.1 96.0 95 100 105 110 115 120 125 130 135 140 145 150 35 65 75 80 Mass-to-Charge (m/z) Phenol, 2-propyl- (NIST20.L) Counts x10²_ 0.9 107.0 0.8 0.7 0.6 0.5 0.4 0.3 136.0 77.0 0.2 0.1 51.0 39.0 63.0 91.0 115.0 100 105 110 115 120 125 130 135 140 145 150 35 40 45 50 55 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (31.0102-31.1594 min, 25 scans) 13.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 136.1 165.0 180.0 0.2 64.0 77.0 97.0 43.0 0.1 125.0 150.0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 31.0752 x10⁵ 1.4 Counts x10⁴ 107.0 Component 107.0 136.1 8-1.2 136.1 7 77.0 НО 6 1



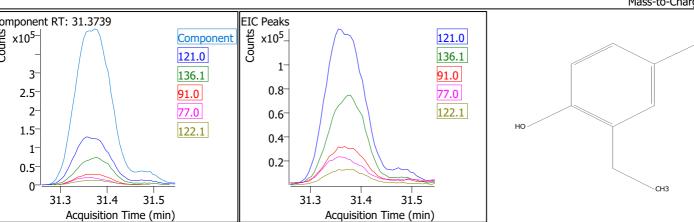
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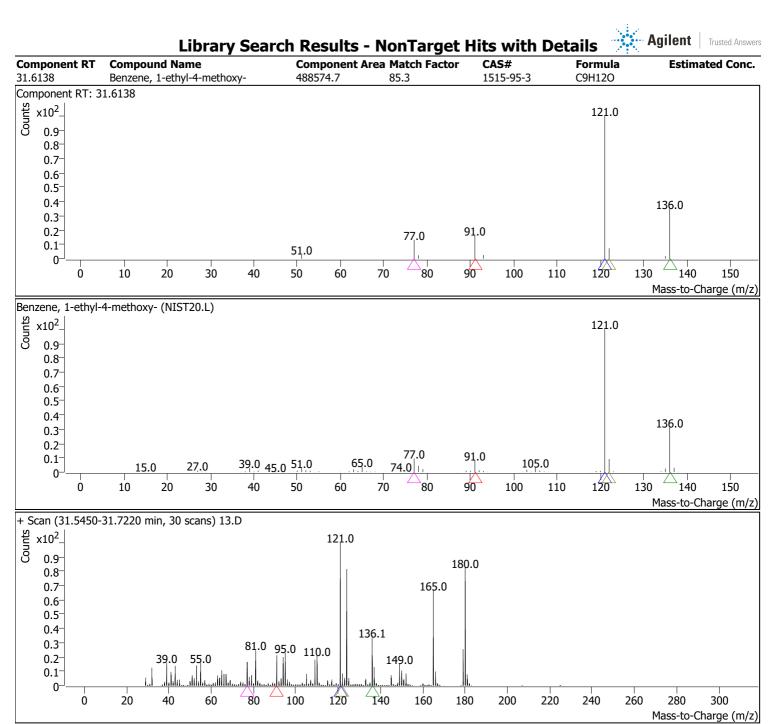
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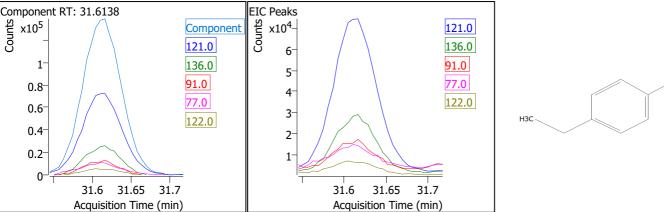
0.4



··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 31.3739 Phenol, 2-ethyl-4-methyl-2397343.8 3855-26-3 C9H12O Component RT: 31.3739 v10² 0.9 121.0 0.8 0.7 0.6 136.1 0.5 0.4 0.3 91.0 0.2 77.0 0.1 107.0 0 90 120 10 20 30 40 50 60 70 100 110 130 140 150 Mass-to-Charge (m/z) Phenol, 2-ethyl-4-methyl- (NIST20.L) Counts x10²_ 0.9 121.0 0.8 0.7 0.6 136.0 0.5 0.4 0.3 0.2 77.0 91.0 0.1 60.065.0 39.0 46.051.0 115.0 74.0 . 83.0 0 10 20 30 40 60 70 80 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (31.2741-31.5331 min, 44 scans) 13.D st x10² 0.9 121.0 0.8 0.7 0.6 0.5 0.4 136.1 165.0 180.0 0.3 91.0 110.0 0.2 43.0 55.0 77.0 0.1 150.0 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 31.3739 Counts x10⁵⁻ x10⁵-121.0 Component 121.0 136.1



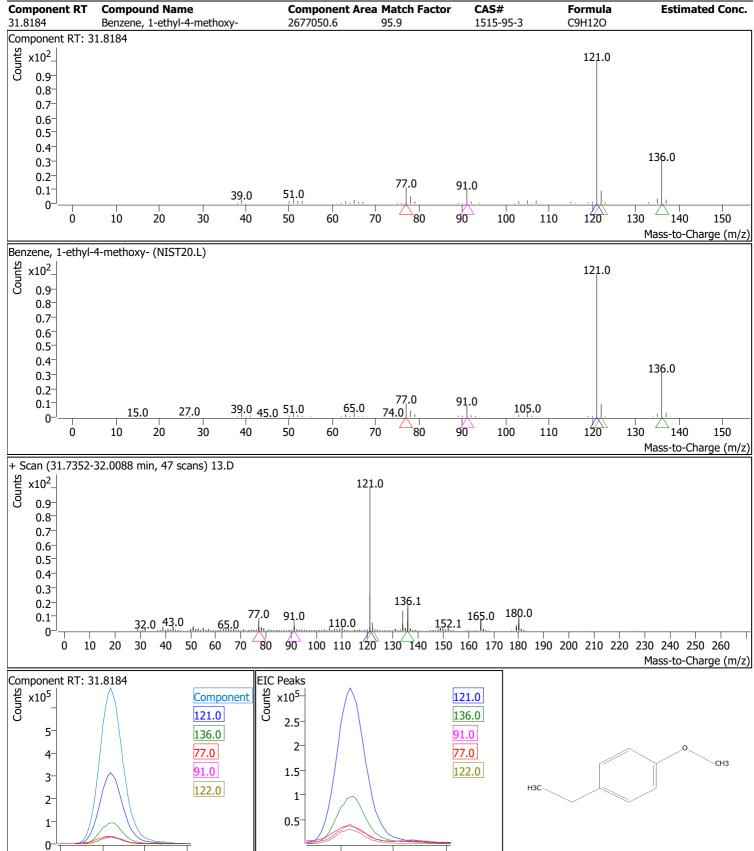




CH3







31.8

31.9 Acquisition Time (min)

31.8

31.9

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.** 88-69-7 32.0999 Phenol, 2-(1-methylethyl)-906542.2 87.6 C9H12O Component RT: 32.0999 v10² 0.9 121.0 0.8 0.7 0.6 0.5 136.0 0.4 0.3 91.0 0.2 77.0 107.0 0.1 39.0 129.0 51.0 50 90 110 130 10 20 30 40 60 70 100 120 140 150 Mass-to-Charge (m/z) Phenol, 2-(1-methylethyl)- (NIST20.L) St x10²_ 0.9 121.0 0.8 0.7 0.6 0.5 0.4 0.3 136.0 0.2 28.0 0.1 39.0 45.0 51.0 31.0 60.065.0 107.0 115.0 110 120 10 20 30 40 50 60 70 80 90 100 130 140 150 Mass-to-Charge (m/z) + Scan (32.0088-32.2376 min, 39 scans) 13.D st x10² 0.9 121.1 0.8 180.0 135.0 0.7 0.6 150.0 165.0 0.5 0.4^{-} 0.3 91.0 0.2 110.1 0.1 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 32.0999 Counts Counts x10⁴ 121.0 Component 121.0 136.0 1.8 136.0 77.0 1.6 6



32.1

Acquisition Time (min)

91.0

107.0

32.2

нзс

CH3

1.4

1.2

0.8

0.6

0.4

32.1

Acquisition Time (min)

1-

91.0

77.0

107.0

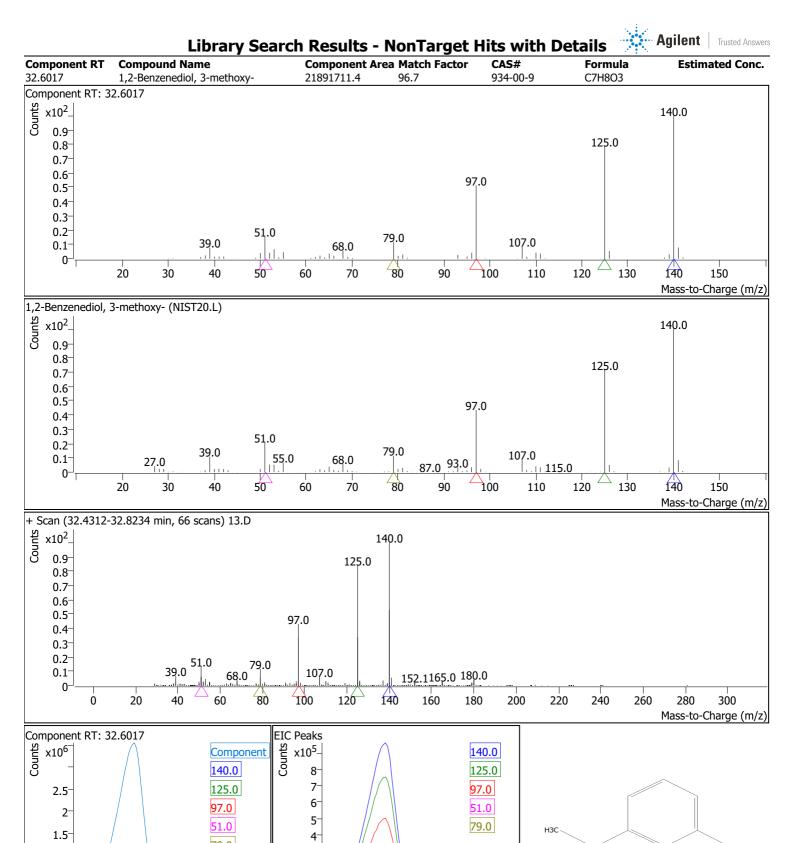
32.2

5

4

3

2





79.0

1-

32.6

32.7

Acquisition Time (min)

0.5

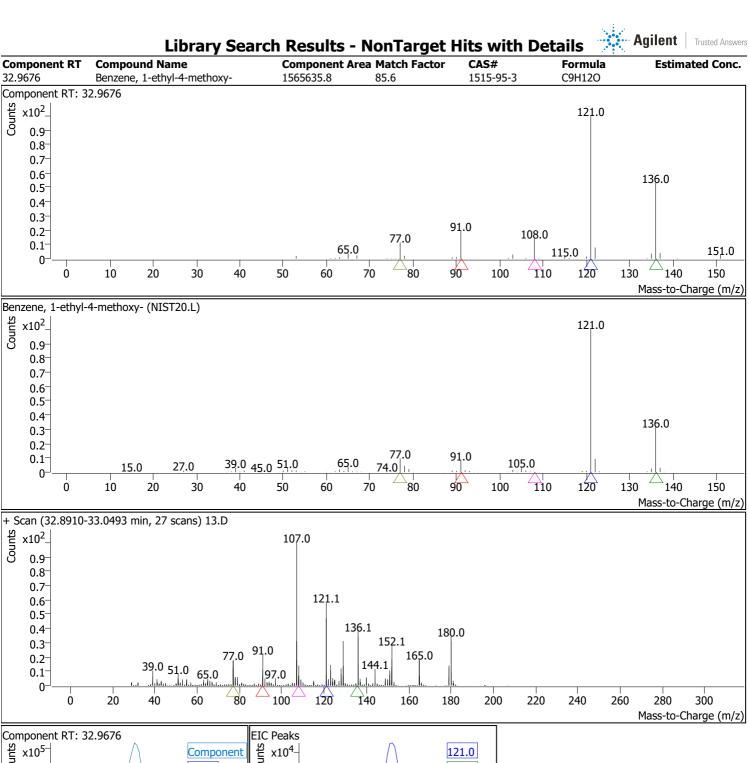
3-

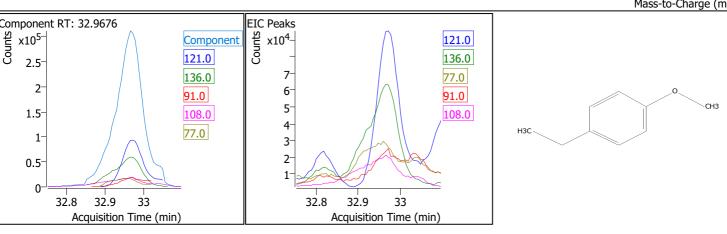
2

32.5

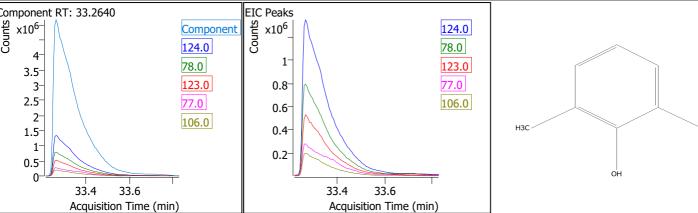
32.6

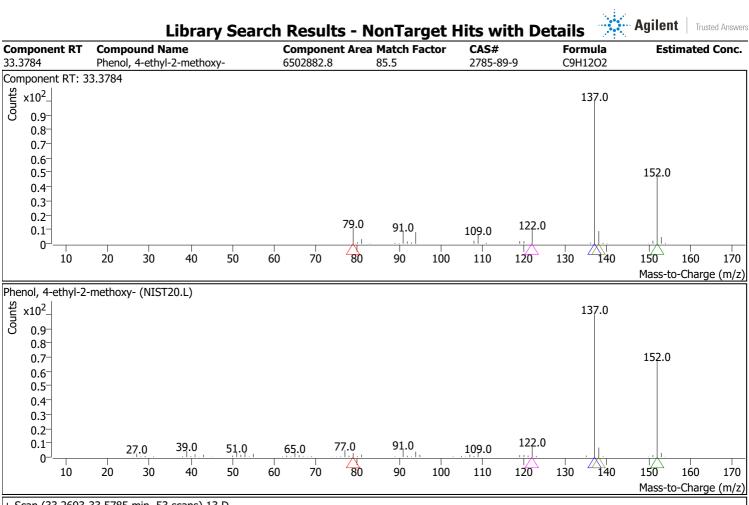
32.7 Acquisition Time (min) ОН

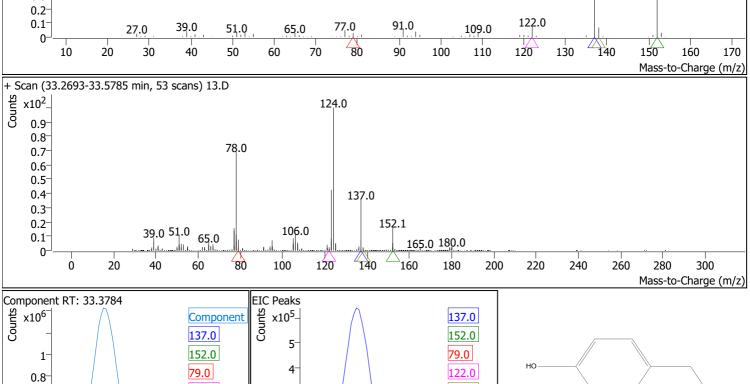


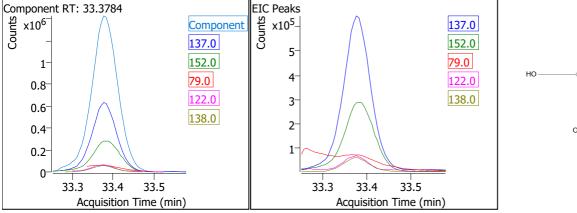


··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 488-17-5 33.2640 1,2-Benzenediol, 3-methyl-38503347.8 96.9 C7H8O2 Component RT: 33.2640 v10² 0.9 124.0 0.8 0.7^{-} 78.0 0.6 0.5 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 78.0 0.4 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 (33.2218-33.8045 min, 99 scans) 13.D st x10² 0.9 124.0 0.8 78.0 0.7 0.6 0.5 0.4 137.0 0.3 0.2 39.0 51.0 65.0 152.1 106.0 0.1 165.0 179.0 194.1 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 33.2640 EIC Peaks Counts Counts x10⁶ 124.0 Component 124.0 78.0 4 1 78.0 123.0 3.5









Library Search Results - NonTarget Hits with Details CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 3864001.9 112-05-0 34.0012 Nonanoic acid 88.9 C9H18O2 Component RT: 34.0012 v10² 0.9 60.0 73.0 0.8 0.7^{-} 57.0 0.6 0.5 41.0 115.0 0.4 129.0 0.3 29.0 0.2 0.1 40 10 20 30 50 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) Nonanoic acid (NIST20.L) st x10²_ 0.9-60.0 73.0 0.8 0.7 0.6 57.0 0.5 0.4 41.0 0.3 0.2 29.0 69.0 129.0 98.0 87.0 0.1 158.0 141.0 18.0 93.0111 111.0 40 10 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (33.7226-34.0839 min, 61 scans) 13.D st x10² 0.9 179.0 0.8 60.0 0.7 43.0 194.1 0.6 0.5 0.4^{-} 121.0 91.0 165.0 0.3 136.1^{149.0} 29.1 0.2 0.1 0 ²80 60 20 40 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 34.0012 Counts x10⁵ x10⁴ 60.0 Component 60.0 71.0 3.5 73.0 73.0 3.5 3 57.0 57.0

41.0

3

2

2.5

1.5

0.5

33.8

33.9

34

Acquisition Time (min)

34.1

71.0

41.0

2.5

1.5

2

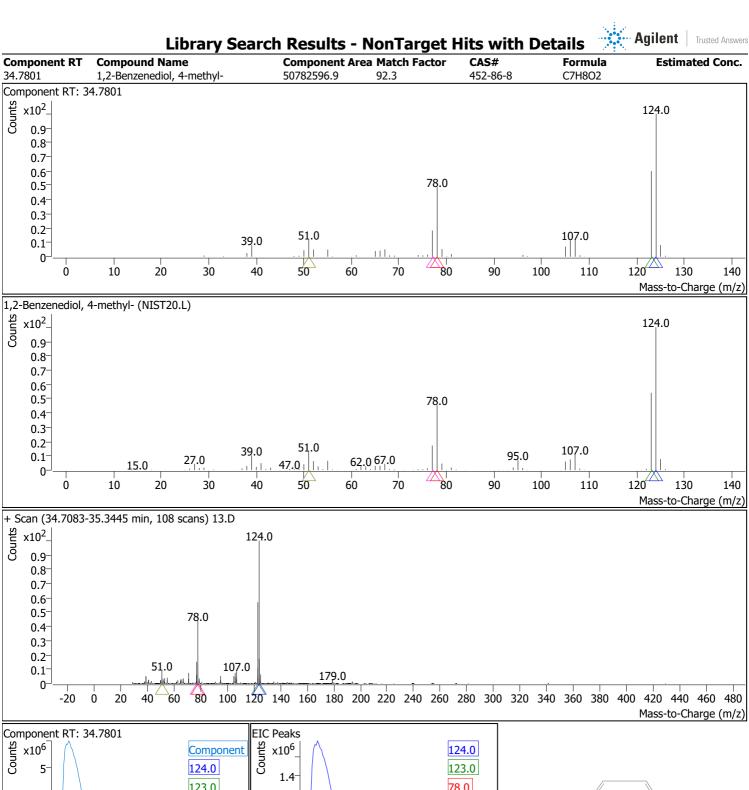
1.5 0.5

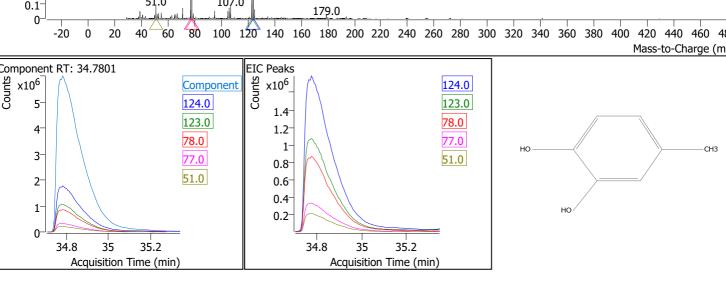
33.8

33.9

34

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.** 1,3-Benzenediol, 2,5-dimethyl-488-87-9 35.4100 22235668.2 93.5 C8H10O2 Component RT: 35.4100 v10² 0.9 138.1 0.8 0.7 0.6 0.5 123.0 91.0 0.4 0.3 0.2 120.0 65.0 0.1 120 20 30 40 50 60 70 80 90 100 110 130 140 150 Mass-to-Charge (m/z) 1,3-Benzenediol, 2,5-dimethyl- (NIST20.L) Counts x10²_ 0.9 138.0 0.8 0.7 0.6 0.5 123.0 0.4 0.3 91.0 0.2 53.0 39.0 65.0 83.0 109.0 0.1 74.0 20 30 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (35.3207-35.6596 min, 58 scans) 13.D st x10² 0.9 138.1 71.0 0.8 0.7 0.6 0.5 91.0 0.4^{-} 123.0 0.3 0.2 43.0 53.0 65.0 77.0 0.1 29.0 107.0 179.0 194.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 35.4100 **EIC Peaks** Counts x10⁶ Counts x10⁶-138.1 Component 138.1 123.0 нзс 3.5 0.8 123.0 91.0 3 0.7 91.0 137.0

35.5

35.6 Acquisition Time (min)

92.0

0.6

0.5

 0.4^{-}

0.3

0.2

 0.1°

35.4

137.0

92.0

2.5

1.5

0.5

2

1

35.4

35.5

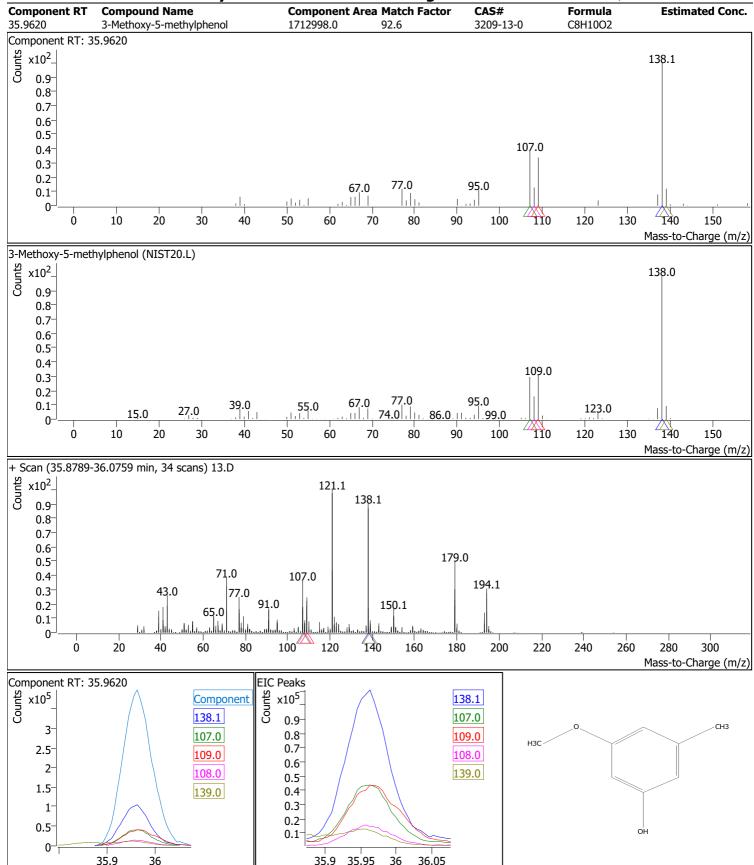
Acquisition Time (min)

35.6

CH3

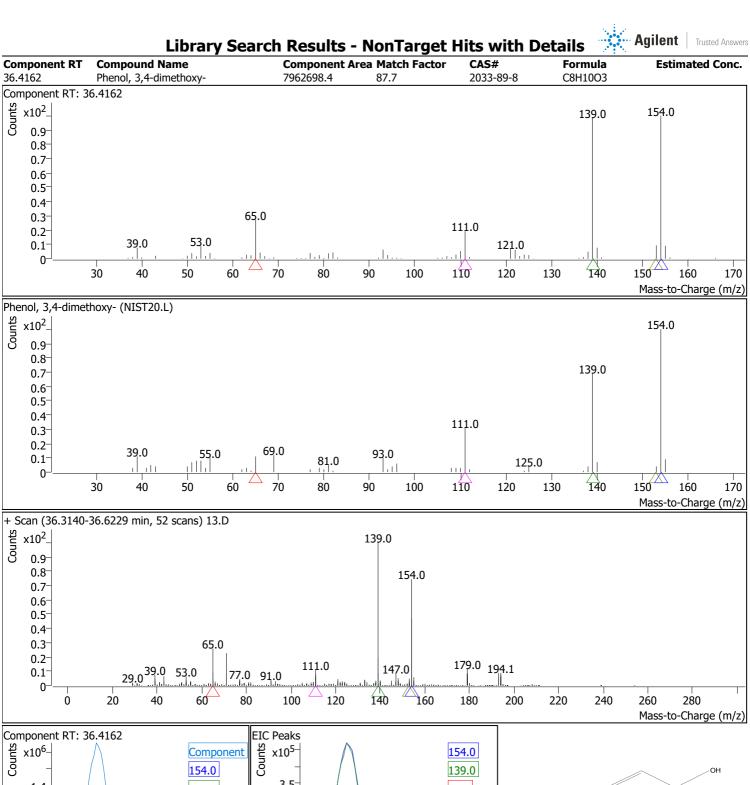


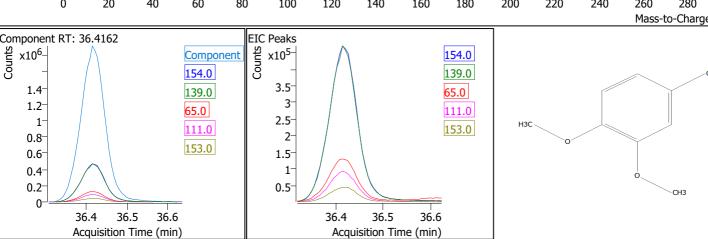




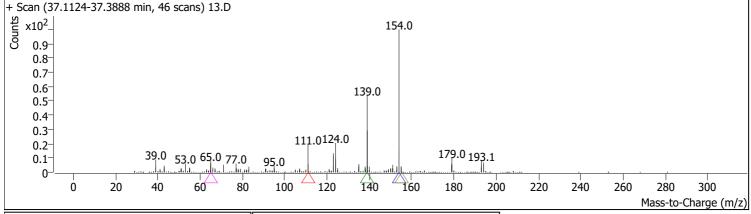
Acquisition Time (min)

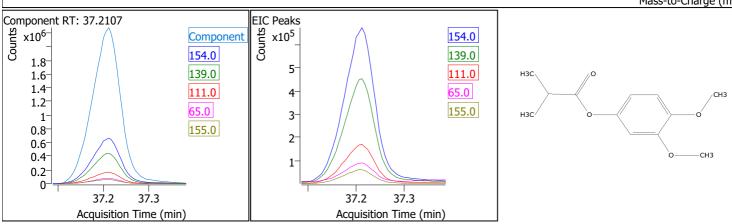
Acquisition Time (min)





Library Search Results - NonTarget Hits with Details --- Agilent Trusted Answers **Compound Name Component Area Match Factor Component RT** CAS# **Formula Estimated Conc.** 37.2107 3,4-Dimethoxyphenol, 2-10174951.8 89.2 1000447-30-5 C12H16O4 methylpropionate Component RT: 37.2107 x10²_ 154.0 0.9 8.0 139.0 0.7 0.6 0.5 0.4 0.3 111.0 0.2^{-} 53.0 0.1 83.0 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 -10 10 20 50 60 80 Mass-to-Charge (m/z) 3,4-Dimethoxyphenol, 2-methylpropionate (NIST20.L) $x10^{2}$ 154.0 0.9 0.8 0.7 0.6 139.0 0.5 0.4 0.3 43.0 0.2 111.0 125.0 0.1 69.0 79.0 95.0 224.0 27.0 53.0 165.0 0 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 10 20 40 50 80 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.** 1,3-Benzenediol, 4,5-dimethyl-527-55-9 37.4751 37475302.6 93.9 C8H10O2 Component RT: 37.4751 v10² 0.9 138.1 0.8 0.7 0.6 123.0 0.5 0.4 91.0 0.3 0.2 65.0 77.0 0.1 120 140 10 20 30 40 50 60 70 80 90 100 110 130 150 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 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 (37.3959-37.7586 min, 62 scans) 13.D st x10² 0.9 138.1 0.8 123.0 0.7 0.6 91.0 0.5 0.4 0.3 0.2 65.0 77.0 39.0 51.0 162.0 179.0 194.1 0.1 109.0 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 37.4751 **EIC Peaks** Counts Counts x10⁶ x10⁶ 138.1 Component НЗС 138.1 123.0 6 1.4 123.0 137.0 5 1.2 137.0 91.0 4 1

37.5

37.6

Acquisition Time (min)

37.7

91.0

92.0

3

2

1

37.4 37.5 37.6 37.7

Acquisition Time (min)

0.8

0.6

0.4

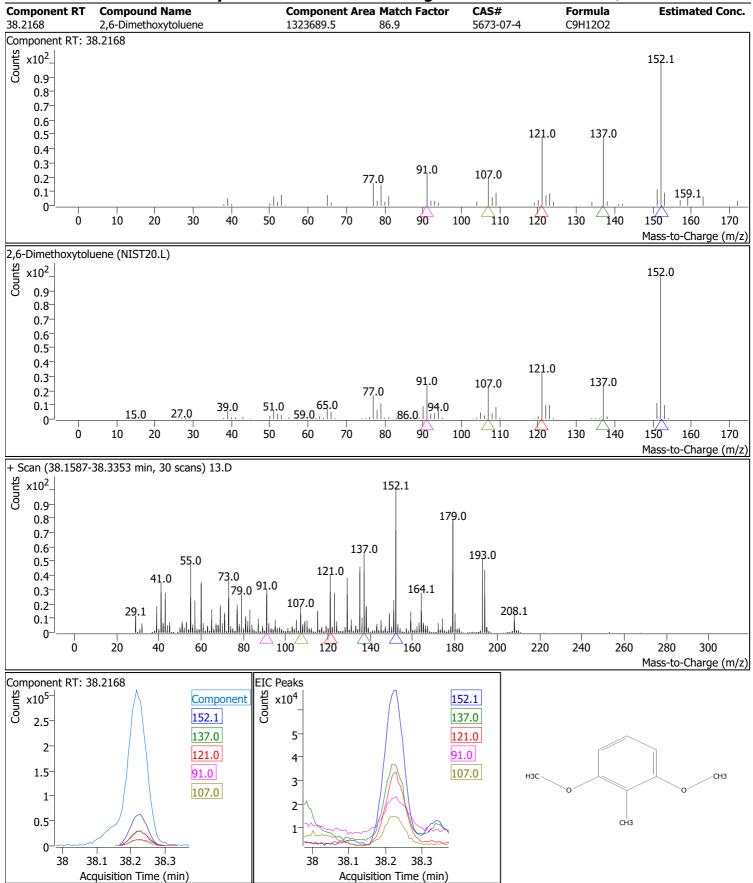
0.2

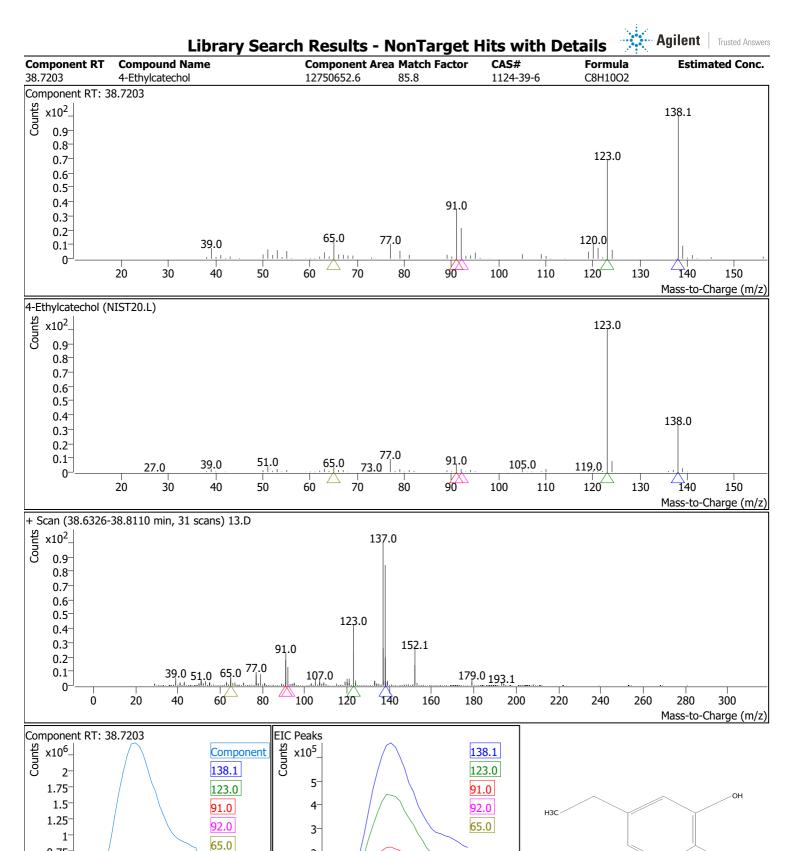
92.0

H3C









38.7

38.75

Acquisition Time (min)

38.8

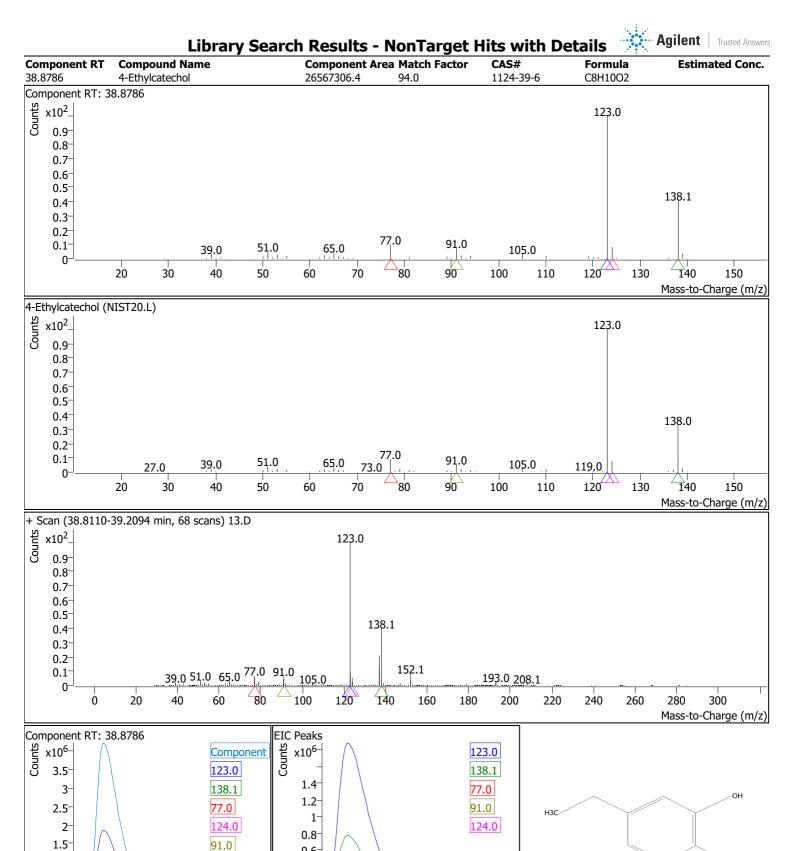
2

0.75

0.5 0.25

38.7 38.75 38.8

Acquisition Time (min)



0.6

0.4

0.2

38.9

39

39.1 Acquisition Time (min)

1

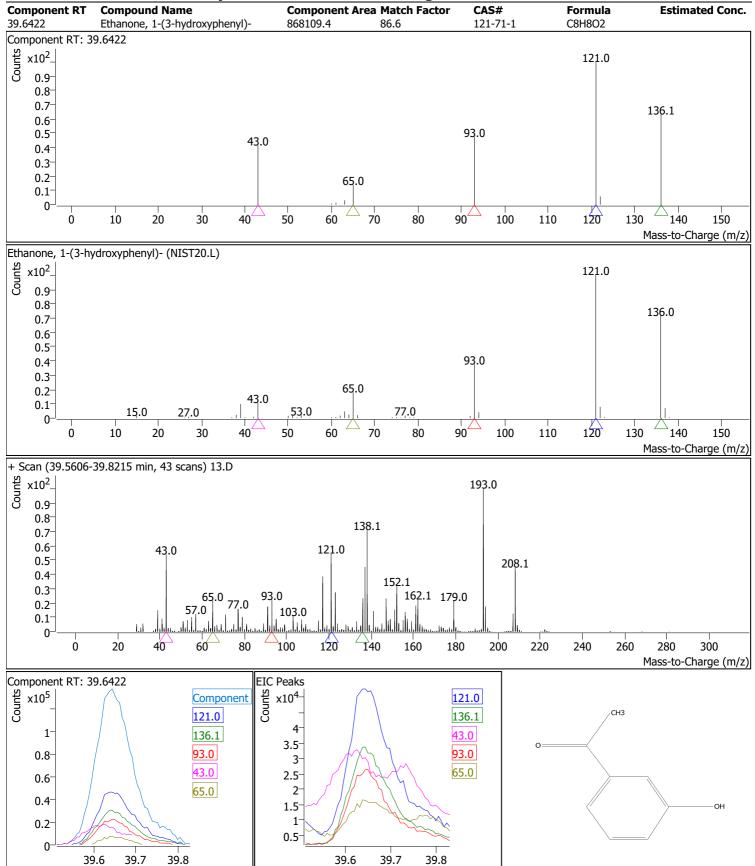
39

Acquisition Time (min)

39.2







Acquisition Time (min)

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 39.9257 1,3-Benzenediol, 4,5-dimethyl-11298478.4 91.0 C8H10O2 Component RT: 39.9257 Counts $x10^{2}$ 138.1 0.9 0.8 123.0 0.7^{-} 0.6 0.5 0.4 0.3 91.0 0.2 39.0 77.0 65.0 0.1 120 140 Ó 10 20 30 40 50 60 70 80 90 100 110 130 150 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 (39.8278-40.1988 min, 63 scans) 13.D st x10² 0.9 138.1 0.8 0.7^{-} 123.0 0.6 0.5 0.4 153.0 0.3 91.0 193.0 0.2 65.0 77.0 168.1 39.0 51.0 208.1 0.1 107.0 179.0 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 39.9257 **EIC Peaks** Counts v10⁶ x10⁵ 138.1 Component НЗС 138.1 123.0 1.6 3.5 1.4 123.0 137.0 3 1.2 137.0 91.0 2.5

40

40.1

Acquisition Time (min)

92.0

H3C

1

0.8

0.6 0.4

0.2

40

40.1

Acquisition Time (min)

91.0

92.0

2-

1

39.9

0.5

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 40.3432 5H-1-Pyrindine, 6,7-dihydro-4-amino-11326319.3 86.2 62732-46-1 C10H14N2 2,3-dimethyl-, hydrate Component RT: 40.3432 x10²_ 161.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 147.0 0.2^{-} 77.0 91.0 105.0 115.0 0.1 0-10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 Mass-to-Charge (m/z) 5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-, hydrate (NIST20.L) $x10^{2}$ 161.0 0.9 0.8 0.7^{-} 0.6 0.5 0.4 0.3 147.0 0.2 54.0 0.1 27.0 65.0 77.0 85.0 93.0 106.0 118.0 15.0 134.0 0 150 160 10 20 30 40 50 60 70 80 90 100 110 120 130 140 170 180 Mass-to-Charge (m/z) + Scan (40.2321-40.5294 min, 51 scans) 13.D st x10² 161.1 0.8 0.7 0.6 0.5 123.0 0.4 147.0 0.3 138.0 193.0 77.0 91.0 105.1 0.2 39.0 51.0 65.0 208.1 0.1 179.0 0 80 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 40.3432 Counts x10⁵ x10⁶ 161.0 Component ತ 162.0 161.0 **Н3С** 2.25 162.0 147.0 1.75 147.0 145.0 4



40.4

Acquisition Time (min)

77.0

40.5

НЗС

NH2

145.0

77.0

3-

2-

40.3

1.25

0.75⁻ 0.5⁻ 0.25⁻

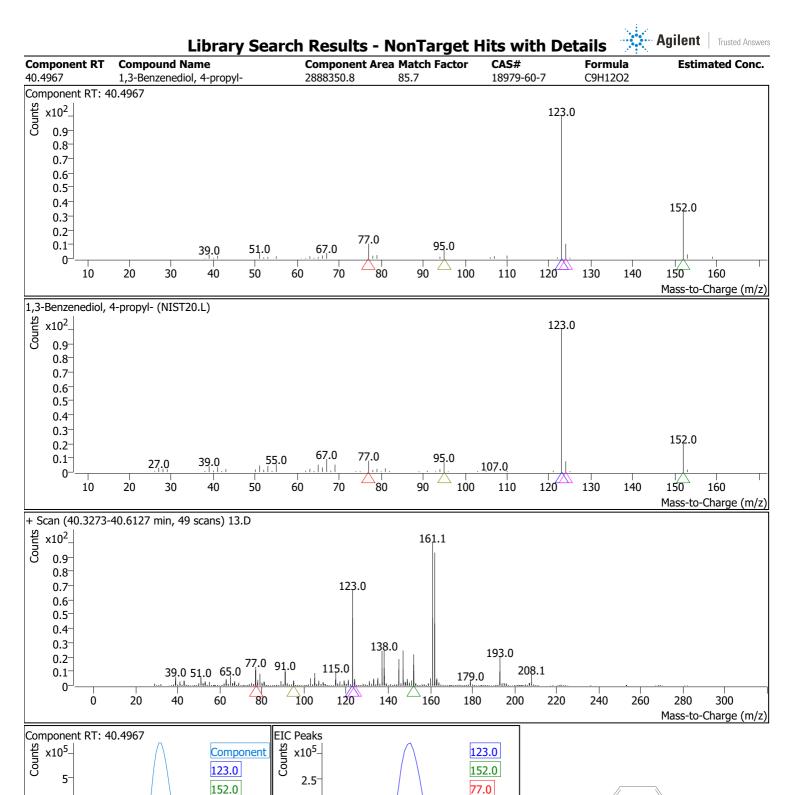
1

0

40.3

40.4

Acquisition Time (min)





124.0

95.0

2

1.5

1

40.4

40.5

Acquisition Time (min)

0.5

77.0

124.0

95.0

4

3

2

1

40.4

40.5

Acquisition Time (min)

НЗС

--- 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 40.6807 4-Methoxy-2,6-dimethylphenol 11509289.2 88.7 C9H12O2 Component RT: 40.6807 y x10² 0.9 137.0 0.8 0.7 152.0 0.6 0.5 0.4 0.3 123.0 0.2 77.0 91.0 109.0 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 (40.5948-40.7673 min, 30 scans) 13.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 152.1 0.4 0.3 0.2 39.0 51.0 65.0 77.0 91.0 109.0 123.0 0.1 179.0 193.0 208.1 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 40.6807 stuno 2.25 Counts x10⁵ 137.0 Component нзс 137.0 152.0 2.25 6 152.0 123.0 1.75 5 138.0 123.0



40.65

40.7

Acquisition Time (min)

40.75

77.0

H₃C

4

3-

2-

138.0

77.0

40.75

1.5

1.25

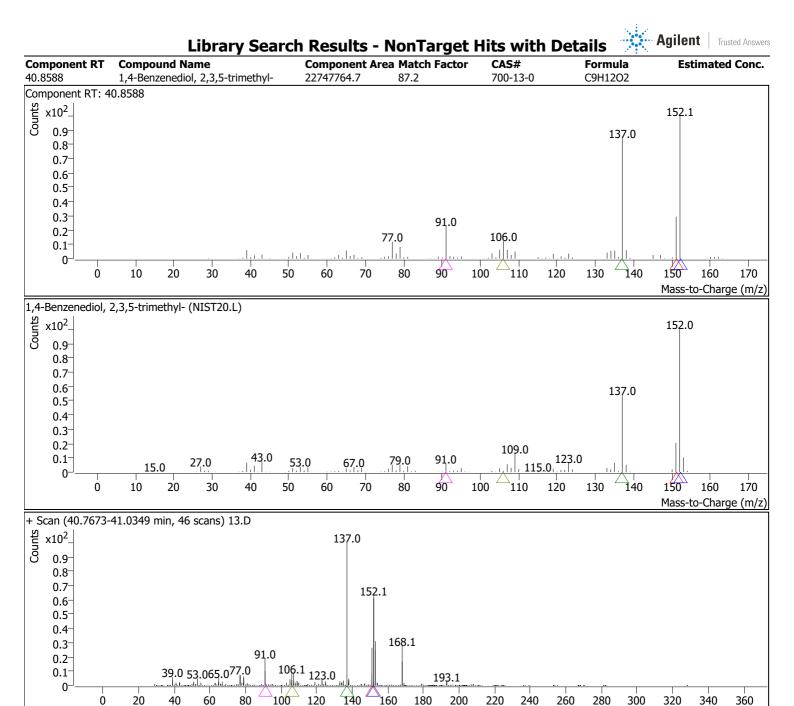
0.75

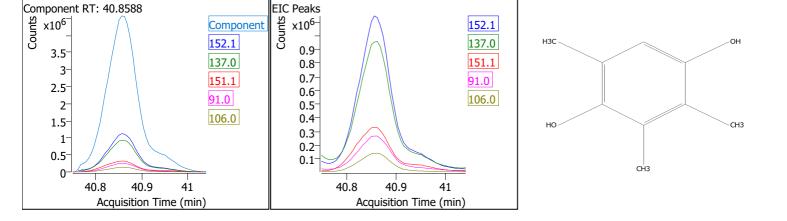
0.5 0.25

40.65 40.7

Acquisition Time (min)

-CH3

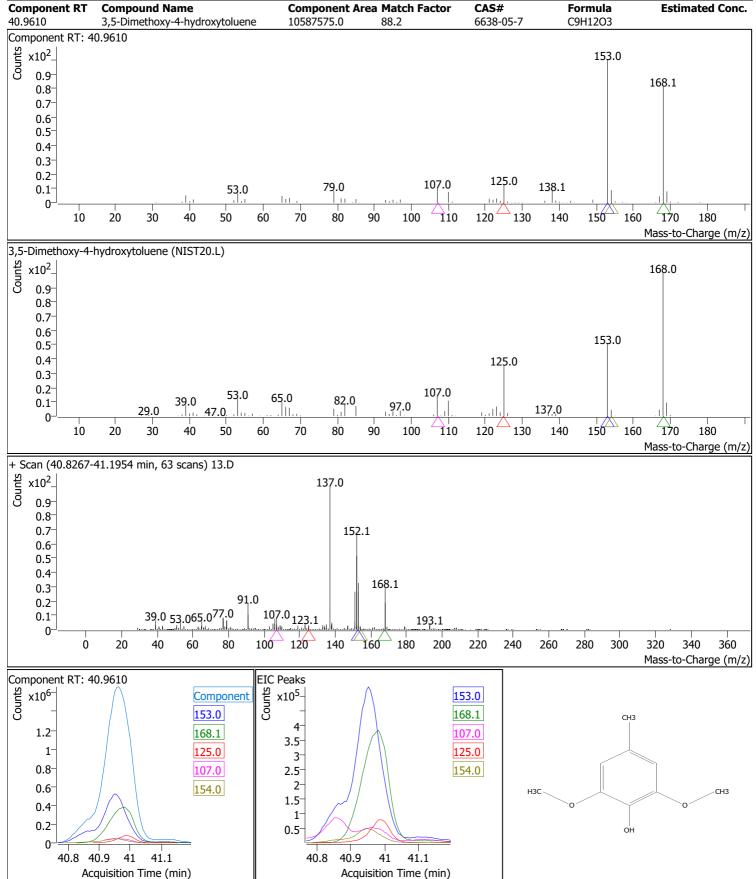


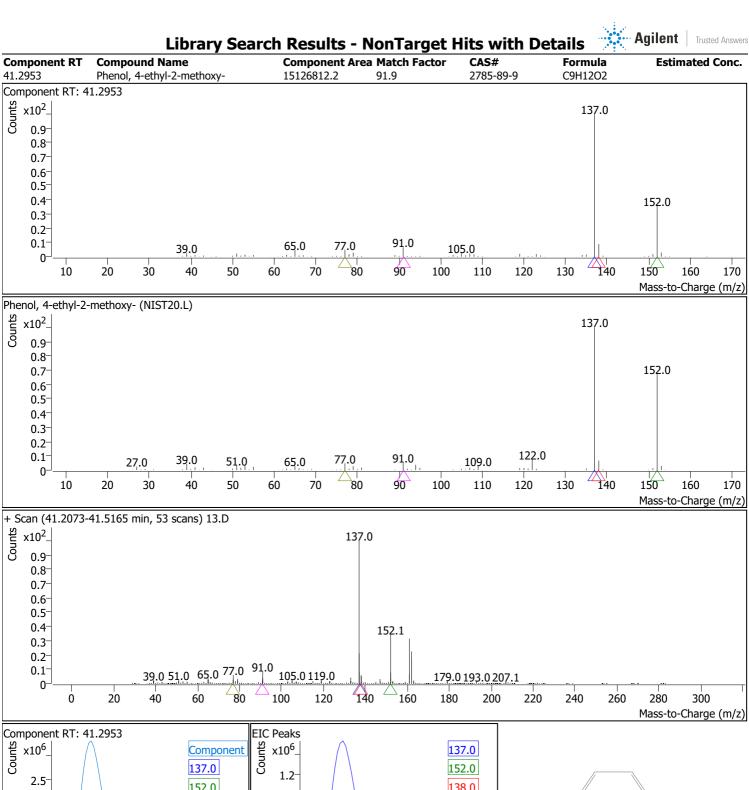


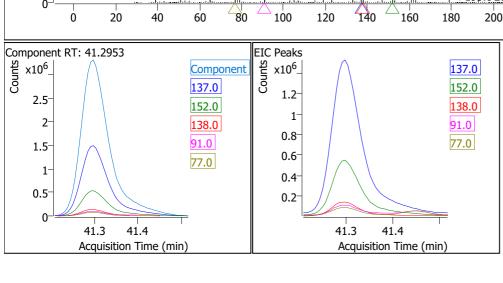
Mass-to-Charge (m/z)

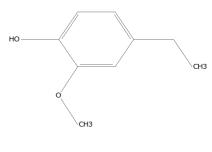












--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 41.4486 5H-1-Pyrindine, 6,7-dihydro-4-amino-8539314.1 86.7 62732-46-1 C10H14N2 2,3-dimethyl-, hydrate Component RT: 41.4486 x10²_ 162.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 147.0 77.0 119.0 133.0 0.1 105.0 0-150 90 10 20 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) 5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-, hydrate (NIST20.L) $x10^{2}$ 161.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 147.0 0.2 0.1 54.0 77.0 85.0 93.0 27.0 65.0 106.0 118.0 15.0 134.0 0 90 150 10 20 30 40 50 60 70 80 100 110 120 130 140 160 170 180 Mass-to-Charge (m/z) + Scan (41.3500-41.6176 min, 46 scans) 13.D st x10² 161.1 0.8 0.7^{-} 0.6 137.0 0.5 0.4 0.3 152.1 0.2 39.0 51.0 65.0 77.0 0.1 115.0 179.0 193.0 207.1 0 100 Ó 20 40 60 80 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 41.4486 **EIC Peaks** Counts Counts x10⁶ x10⁵ 162.0 Component 161.0 162.0 **Н3С** 4.5 1.4 161.0 147.0 1.2 3.5 147.0 163.0 1 3

НЗС

91.0

163.0

91.0

0.8

0.6

0.4

41.4

41.5

Acquisition Time (min)

2.5

1.5

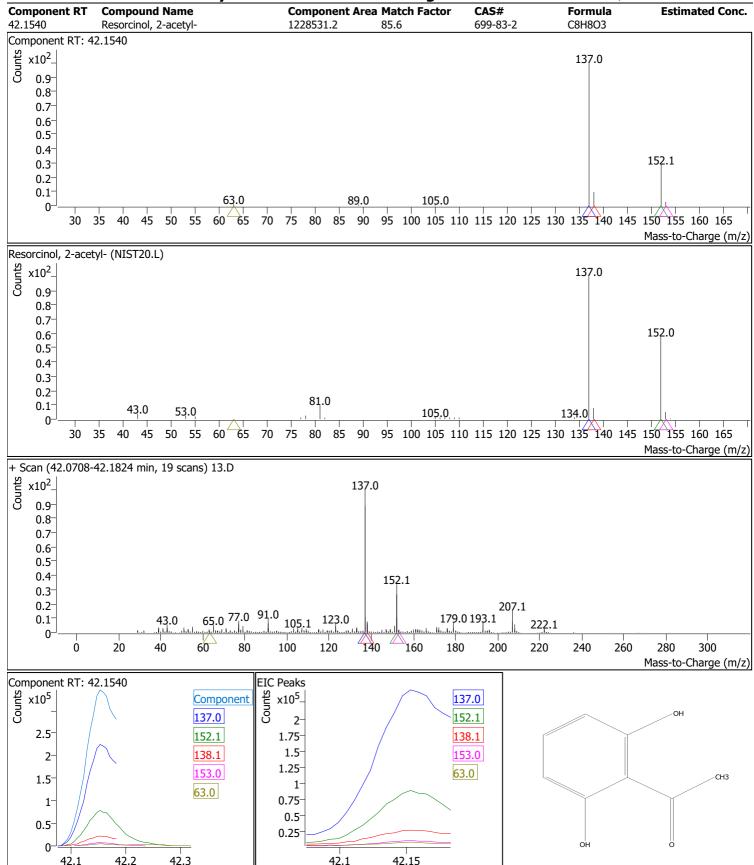
0.5

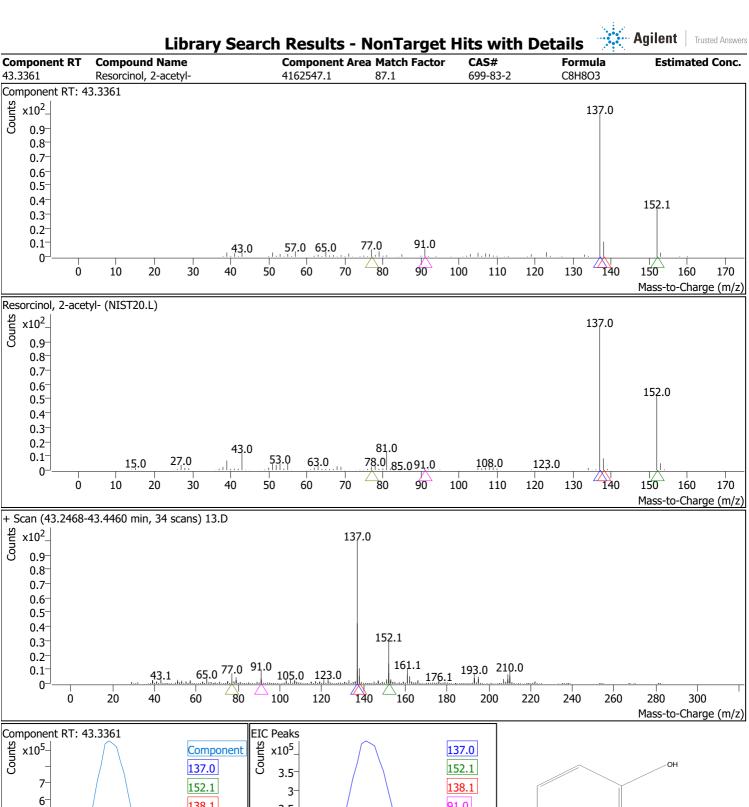
41.4

2









2.5

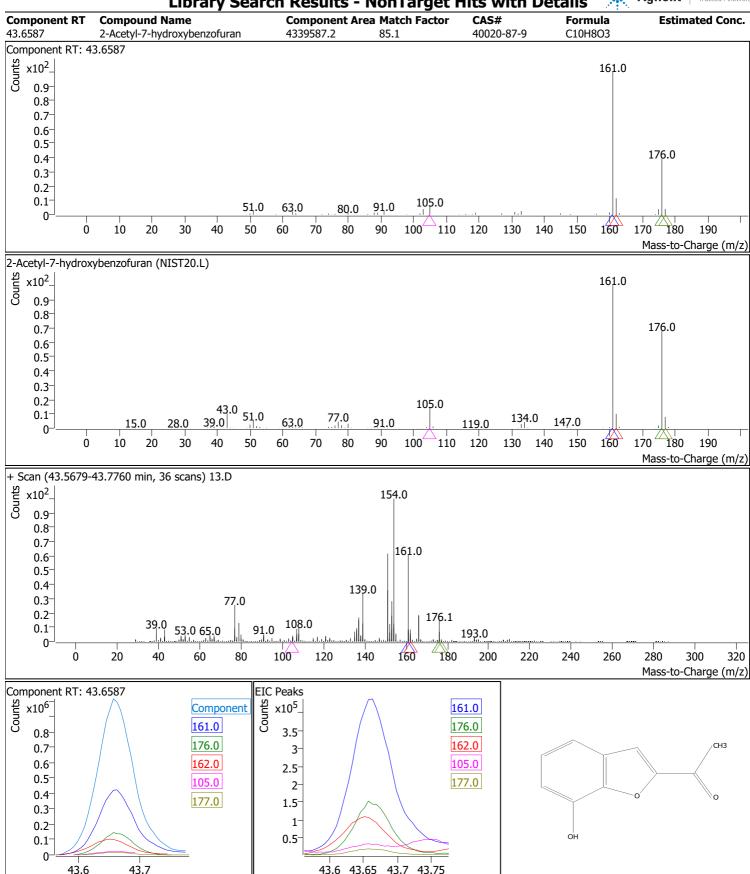
138.1

5

91.0







--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.3768 Dodecanoic acid, methyl ester 8849443.4 93.8 111-82-0 C13H26O2 Component RT: 44.3768 y x10² 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 69.1 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 70 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 55.0 0.2 29.0 69.0 101.0 115.0 129.0 143.0 157.0 171.0 183.0 0.1 214.0 $\stackrel{\sim}{80}$ $\stackrel{\frown}{90}$ 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 30 40 50 60 70 Mass-to-Charge (m/z) + Scan (44.2873-44.5546 min, 45 scans) 13.D st x10² 0.9 161.0 175.1 74.0 0.8 87.0 0.7^{-} 0.6 0.5 0.4^{-} 0.3 43.0 55.0 115.0 144.1 0.2 129.1 0.1 103.0 214.2 20 60 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) EIC Peaks Component RT: 44.3768 Counts Counts x10⁵ 74.0 Component



44.4

87.0

43.0

55.0

41.0

44.5

Acquisition Time (min)

74.0

87.0

43.0

55.0

41.0

2

1.75

1.5

1.25

0.75 0.5 0.25

1

44.4

Acquisition Time (min)

44.5

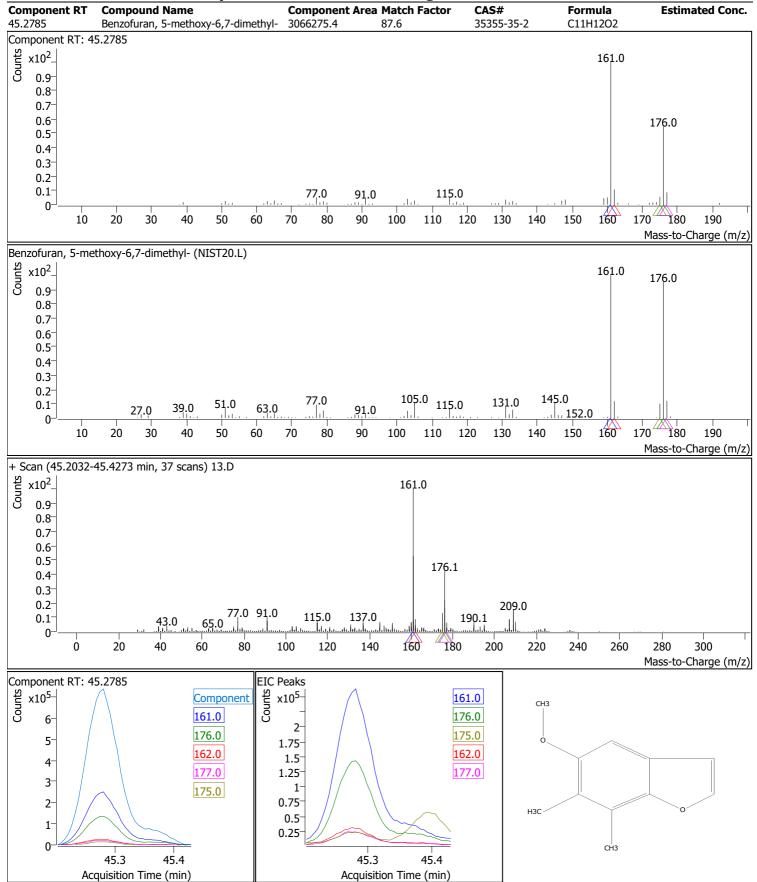
5

3

2

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.** 47.4453 Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-1048188.3 89.1 65996-50-1 C6H5N3O2 dione Component RT: 47.4453 x10²_ 151.1 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 0.1 0-40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione (NIST20.L) $x10^{2}$ 151.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 80.0 108.0 0 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 Mass-to-Charge (m/z) + Scan (47.3733-47.5160 min, 25 scans) 13.D x10². 175.1 0.9 0.8 0.7 151.1 0.6 0.5 0.4 190.1 0.3 0.2 167.0 65.0⁷⁷.0 ⁹¹.0 0.1 43.0 115.0 135.1 n 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 Mass-to-Charge (m/z) Component RT: 47.4453 **EIC Peaks** Counts Counts x10⁵x10⁵-151.1 Component 152.1 151.1 2 2 152.1 149.0 1.75 1.75 149.0 1.5 1.5

47.45

Acquisition Time (min)

47.5

1.25 1

0.75

0.5

47.4

0.25

1.25

0.75

0.5

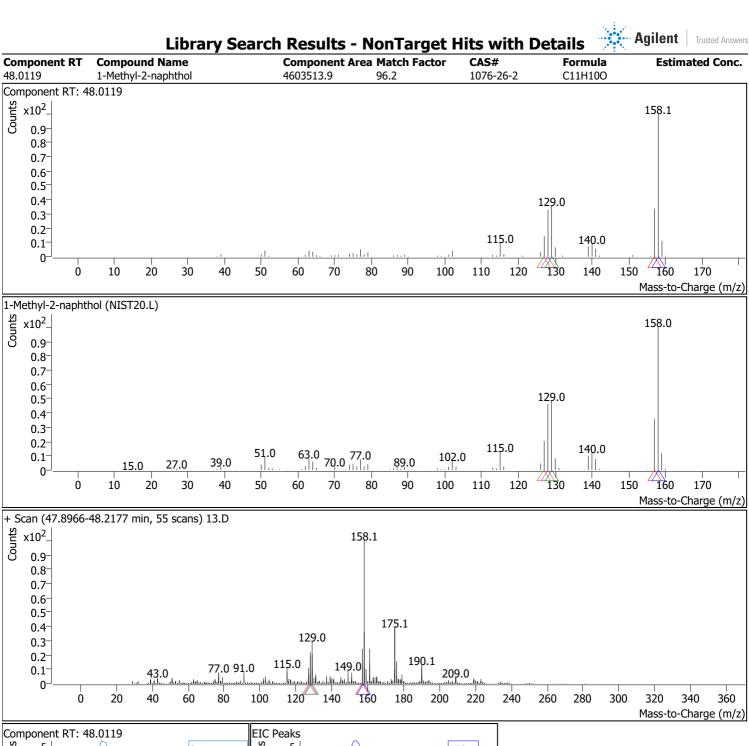
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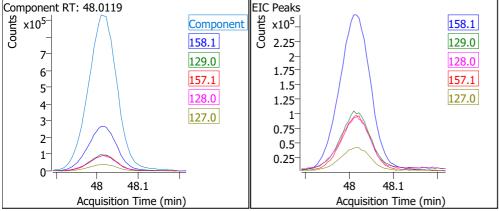
47.5

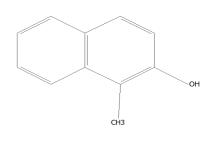
Acquisition Time (min)

47.6

0.25

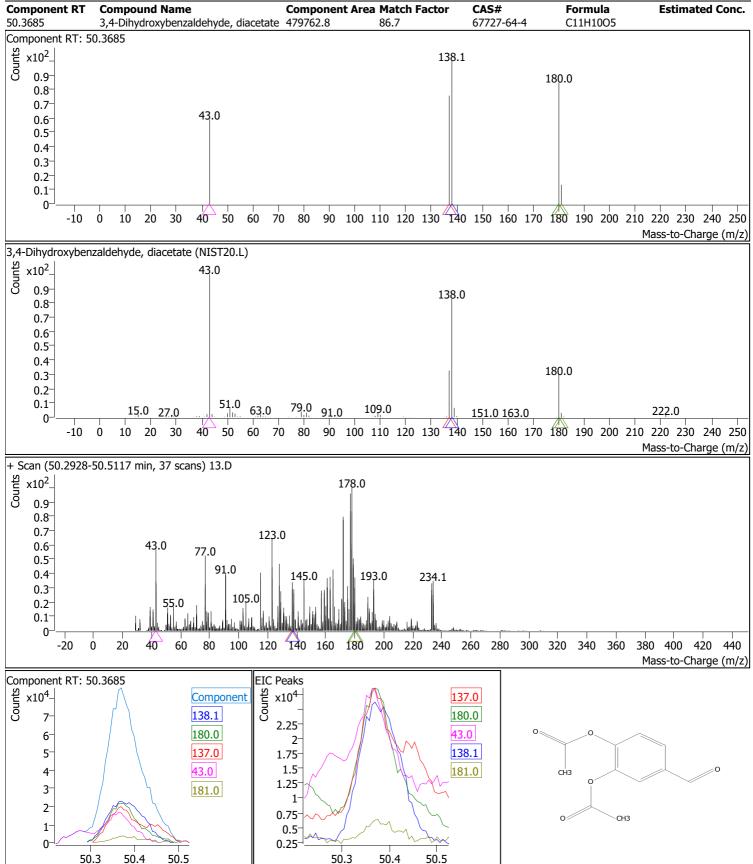




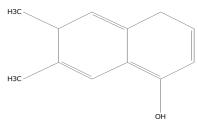


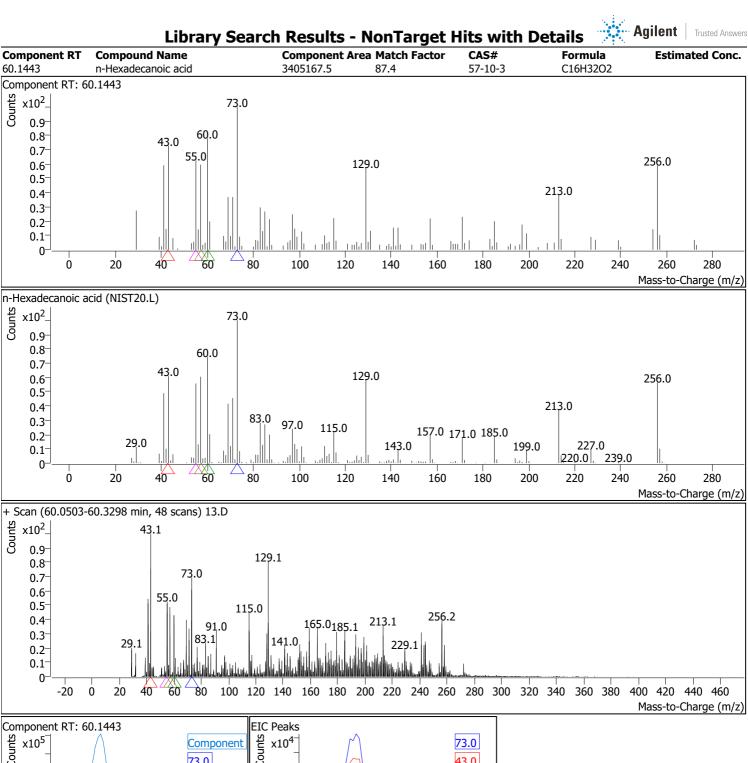


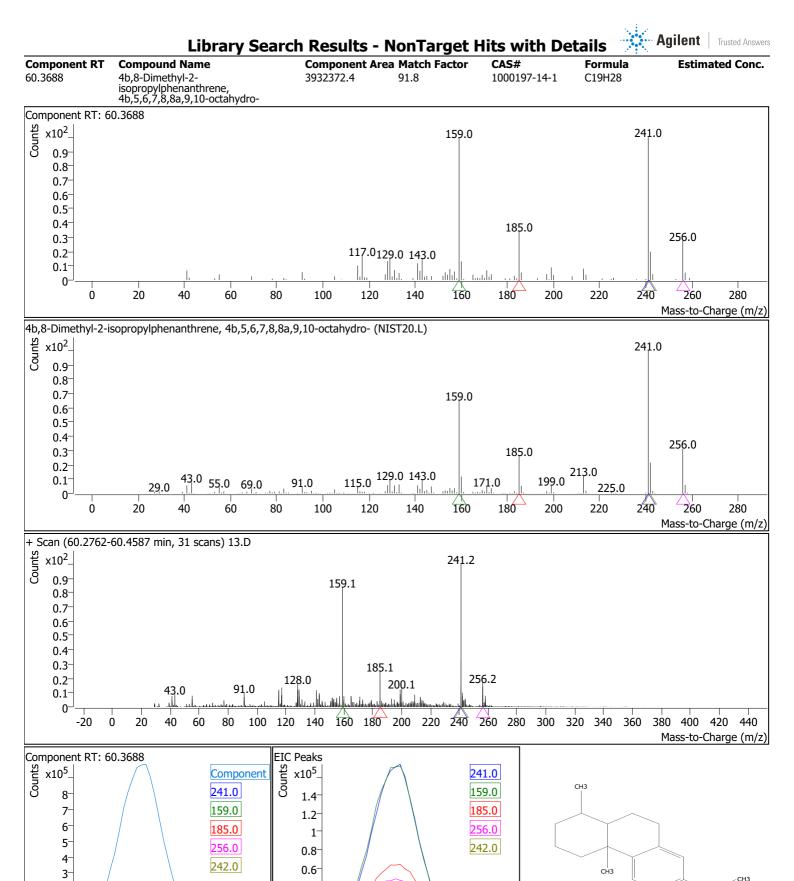




··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 52.5430 1-Naphthol, 6,7-dimethyl-4343396.2 90.5 31776-14-4 C12H12O Component RT: 52.5430 v10² 0.9 172.1 0.8 0.7 0.6 0.5 157.1 0.4 128.0 0.3 0.2 115.0 141.0 0.1 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 180 Mass-to-Charge (m/z) 1-Naphthol, 6,7-dimethyl- (NIST20.L) Counts x10²_ 0.9 172.0 0.8 0.7 0.6 0.5 0.4 0.3 157.0 129.0 0.2 115.0 143.0 0.1 63.0 72.079.086.0 39.0 51.0 102.0 18.0 29.0 160 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 170 180 190 Mass-to-Charge (m/z) + Scan (52.4552-52.6770 min, 37 scans) 13.D st x10² 0.9 172.1 0.8 0.7^{-} 0.6 0.5 0.4^{-} 137.0 ^{157.0} 128.0 0.3 115.0 63.0^{77.0}^{91.0} 0.2 ^{189.1} 207.1 43.0 0.1 0 160 20 40 60 80 100 120 140 180 200 220 240 260 280 300 320 340 360 380 Mass-to-Charge (m/z) EIC Peaks Component RT: 52.5430 Counts Counts x10⁵ 172.1 Component 172.1 157.1 Н3С 2 7 157.1 128.0 1.75 6







60.35

60.4

Acquisition Time (min)

0.4

0.2

2

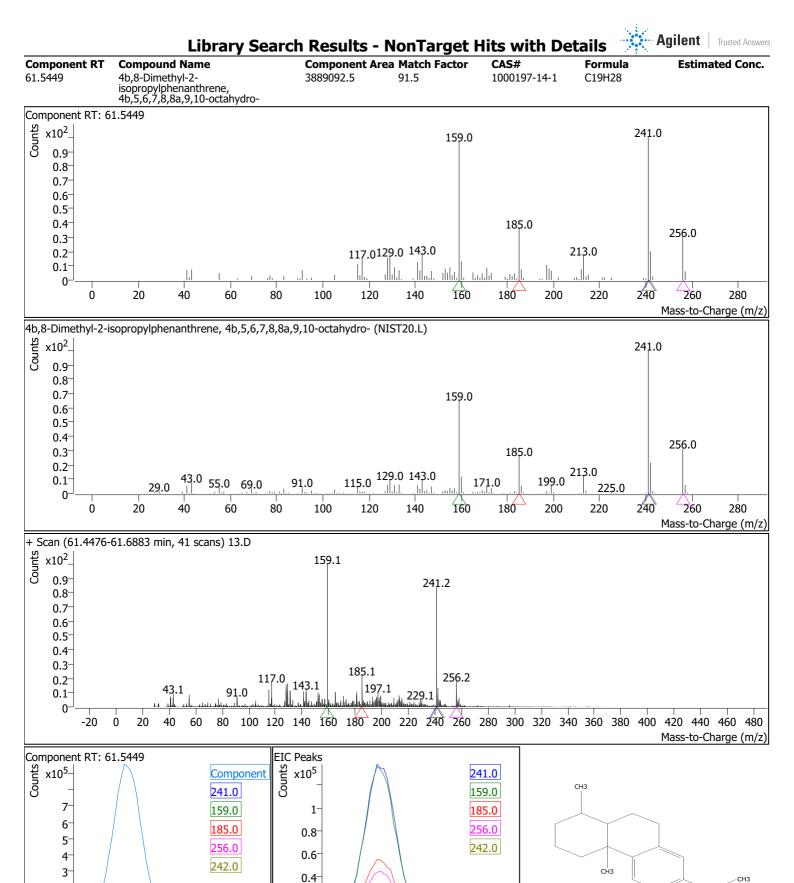
60.3

60.35

60.4

Acquisition Time (min)

СНЗ



61.6

Acquisition Time (min)

0.2

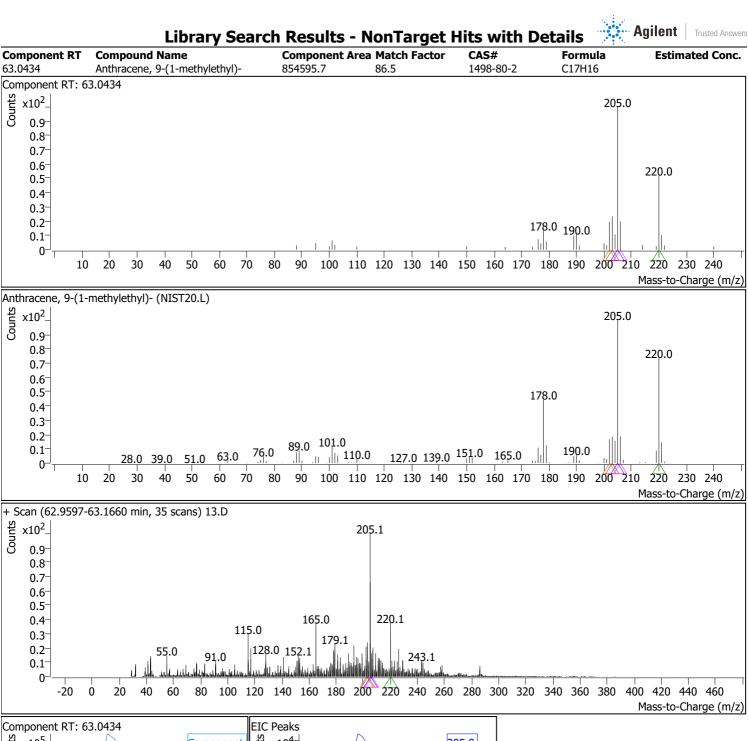
61.5

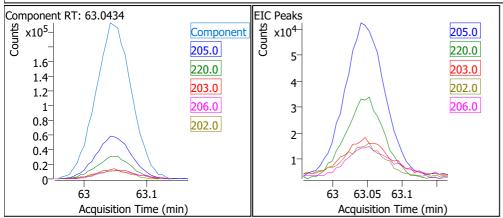
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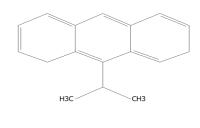
61.5

Acquisition Time (min)

СНЗ







--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 64.3737 Heneicosane 1587679.9 88.6 629-94-7 C21H44 Component RT: 64.3737 v10² 0.9 57.0 71.0 0.8 0.7^{-} 43.0 85.0 0.6 0.5 0.4 0.3 99.0 0.2 0.1 260 300 -20 20 80 100 120 140 160 180 200 220 240 280 320 Mass-to-Charge (m/z) Heneicosane (NIST20.L) Counts x10²_ 0.9 57.0 43.0 0.8 0.7 71.0 0.6 0.5 85.0 0.4 0.3 29.0 99.0 0.2 0.1 141.0 169.0 197.0 296.0 225.0 253.0 60 40 -20 0 20 80 100 120 140 160 180 200 220 240 260 280 300 320 Mass-to-Charge (m/z) + Scan (64.2941-64.4618 min, 28 scans) 13.D St x10² 0.9 57.1 197.1 0.8 0.7 0.6 85.1 0.5 254.2 0.4^{-} 212.1 0.3 165.1 239.1 0.2 115.0 179.0 151.0 29.1 0.1 -20 40 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 Mass-to-Charge (m/z) EIC Peaks Component RT: 64.3737 Counts stuno x10⁵x10⁴ 57.0 Component 71.0 57.0 6 3 71.0 43.0 5 85.0 2.5 43.0

64.4

64.5

Acquisition Time (min)

41.0

2

0.5

64.4

Acquisition Time (min)

64.5

1.5

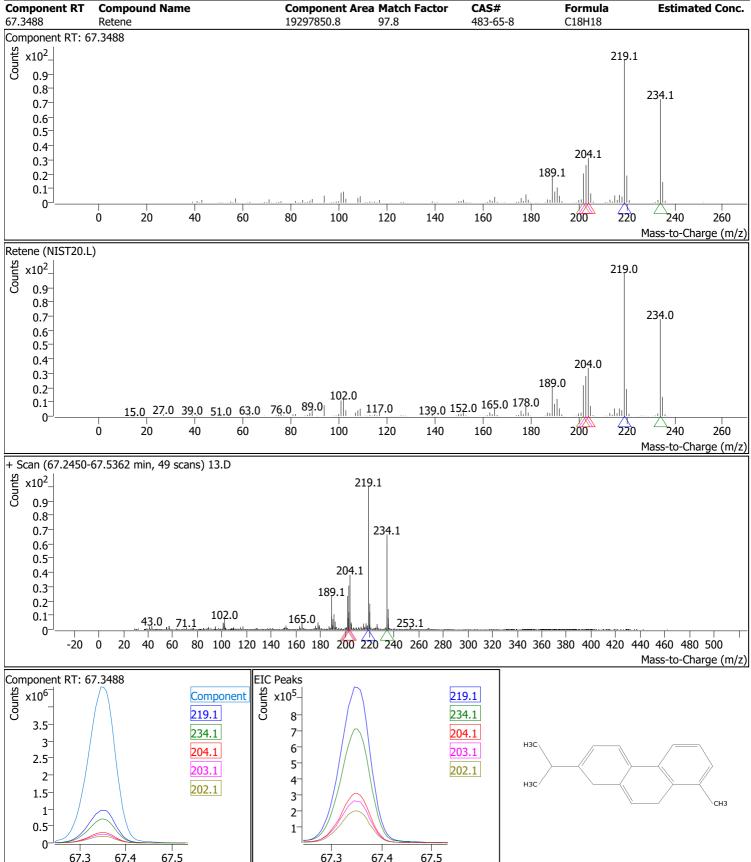
85.0

41.0

3

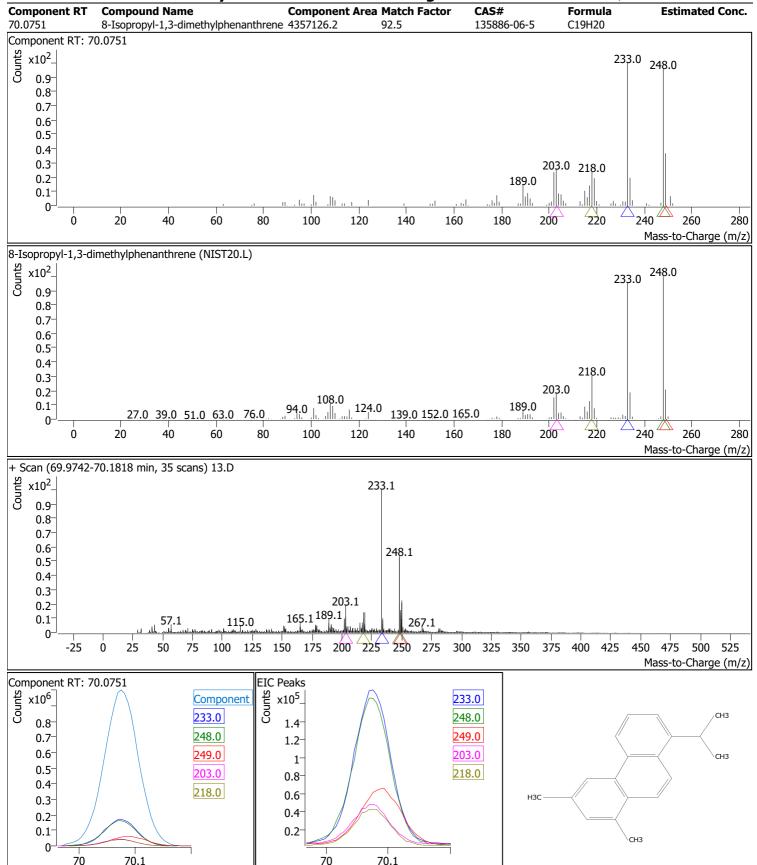
2

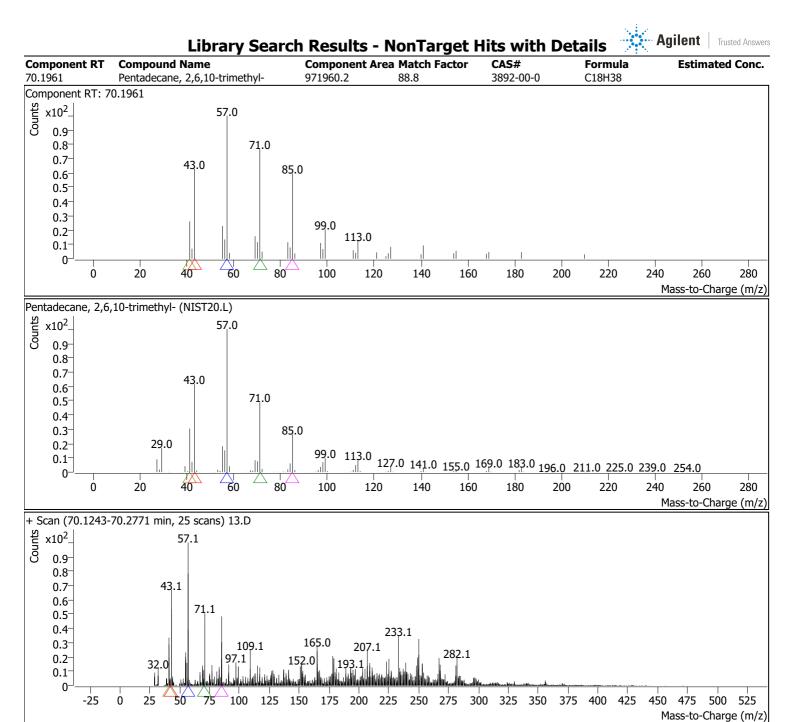














70.15 70.2 70.25 70.3

Acquisition Time (min)

57.0

43.0

71.0

85.0

41.0

EIC Peaks

x10⁴

3.5

2.5

1.5

3

2

1

 0.5°

Counts

Component 57.0

71.0

43.0

85.0

41.0

Component RT: 70.1961

Counts

2

1.75

1.5

1.25

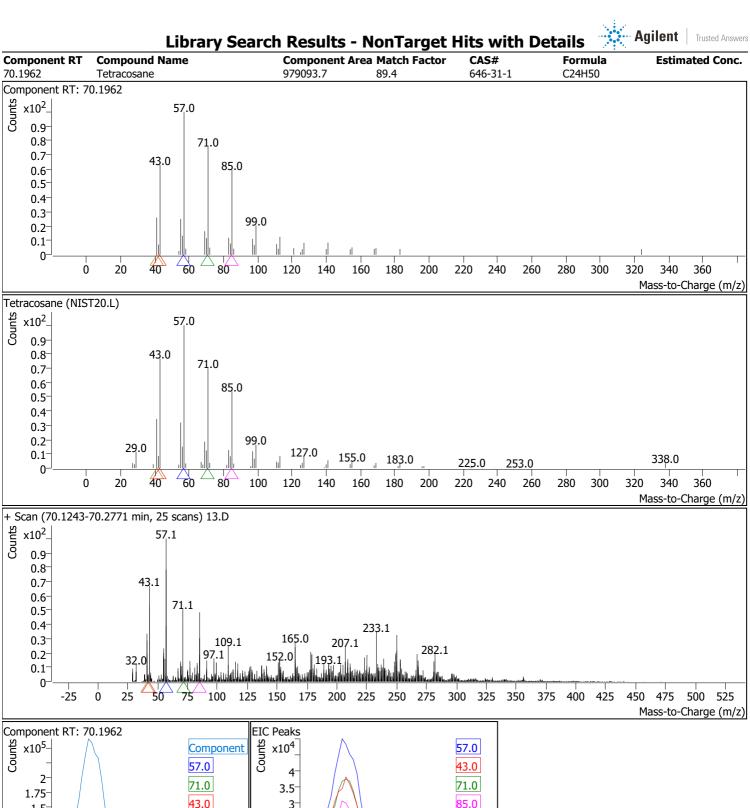
0.75

0.25

0.5

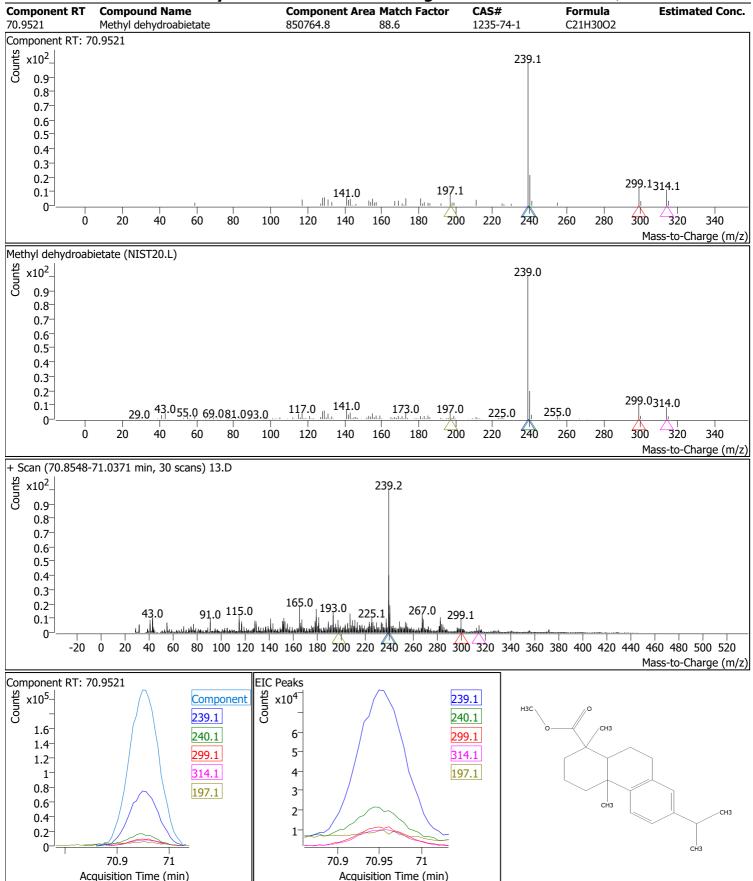
70.2

70.3









Compound Name Component RT Component Area Match Factor CAS# **Formula Estimated Conc.** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6745 7845639.3 5155-70-4 C20H28O2 Component RT: 73.6745 $x10^{2}$ 239.1 285.2 0.9 0.8 0.7 0.6 0.5 0.4^{-} 197.1 300.1 0.3 141.0 0.2 0.1 200 240 280 300 320 0 20 40 60 80 100 120 140 160 180 220 260 Mass-to-Charge (m/z) 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L) Counts x10²_ 285.0 0.9 0.8 239.0 0.7° 0.6 0.5 0.4 300.0 0.3 197.0 43.0 0.2 141.0 55.0 _{69.0} 91.0 183.0 0.1 225.0 255.0 240 280 300 0 20 40 60 80 100 120 140 160 180 200 220 260 320 Mass-to-Charge (m/z) + Scan (73.5543-73.9165 min, 61 scans) 13.D 돌 x10². 285.2 0.9 0.8 0.7 0.6 239.2 0.5 0.4 0.3 300.2 197.1 0.2 179.0 43.1 0.1 253.1 200 225 250 275 -25 50 75 100 125 175 300 325 350 375 400 425 450 475 500 525 550 25 150 Mass-to-Charge (m/z) Component RT: 73.6745 EIC Peaks x10⁶ x10⁵ 239.1 Component 239.1 285.2 1.2 СНЗ 1.6 285.2 197.1 1.4 1 197.1 300.1 1.2 0.8 300.1 141.0 1 0.6^{-} 0.8 141.0 0.4 0.6 0.4

73.6

73.7

73.9

73.8

Acquisition Time (min)

0.2

73.6

73.7 73.8 73.9

Acquisition Time (min)

СНЗ

Library Search Results - NonTarget Hits with Details Component Area Match Factor CAS# **Component RT Compound Name Formula Estimated Conc.** 75.3839 1-Octadecanol 1645129.4 90.9 112-92-5 C18H38O Component RT: 75.3839 y x10² 0.9 83.0 97.0 57.0 69.1 0.8 43.0 0.7^{-} 0.6 111.0 0.5 0.4 0.3 0.2 0.1 20 40 120 160 180 200 220 240 260 280 Mass-to-Charge (m/z) 1-Octadecanol (NIST20.L) Counts x10²_ 0.9 43.0 55.0 83.0 0.8 97.0 0.7 69.0 0.6 0.5 111.0 0.4 0.3 29.0 125.0 0.2 0.1 154.0 168.0 182.0 196.0 210.0 224.0 19.0 100 200 0 20 40 80 120 140 160 180 220 240 260 280 Mass-to-Charge (m/z) + Scan (75.3138-75.4971 min, 31 scans) 13.D st x10² 0.9 43.1 0.8 0.7 69.1 97.1 0.6 207.0 0.5 0.4^{-} 249.0 281.0 111.1 151.0 0.3 0.2 0.1 -25 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 Mass-to-Charge (m/z) Component RT: 75.3839 EIC Peaks Counts Counts x10⁵ x10⁴ Component 97.0 83.0 83.0 3 97.0 55.0 2.5 2.5 57.0 57.0 2 2

75.4

75.5 Acquisition Time (min)

55.0

69.1

1.5

1

0.5

1.5

0.5

0-

75.4

75.5

Acquisition Time (min)

1

69.1

