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Analysis File Name 240502 data.uaf

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

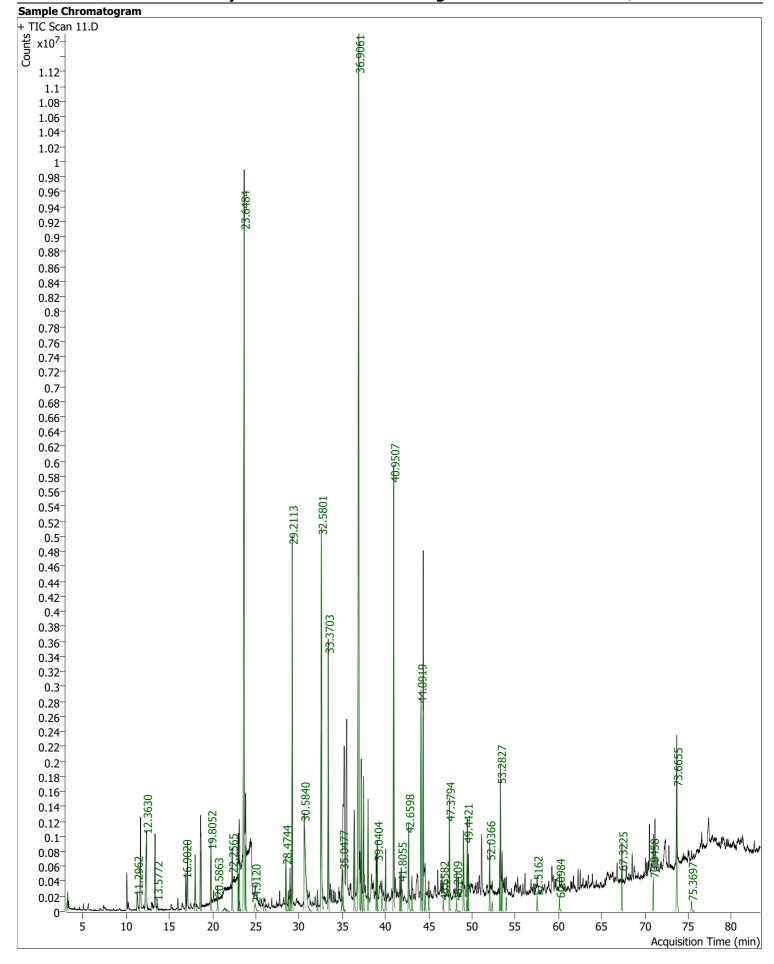
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Instrument Name GCMSD Dil. 1

Instrument Na	me GCMSD	Dil.		1		
Component RT	Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
3.2627	Propanoic acid	79-09-4	C3H6O2	857581.6	98.1	
11.2962	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	1561130.6	88.4	
12.3630	Butyrolactone	96-48-0	C4H6O2	7883171.4	97.6	
12.9351	Methyltartronic acid	595-98-2	C4H6O5	856490.1	94.8	
13.5772	2,5-Hexanedione	110-13-4	C6H10O2	689669.5	90.8	
15.9772	2-Cyclopenten-1-one, 3-methyl-	2758-18-1	C6H8O	715614.8	97.9	
16.9020	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	1789118.6	85.1	
17.9700	Phenol	108-95-2	C6H6O	3359112.1	97.5	
18.6586	Diisoamyl ether	544-01-4	C10H22O	2971737.3	85.3	
19.8052	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	3481815.1	95.0	
20.5863 21.3957	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7 110-88-3	C7H10O C3H6O3	916763.5 669705.4	91.1 81.7	
22.2565	1,3,5-Trioxane	95-48-7	C7H8O	2070659.2	95.1	
	Phenol, 2-methyl-					
22.9523	1-Propanol, 2-(2-hydroxypropoxy)-	106-62-7	C6H14O3	1962313.9	80.4	
23.0797	Acetic acid, trifluoro-, anhydride	407-25-0	C4F6O3	722657.2	83.5	
23.0842	1-Octanol	111-87-5	C8H18O	3701878.6	97.3	
23.6484	Phenol, 2-methoxy-	90-05-1	C7H8O2	46803547.3	98.4	
23.8237	Ethanone, 1-(3-thienyl)-	1468-83-3	C6H6OS	3099943.1	93.8	
24.9120	1,2,3-Propanetriol, 1-acetate	106-61-6	C5H10O4	1142009.2	88.6	
26.0658	Pentanoic acid, 2-methyl-4-oxo-	6641-83-4	C6H10O3	787634.2	82.0	
28.4744	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	2402147.8	95.2	
28.7549	Naphthalene	91-20-3	C10H8	670341.7	93.6	
28.9486	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	1687369.7	95.3	
29.2113	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	19787309.1	99.1	
30.5840	Catechol	120-80-9	C6H6O2	15015507.5	96.5	
32.1161	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1450-72-2	C9H10O2	762312.7	92.7	
32.5801	1,2-Benzenediol, 3-methoxy-	934-00-9	C7H8O3	28168839.6	96.2	
33.3703	Phenol, 4-ethyl-2-methoxy-	2785-89-9	C9H12O2	13973837.1	96.8	
35.0101	4-Methoxy-2,6-dimethylphenol	2431-91-6	C9H12O2	1221125.0	80.1	
35.0477	1,2-Benzenediol, 4-methyl-	452-86-8	C7H8O2	4827313.6	92.3	
36.3966	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	4447071.1	85.8	
36.9061	Phenol, 2,6-dimethoxy-	91-10-1	C8H10O3	64172540.1	98.6	
37.1870	Phenol, 3,4-dimethoxy-	2033-89-8	C8H10O3	7099504.0	88.6	
37.1870	3,4-Dimethoxyphenol, 2-methylpropionate	1000447-30-5	C12H16O4	7116634.6	87.8	
37.4457	Phenol, 2-methoxy-4-propyl-	2785-87-7	C10H14O2	5418466.3	93.8	
37.9713	1,2,3-Trimethoxybenzene	634-36-6	C9H12O3	4698839.4	91.4	
38.9112	4-Ethylcatechol	1124-39-6	C8H10O2	2504636.4	94.0	
39.0404	Benzaldehyde, 3-hydroxy-4-methoxy-	621-59-0	C8H8O3	2975405.9	90.2	
39.5716	Ethanone, 1-(3-hydroxyphenyl)-	121-71-1	C8H8O2	1302024.5	95.0	
40.0056	4-Methoxy-2-methyl-1-(methylthio)benzene	22583-04-6	C9H12OS	2455888.4	86.0	
40.9507	3,5-Dimethoxy-4-hydroxytoluene	6638-05-7	C9H12O3	23919736.5	94.0	
41.6649	Ethanone, 1-(2,3,4-trihydroxyphenyl)-	528-21-2	C8H8O4	1113823.2	82.7	
41.8055	Eugenol	97-53-0	C10H12O2	1556733.5	81.9	
42.6598	Apocynin	498-02-2	C9H10O3	4931034.4	98.1	
43.0430	Benzene, 1,2,3-trimethoxy-5-methyl-	6443-69-2	C10H14O3	1044668.7	89.3	
44.0919	4-Ethyl-2,6-dimethoxyphenol	14059-92-8	C10H14O3	10507765.9	99.0	
44.3530	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	12225428.5	88.4	
44.5738	Flopropione	2295-58-1	C9H10O4	1066632.3	83.6	
44.9967	3,4-Dimethoxyphenylacetone	776-99-8	C11H14O3	894330.2	81.3	
46.6582	Butyrovanillone	64142-23-0	C11H14O3	610759.5	86.8	
47.3794	2,6-Dimethoxy-4-propylphenol	6766-82-1	C11H16O3	4546136.1	93.7	
48.2009	8-Methoxy-1-naphthol	1000482-13-1	C11H10O2	641820.7	82.6	
49.0032	Benzenepropanol, 4-hydroxy-3-methoxy-	2305-13-7	C10H14O3	3980098.9	87.4	
49.4053	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	134-96-3	C9H10O4	649530.2	84.0	
49.4421	2-Naphthalenol, 3-methoxy-	18515-11-2	C11H10O2	3915905.9	95.5	
49.5789	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	20675-95-0	C11H14O3	1916441.2	83.1	
52.0366	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	2478-38-8	C10H12O4	2751823.6	96.9	
52.3254	.beta(4-Hydroxy-3-methoxyphenyl)propionic acid	1135-23-5	C10H12O4	627806.6	87.9	
53.2008	1,6-Dimethoxynaphthalene	3900-49-0	C12H12O2	1708316.2	83.5	
53.2827	Syringylacetone	19037-58-2	C11H14O4	6551892.8	97.1	
53.4722	Naphthalene, 2,3-dimethoxy-	10103-06-7	C12H12O2	2240360.9	87.0	
53.9540	1,6-Dimethoxynaphthalene	3900-49-0	C12H12O2	749797.8	80.5	
57.5162	Dihydrosyringenin	20736-25-8	C11H16O4	879316.4	90.0	
60.0984	n-Hexadecanoic acid	57-10-3	C16H32O2	754579.4	87.3	

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Component	t RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
67.3225	2-Isopropyl-10-methylphenanthrene	66552-97-4	C18H18	2171235.6	95.5	
70.9458	Methyl dehydroabietate	1235-74-1	C21H30O2	1764651.8	93.4	
73.6655	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	8672669.1	93.4	
75.3697	n-Heptadecanol-1	1454-85-9	C17H36O	686811.9	81.1	



-- 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 3.2627 Propanoic acid 857581.6 98.1 Component RT: 3.2627 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 0.1 42.1 55 15 20 35 70 10 25 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 (3.1053-3.3071 min, 34 scans) 11.D st x10² 0.9 29.1 0.8 0.7 45.0 0.6 0.5 0.4^{-} 57.0 0.3 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: 3.2627 Counts Counts x10⁵ x10⁴ 74.0 Component 74.0 29.0 1.6 ОН 29.0 73.0 1.4 3.5 45.0 73.0 1.2 3 57.0

45.0

57.0

0.8

0.6 0.4

0.2

3.2

3.15

3.25

Acquisition Time (min)

3.3

2.5

1.5

0.5

2

1

3.15

3.2

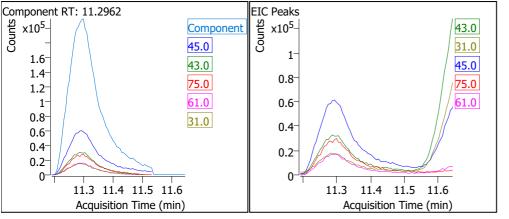
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Acquisition Time (min)

3.3

CH3

--- 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 11.2962 1,2-Propanediol, 3-methoxy-1561130.6 88.4 C4H10O3 Component RT: 11.2962 v10² 0.9 45.0 0.8 0.7^{-} 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 0.2 29.0 33.0 0.1 88.0 75 10 15 25 30 35 55 60 65 80 85 100 105 110 115 Mass-to-Charge (m/z) 1,2-Propanediol, 3-methoxy- (NIST20.L) Square value of the counts of 45.0 0.8 0.7 0.6 43.0 0.5 75.0 0.4 0.3 61.0 31.0 15.0 0.2 33.0 18.0 0.1 88.0 63.0 103.0 71.0 10 15 20 25 30 35 40 50 55 60 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (11.2062-11.5357 min, 55 scans) 11.D St x10² 0.9 45.0 0.8 0.7 0.6 0.5 75.0 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) EIC Peaks Component RT: 11.2962 x10⁵-Component 43.0



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12.3

12.4

Acquisition Time (min)

56.0

1.5

1

0.5

12.2

29.0

56.0

0.5

0.4

0.3

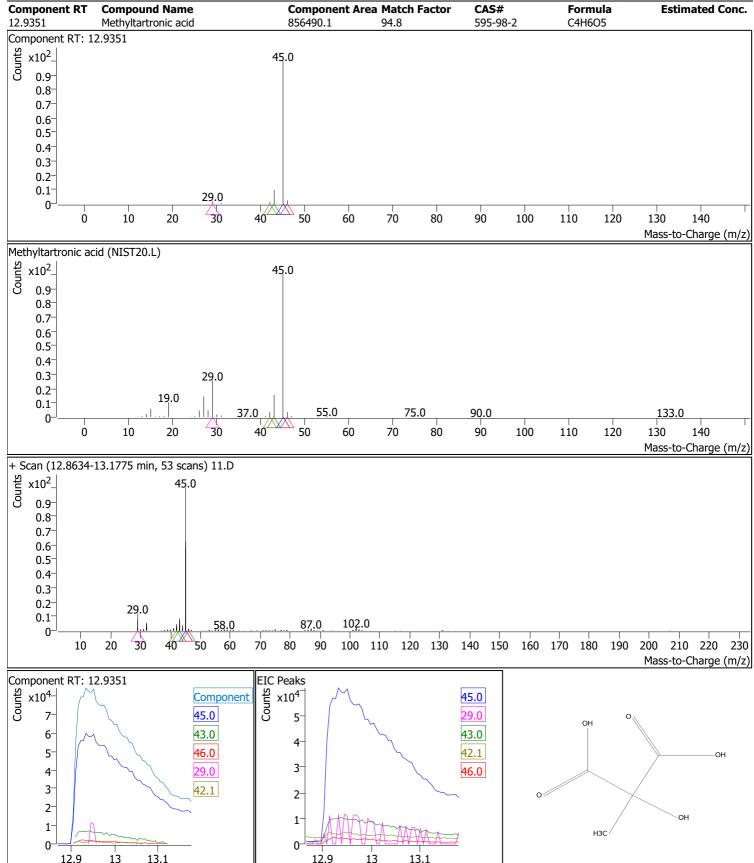
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12.2

12.3

12.4

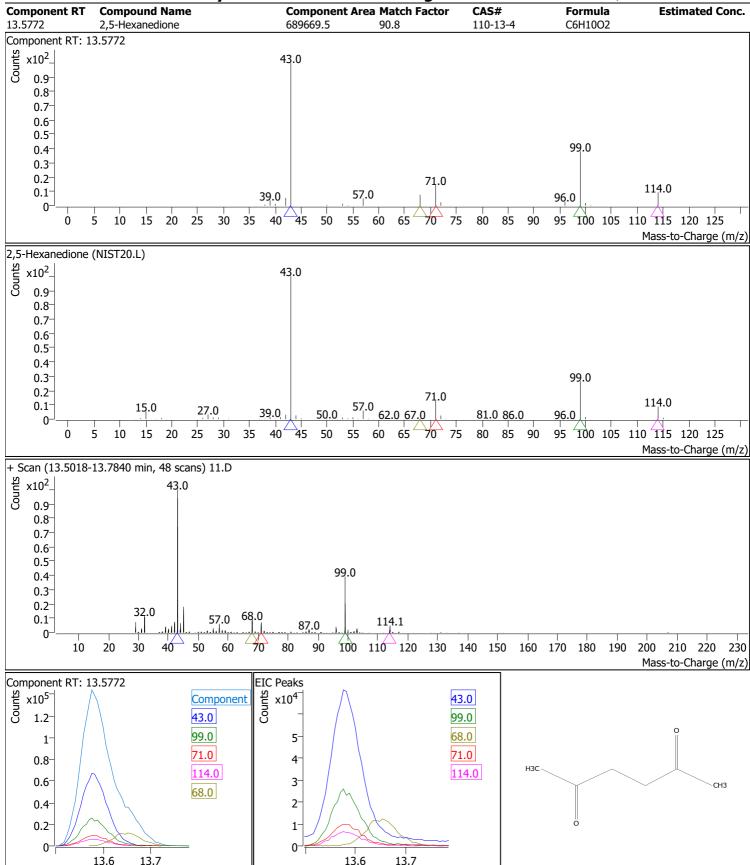




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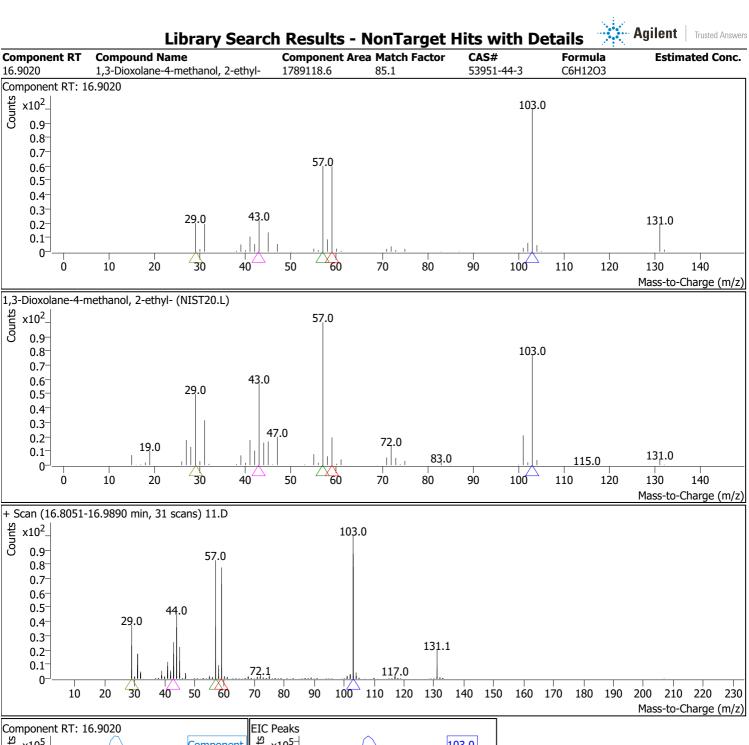


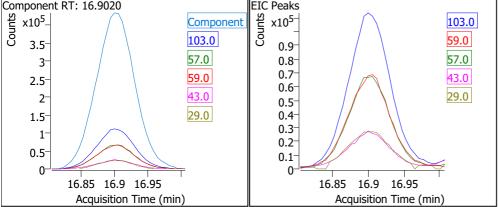




Acquisition Time (min)

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2758-18-1 2-Cyclopenten-1-one, 3-methyl-715614.8 97.9 C6H8O Component RT: 15.9772 v10² 0.9 96.0 0.8 0.7 67.0 0.6 0.5 53.0 0.4 81.0 39.0 0.3 0.2 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) Square value of the counts of 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 (15.9099-16.1565 min, 42 scans) 11.D st x10² 0.9 96.0 0.8 0.7 0.6 67.0 0.5 53.0 0.4^{-} 81.0 39.0 0.3 0.2 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 15.9772 **EIC Peaks** stuno x10⁵⁻ Counts x10⁴ 96.0 Component 96.0 67.0 1.2 2.5 67.0 53.0 CH3





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18.1

Acquisition Time (min)

18.2

40.0

39.0

40.0

1.25

0.75 · 0.5

0.25

1

3

2-

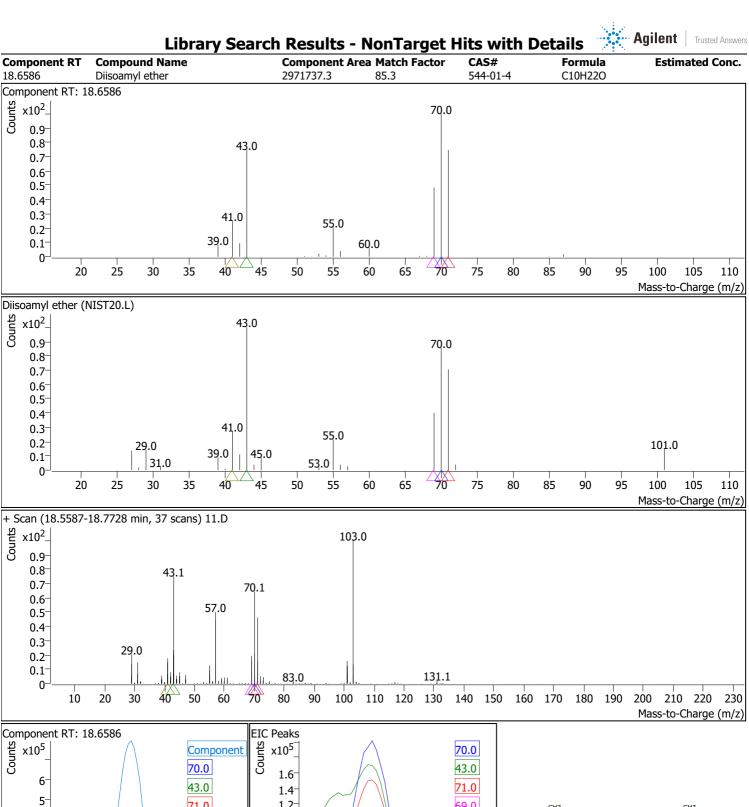
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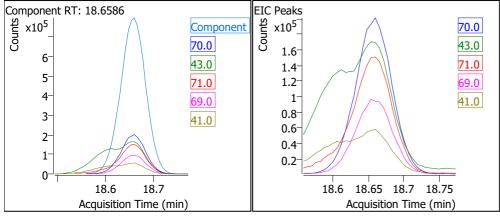
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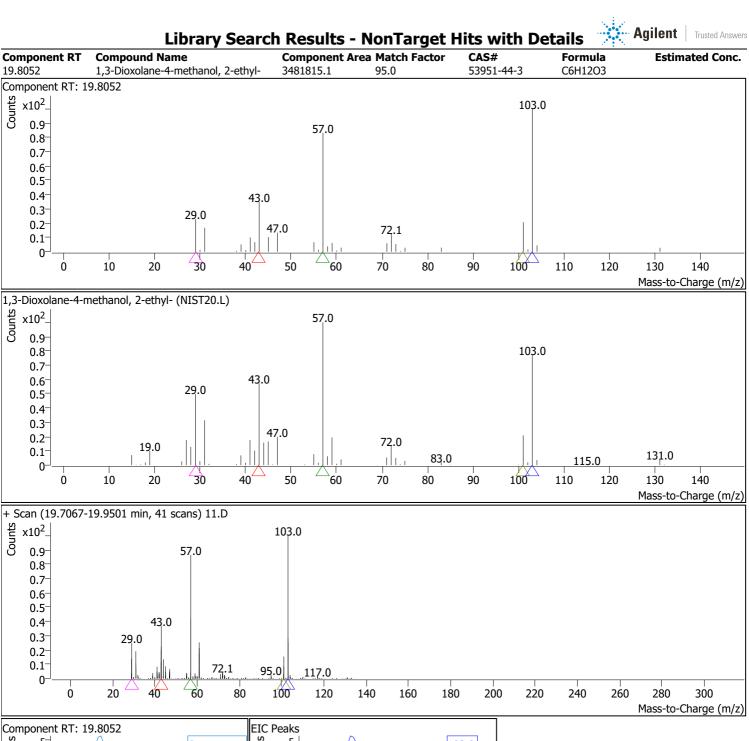
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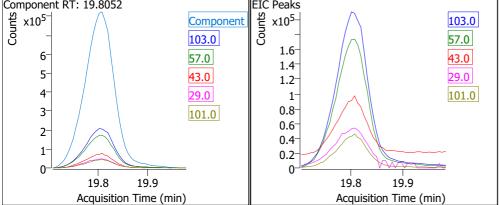
Acquisition Time (min)

18.2

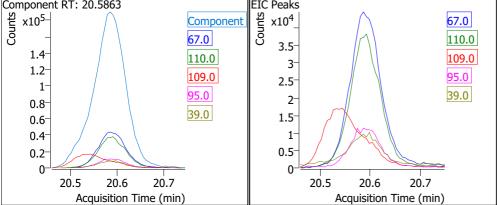


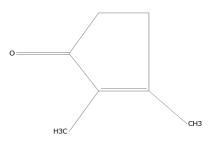


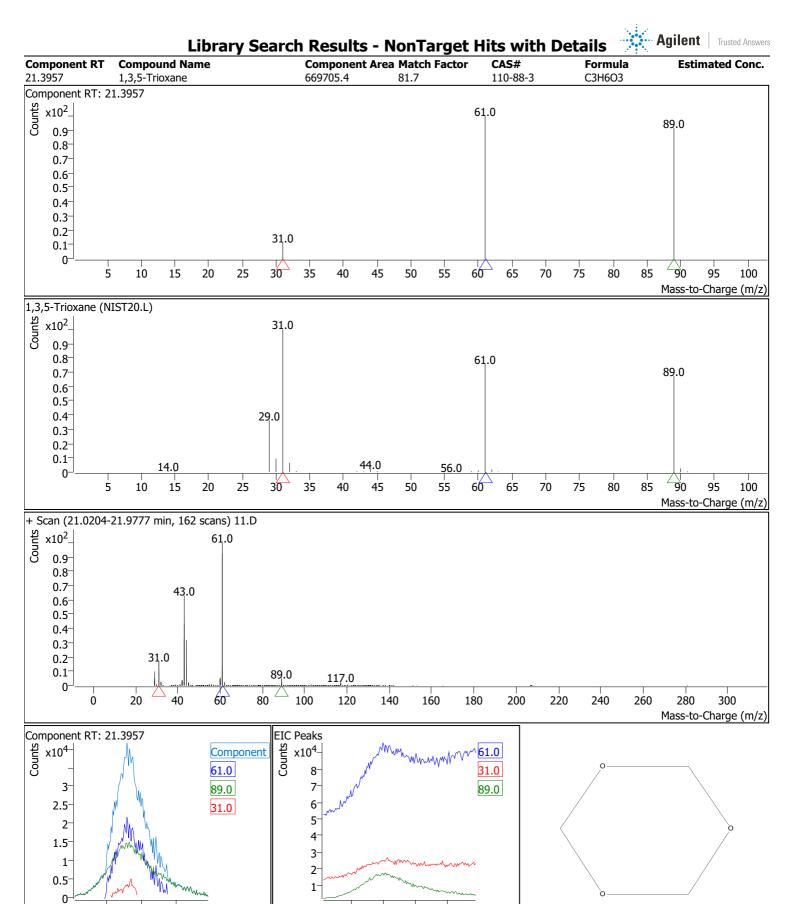




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21.2 21.4 21.6 21.8

Acquisition Time (min)

21.25 21.5 21.75

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22.3

Acquisition Time (min)

22.4

90.0

0.6

 0.5^{-}

 0.4^{-}

0.3

0.2

22.2

77.0

90.0

2.5

1.5

0.5

2

1

22.3

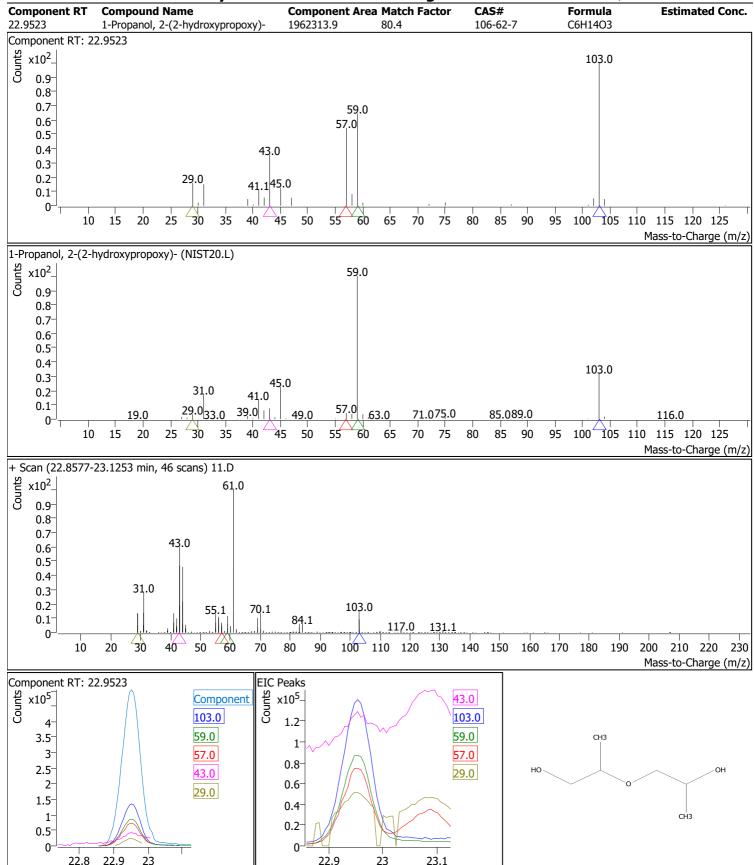
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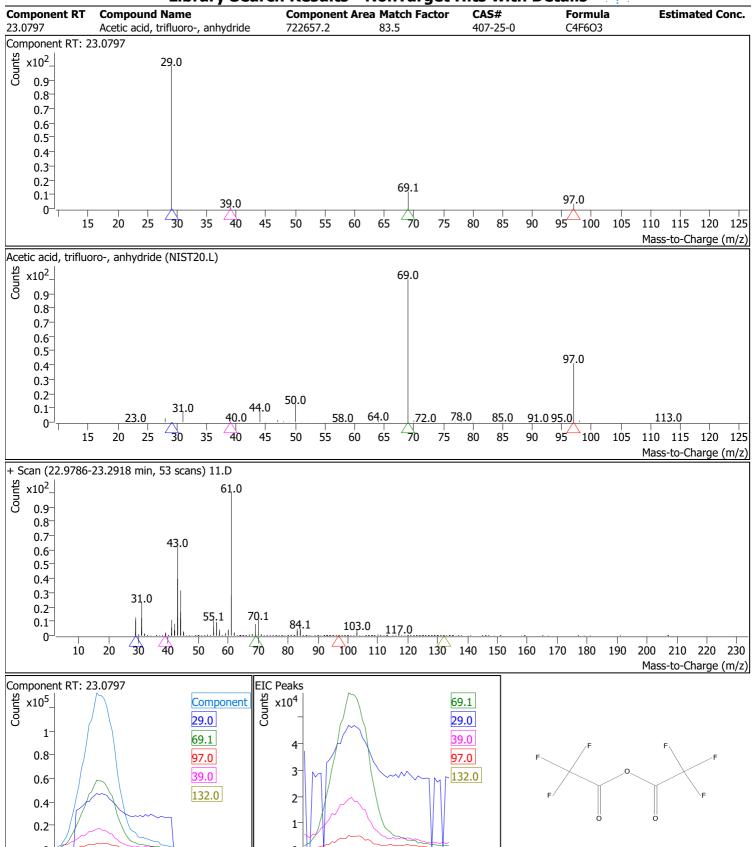






Acquisition Time (min)





23.1

23.2

Acquisition Time (min)

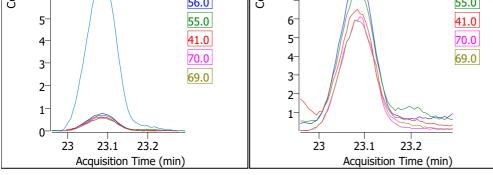
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23.1

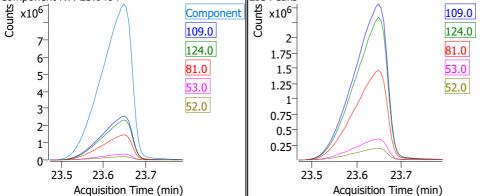
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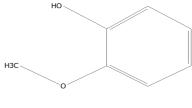
23.2

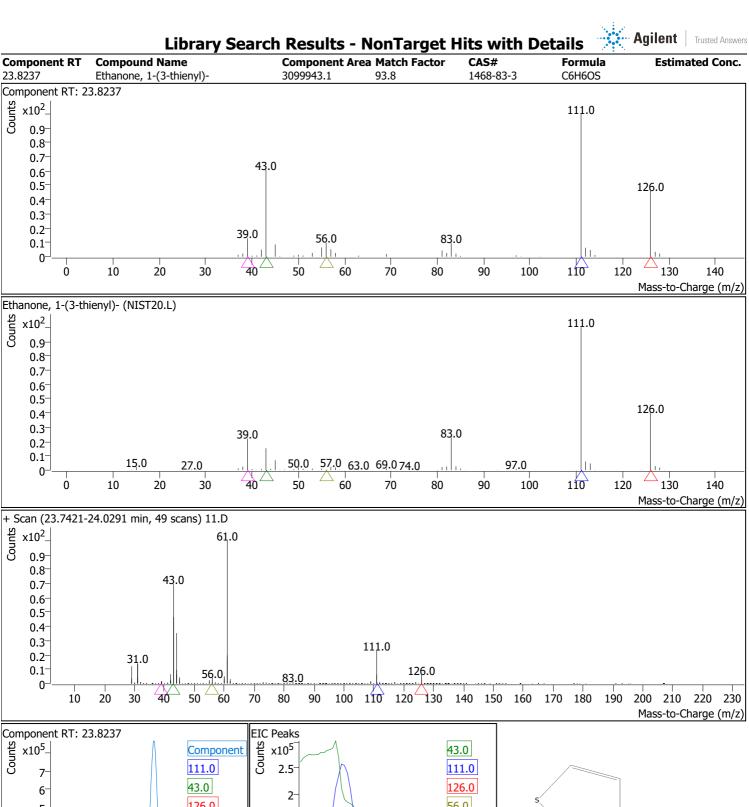
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 23.0842 1-Octanol 3701878.6 111-87-5 C8H18O Component RT: 23.0842 v10² 0.9 56.0 41.0 70.0 0.8 29.0 0.7 84.0 0.6 0.5 0.4 0.3 0.2 0.1 55 100 105 110 115 120 125 130 135 140 50 65 75 80 85 90 95 60 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Square value of the counts of 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 35 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (22.9707-23.2728 min, 51 scans) 11.D St x10²_ 0.9 0.8 0.7 43.0 0.6 0.5 0.4^{-} 0.3 31.0 0.2 55.1 70.1 103.0 0.1 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 180 190 200 210 220 230 90 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.0842 Counts Counts x10⁵ x10⁴ 56.0 Component 56.0 55.0 5 55.0 6 41.0

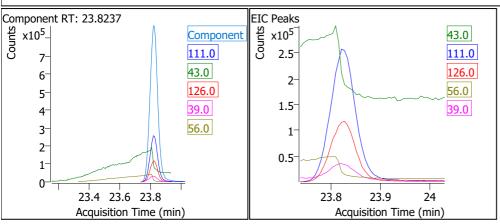


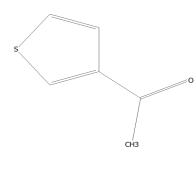
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6484 Phenol, 2-methoxy-46803547.3 98.4 C7H8O2 Component RT: 23.6484 v10² 0.9 109.0 124.0 0.8 0.7^{-} 81.0 0.6 0.5 0.4 0.3 0.2 0.1 39.0 65.0 80 110 10 20 30 40 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) St x10²_ 0.9 109.0 124.0 0.8 0.7 0.6 0.5 81.0 0.4 0.3 0.2 53.0 27.0 39.0 0.1 65.0 18.0 77.0 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4701-23.7853 min, 54 scans) 11.D st x10² 0.9 109.0 124.0 0.8 81.0 0.7 0.6 0.5 61.0 0.4^{-} 43.0 0.3 0.2 53.0 0.1 31.0 95.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 23.6484 EIC Peaks Counts Counts x10⁶ 109.0 Component 109.0 124.0 2 7 124.0 81.0 1.75 6





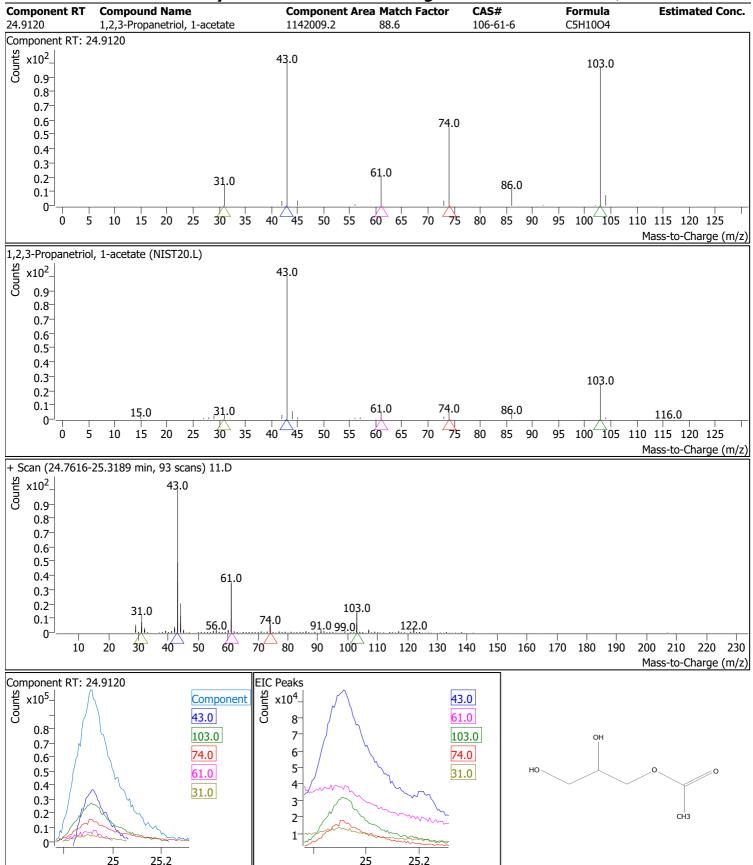






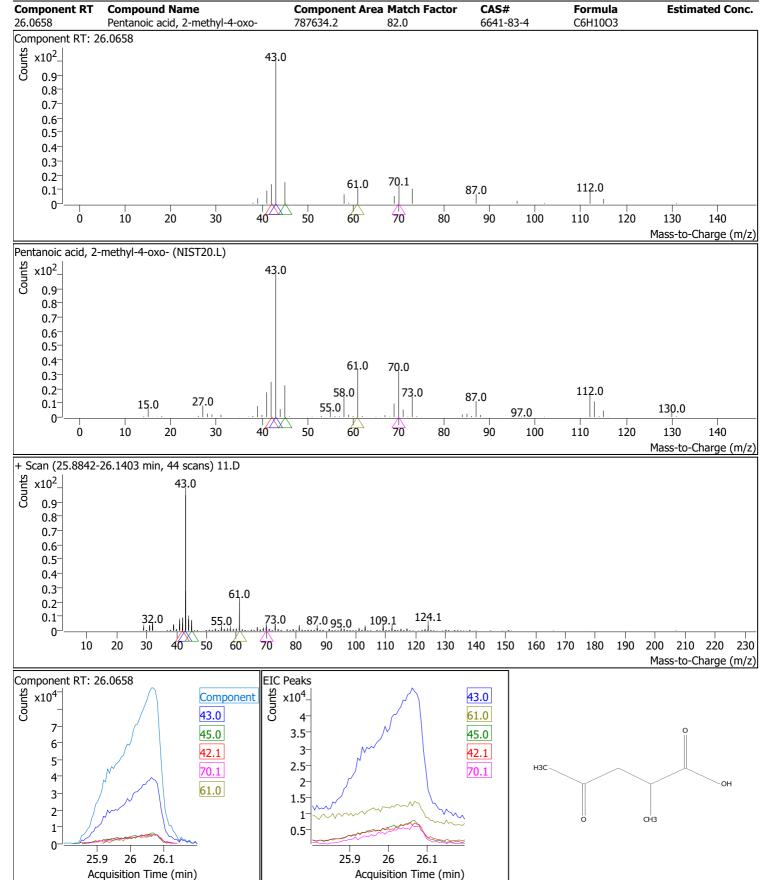


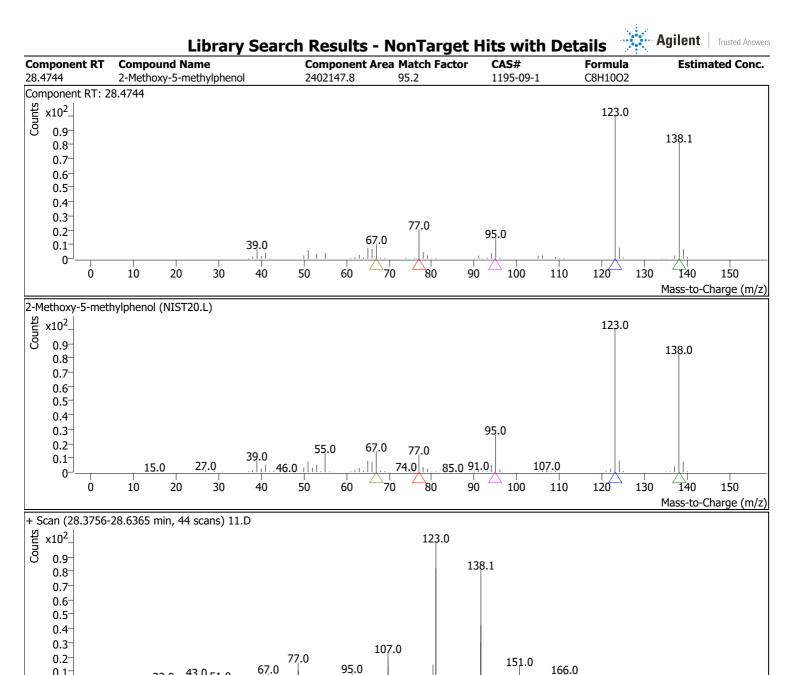




Acquisition Time (min)







0.1

Counts x10⁵

5

3

2-

1-

28.4

28.5

Acquisition Time (min)

28.6

10

Component RT: 28.4744

20

50

60

Component 123.0

138.1

77.0

95.0

67.0

90

EIC Peaks

x10⁵-

1.6

1.4

1.2

0.8

0.6 0.4

0.2

28.4

1

100 110

120 130

28.6

140 150

123.0

138.1

77.0

95.0

67.0

160 170

нзс

180

190

200

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

28.5

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Naphthalene 91-20-3 28.7549 670341.7 93.6 C10H8 Component RT: 28.7549 v10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 64.0 51.0 50 75 45 55 60 65 70 85 100 105 110 115 120 135 Mass-to-Charge (m/z) Naphthalene (NIST20.L) x10²_ 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 51.0 63.0 75.0 87.0 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 135 140 Mass-to-Charge (m/z) + Scan (28.6639-28.8751 min, 36 scans) 11.D st x10² 0.9 128.1 0.8 0.7 0.6 0.5 0.4^{-} 0.3 151.0 122.0 0.2 77.0 105.0 166.0 43.0 0.1 57.0 136.0 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) EIC Peaks Component RT: 28.7549 st x10⁵ Counts x10⁵ 128.0 Component 128.0 127.0 1.4 0.8 127.0 129.0 1.2 0.7 129.0 102.0 0.6 1 0.5 102.0 126.0 0.8

7 28.75 28.8 28.85 Acquisition Time (min)

 0.4^{-}

0.3

0.2

0.1

126.0

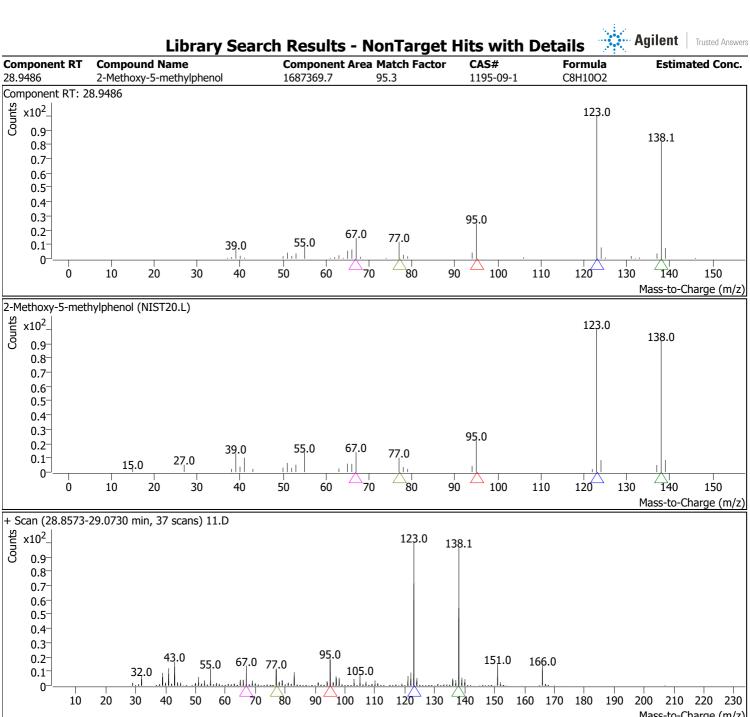
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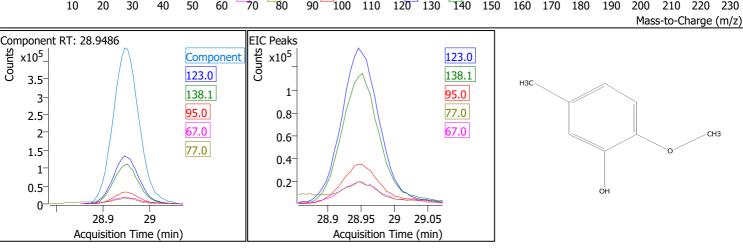
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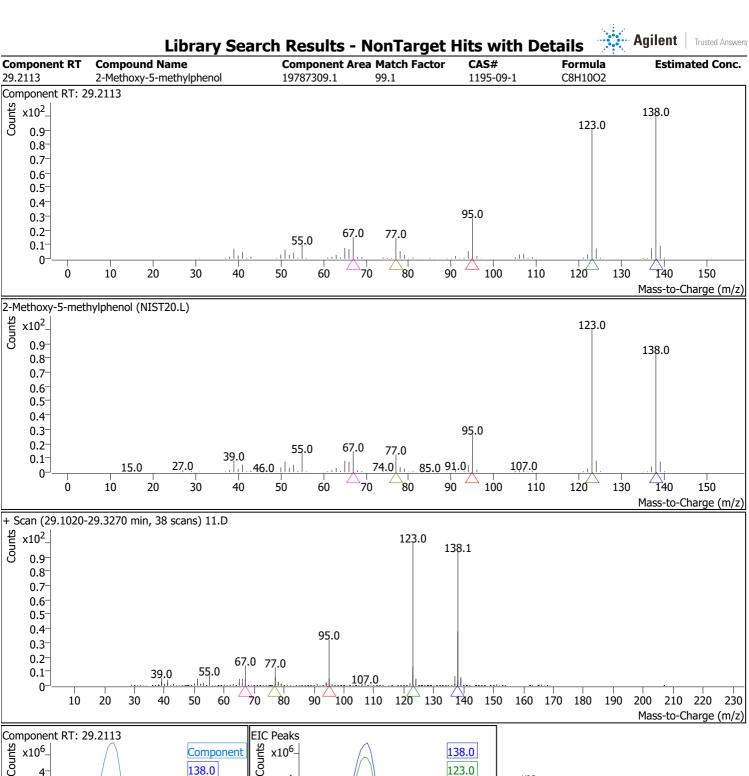
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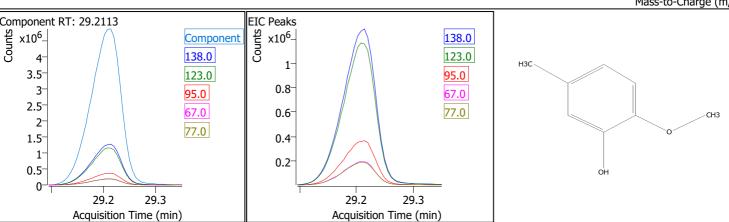
28.7

28.8

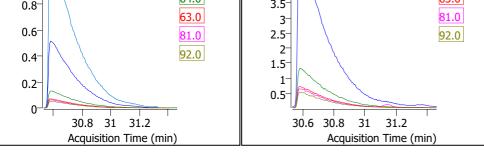




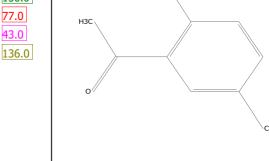




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.5840 Catechol 15015507.5 96.5 C6H6O2 Component RT: 30.5840 v10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 ² 95 110 115 120 125 10 15 35 45 50 55 75 80 85 90 100 105 Mass-to-Charge (m/z) Catechol (NIST20.L) st v10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 64.0 0.3 0.2 92.0 0.1 ∠65 10 15 25 30 35 40 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.5340-31.3249 min, 134 scans) 11.D st x10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4^{-} 0.3 64.0 0.2 81.092.0 _{39.0} 53.0 0.1 Ó 20 40 60 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 30.5840 **EIC Peaks** Counts Counts x10⁶ x10⁵ 110.0 Component 110.0 64.0 4 64.0 63.0 3.5 0.8



--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1450-72-2 32.1161 Ethanone, 1-(2-hydroxy-5-762312.7 92.7 C9H10O2 methylphenyl)-Component RT: 32.1161 x10²_ 135.0 0.9 8.0 0.7 0.6 150.0 0.5 0.4 0.3 77.0 0.2^{-} 43.0 0.1 39.0 107.0 121.0 0-150 10 20 30 40 50 60 70 80 90 100 110 120 130 140 160 170 Mass-to-Charge (m/z) Ethanone, 1-(2-hydroxy-5-methylphenyl)- (NIST20.L) Counts $x10^{2}$ 135.0 0.9 0.8 0.7 0.6 150.0 0.5 0.4 0.3 107.0 0.2 77.0 43.0 51.0 0.1 27.0 63.0 85.091.0 131.0 121.0 0 130 150 10 20 30 50 60 70 80 90 100 110 120 140 160 170 Mass-to-Charge (m/z) + Scan (32.0393-32.2524 min, 36 scans) 11.D x10². 135.0 0.9 0.8 0.7 0.6 0.5 150.0 0.4 0.3 43.0 0.2 32.0 180.0 0.1 165.0 110.0 121.0 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 10 20 30 40 50 60 70 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 32.1161 Counts Counts x10⁴_ 135.0 x10⁵ Component НО 150.0 135.0 1.6 6 150.0 77.0 1.4 **Н3С** 5 1.2 77.0 43.0 4 1



32.1 32.15 32.2

Acquisition Time (min)

43.0

136.0

3

2-

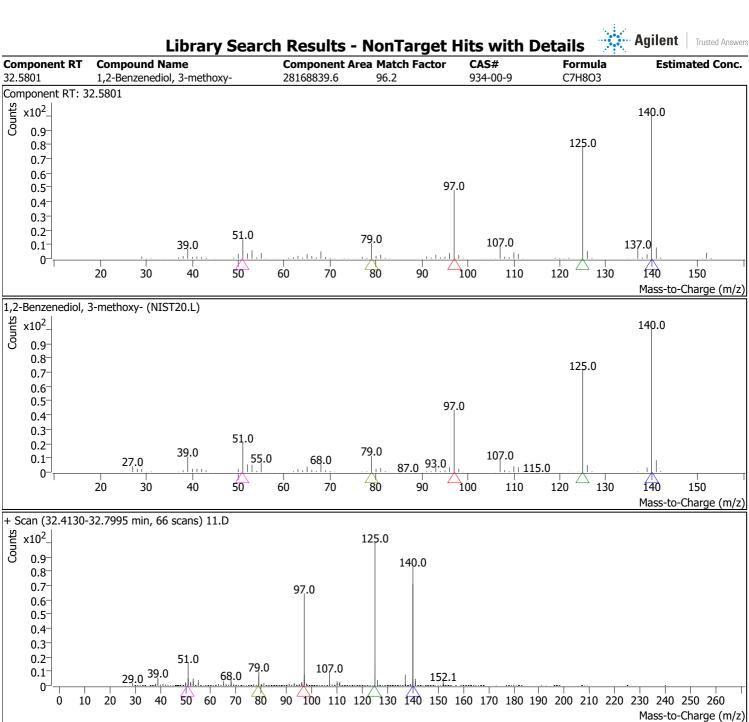
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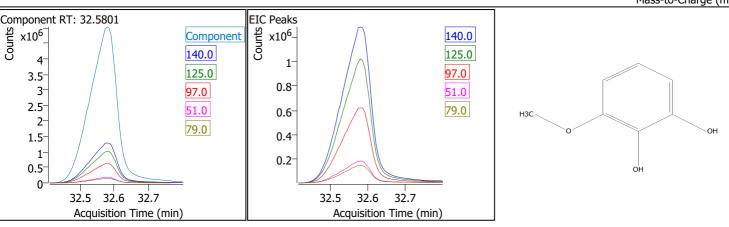
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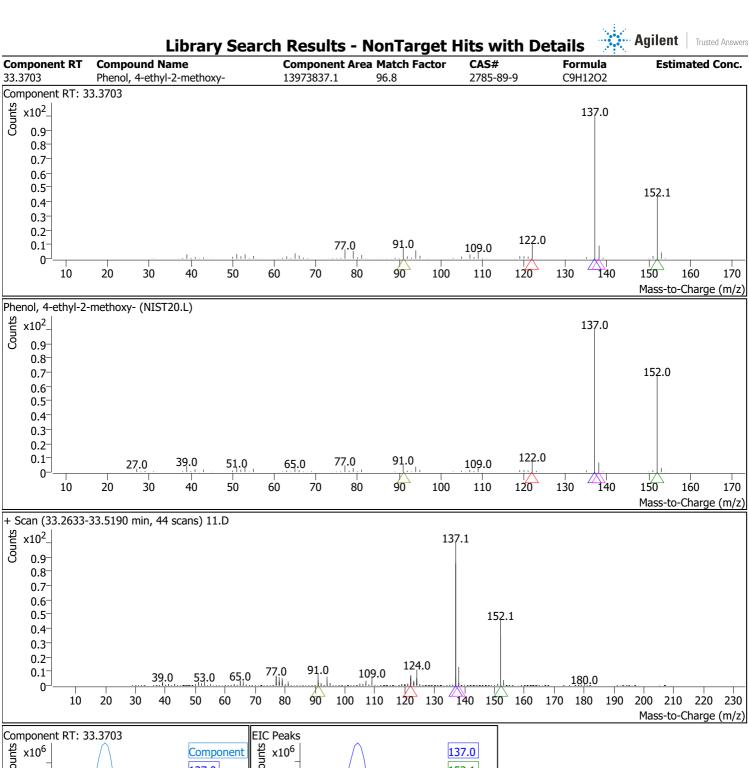
0.4 0.2

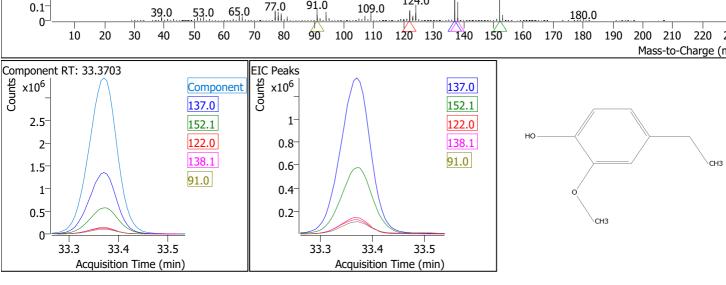
32.1

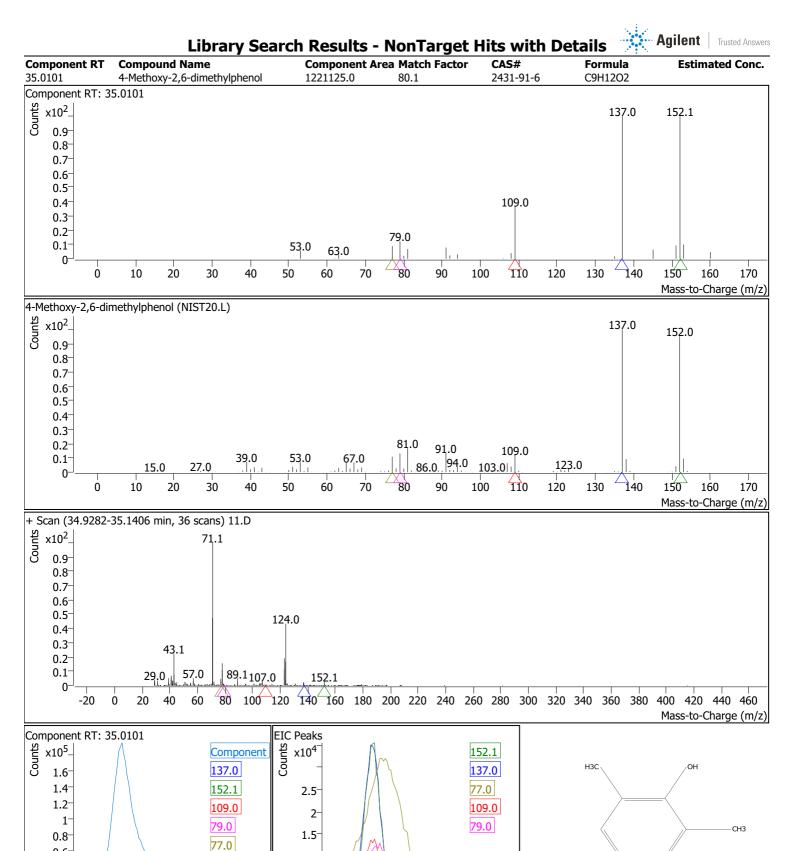
32.2













35

35.1 35.2

Acquisition Time (min)

1-

0.5

0.6

0.4

0.2

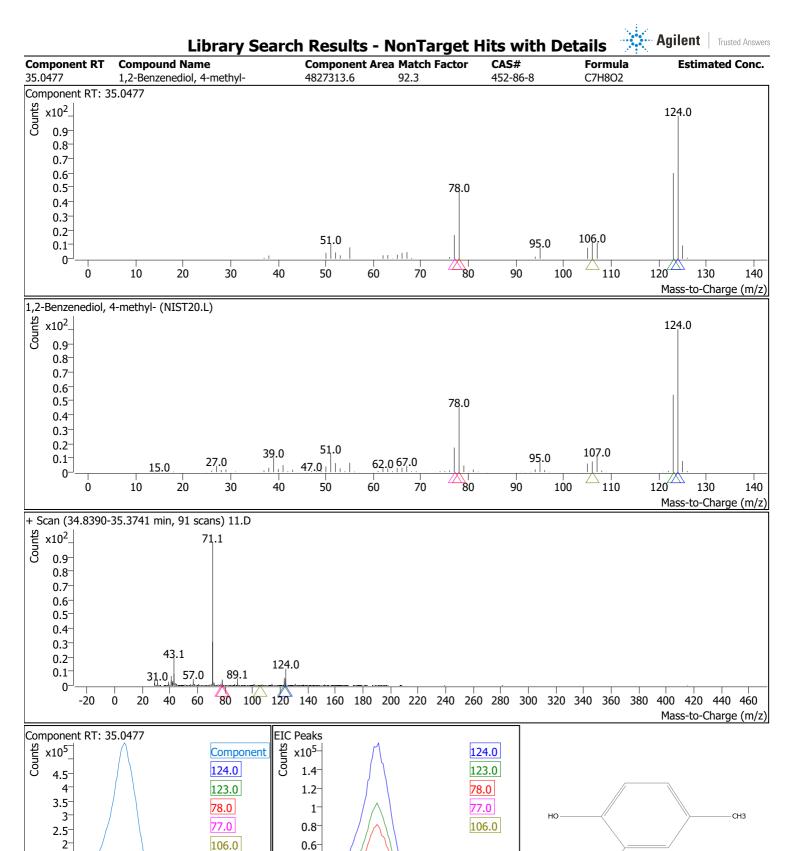
34.9

35

35.1 35.2

Acquisition Time (min)

H₃C



35.2

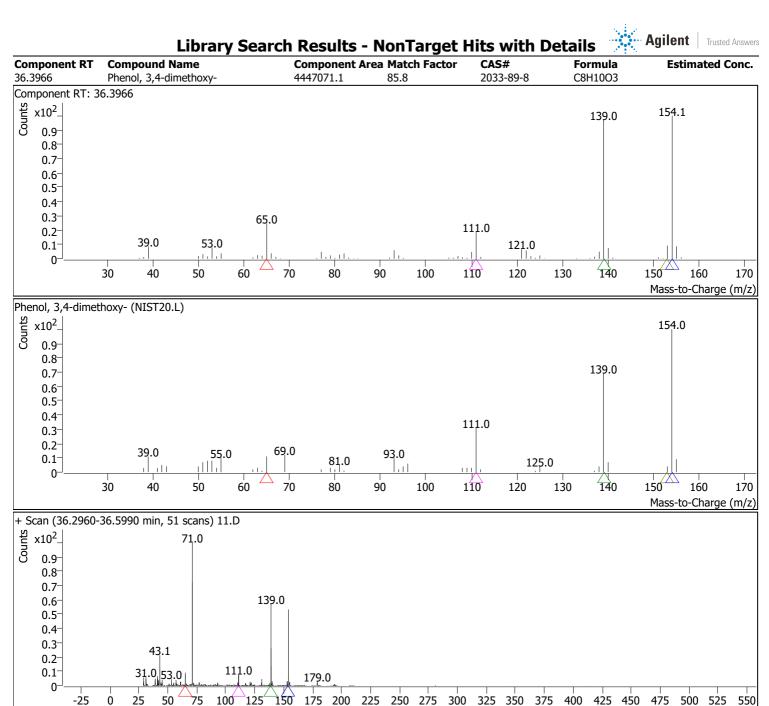
Acquisition Time (min)

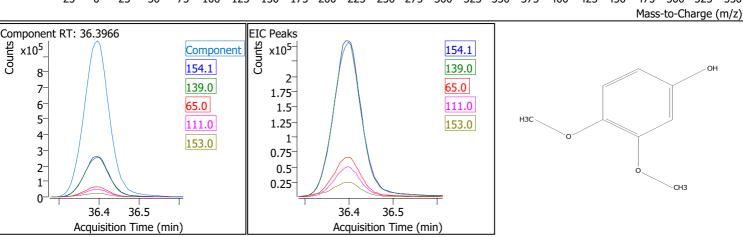
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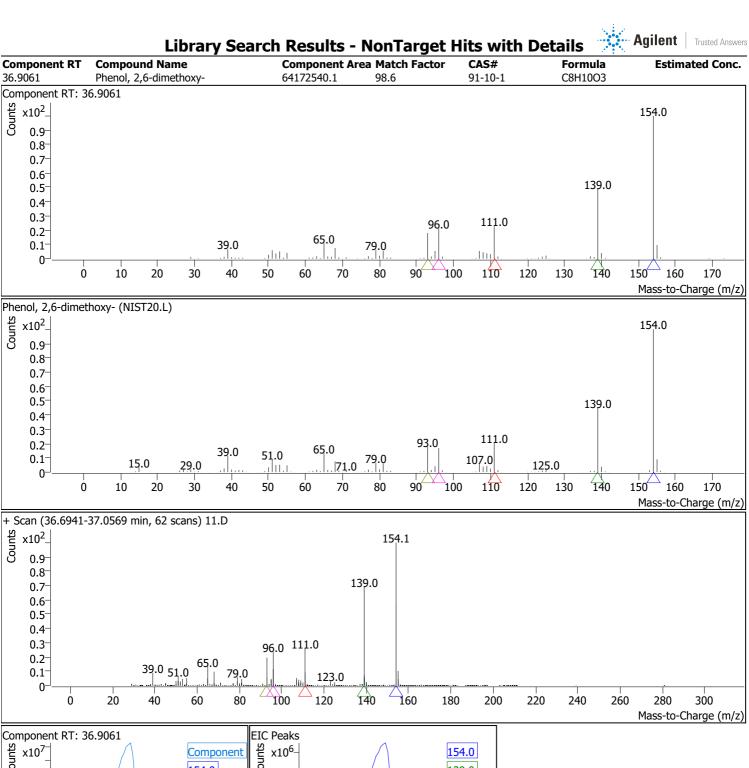
1.5

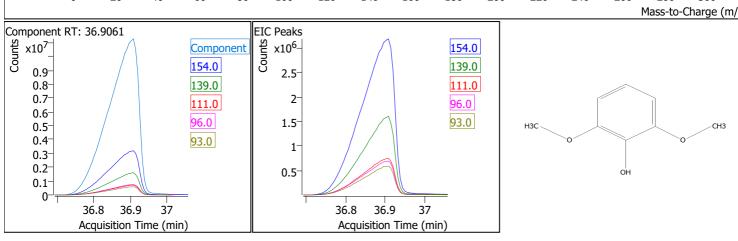
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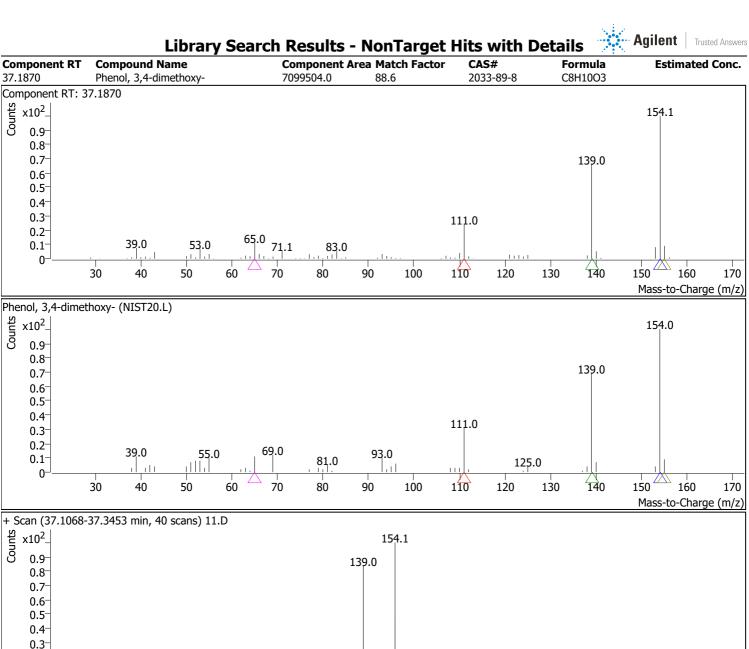
35.2

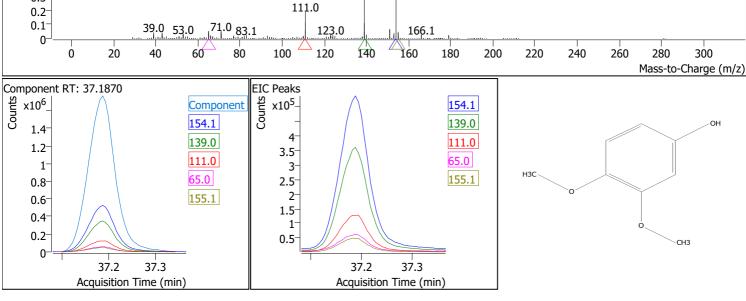






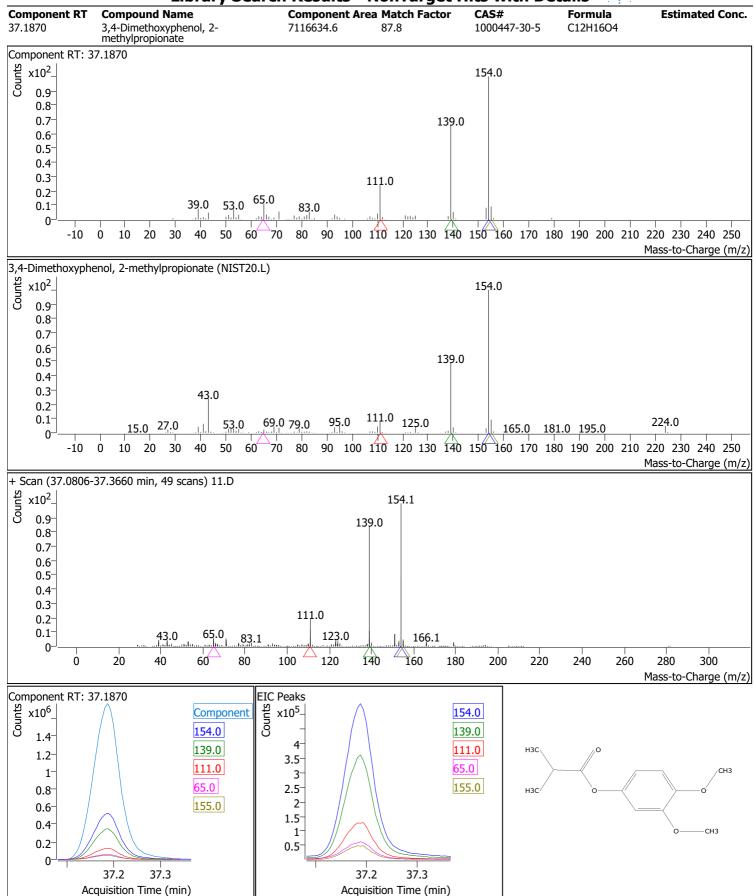




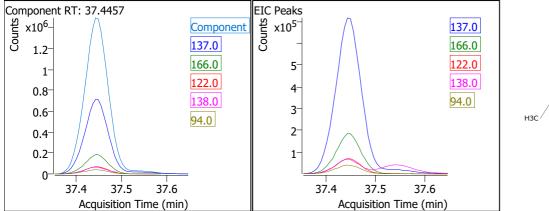


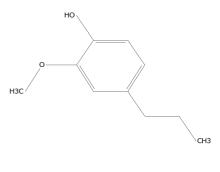
Library Search Results - NonTarget Hits with Details





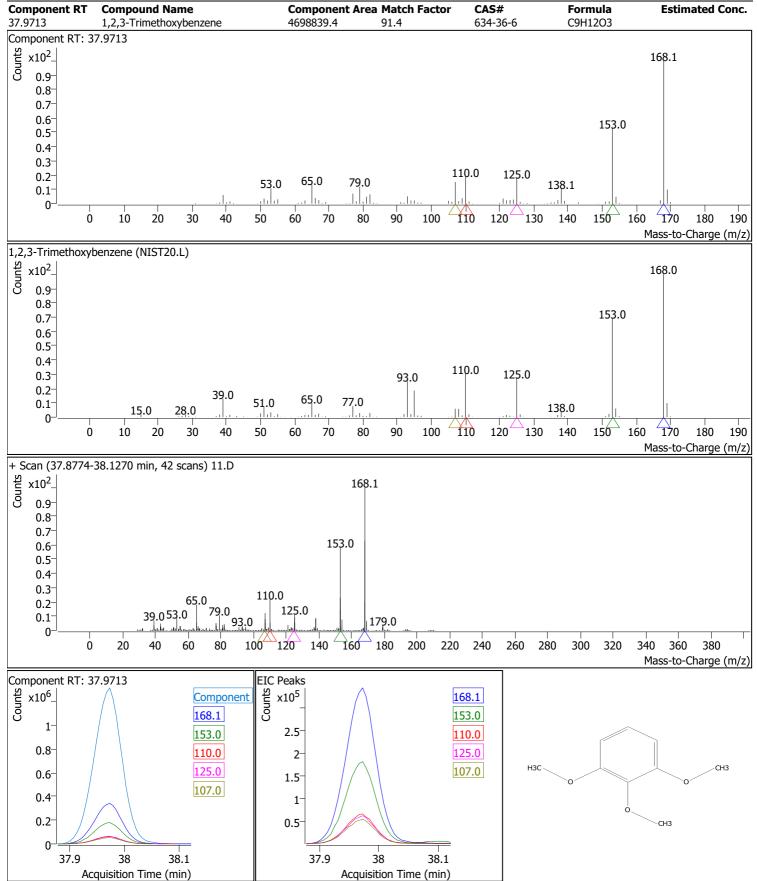
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 37.4457 Phenol, 2-methoxy-4-propyl-5418466.3 93.8 2785-87-7 C10H14O2 Component RT: 37.4457 y x10² 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 0.1 77.0 51.0 105.0 160 - 170 50 120 10 20 30 40 60 70 100 110 130 180 Mass-to-Charge (m/z) Phenol, 2-methoxy-4-propyl- (NIST20.L) Counts x10²_ 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 166.0 0.2 122.0 94.0 77.0 27.0 39.0 51.0 15.0 0.1 66.0 107.0 150.0 160 170 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 180 Mass-to-Charge (m/z) + Scan (37.3579-37.6455 min, 49 scans) 11.D st x10² 0.9 137.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 166.1 122.0 0.1 71.0 154.0 179.0 -20 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 Mass-to-Charge (m/z) EIC Peaks Component RT: 37.4457 x10⁶-Counts x10⁵ 137.0 Component 137.0 166.0 1.2 166.0 122.0 5 1

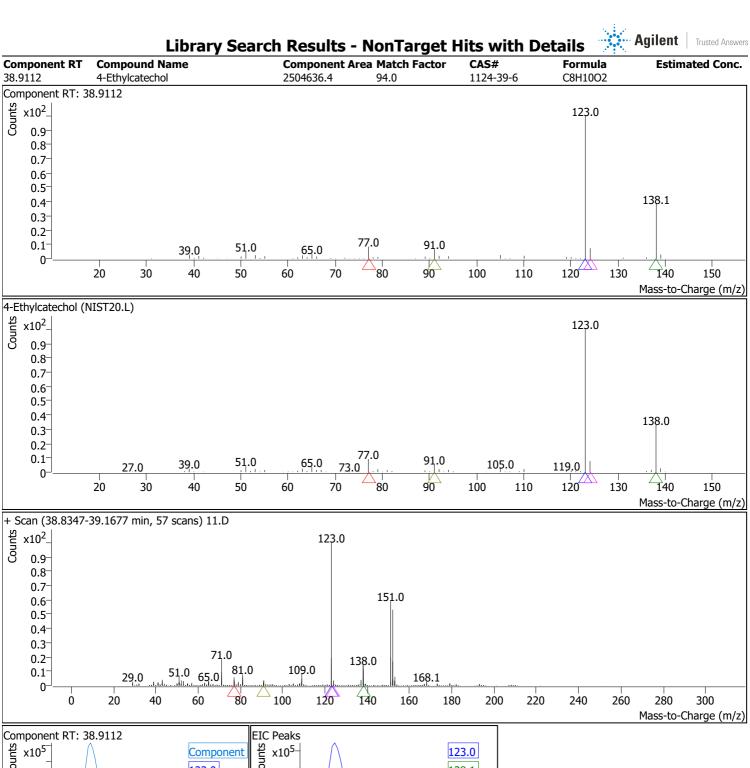


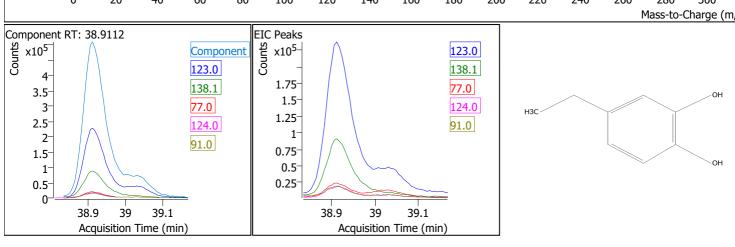












--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 621-59-0 39.0404 Benzaldehyde, 3-hydroxy-4-methoxy-2975405.9 90.2 C8H8O3 Component RT: 39.0404 v10² 0.9 151.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 81.0 109.0 0.2 168.1 0.1 80 170 10 20 30 60 100 110 120 130 140 150 160 Mass-to-Charge (m/z) Benzaldehyde, 3-hydroxy-4-methoxy- (NIST20.L) st x10² 0.9 151.0 0.8 0.7 0.6 0.5 0.4 81.0 0.3 109.0 0.2 123.0 39.0 0.1 15.0 119.0 128.0 137.0 74.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (38.9482-39.1618 min, 36 scans) 11.D st x10² 0.9 151.0 0.8 0.7 0.6 0.5 0.4^{-} 123.0 0.3 0.2 109.0 51.0 65.0 138.1 0.1 168.1 91.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 39.0404 Counts x10⁵ Counts x10⁵ 151.0 Component 151.0 152.1 1.4 5 152.1 81.0 1.2

3

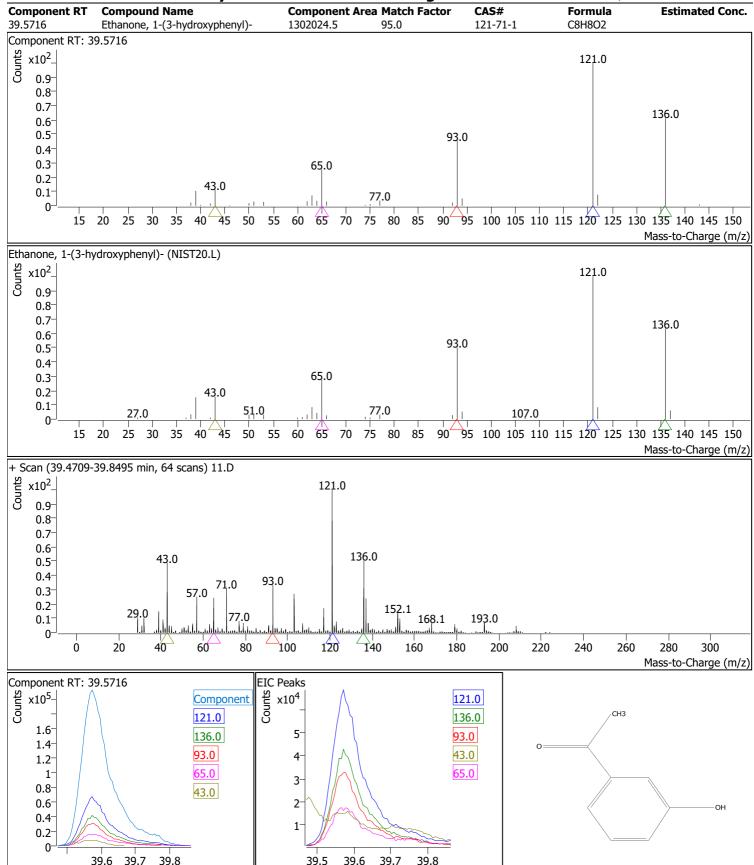
2

1

39.1







--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4-Methoxy-2-methyl-1-(methylthio)benzene 40.0056 2455888.4 86.0 22583-04-6 C9H12OS Component RT: 40.0056 x10²_ 153.0 0.9 8.0 0.7 0.6 0.5 168.0 0.4 0.3 138.0 0.2^{-} 107.0 0.1 0-110 170 140 150 0 10 20 30 50 80 90 100 120 130 160 180 190 Mass-to-Charge (m/z) 4-Methoxy-2-methyl-1-(methylthio)benzene (NIST20.L) $x10^{2}$ 168.0 0.9 0.8 0.7 153.0 0.6 0.5 0.4 0.3 138.0 0.2 109.0 45.0 0.1 77.0 84.0 91.0 65.0 125.0 28.0 0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 180 190 Mass-to-Charge (m/z) + Scan (39.9257-40.1250 min, 34 scans) 11.D st x10² 0.9 153.0 0.8 0.7 0.6 0.5 0.4 168.1 0.3 0.2 138.0 0.1 107.0 39.0 53.0 65.0 77.0 91.0 0 140 Ó 40 60 80 100 120 20 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 40.0056 **EIC Peaks** Counts Counts x10⁵x10⁵ 153.0 Component 168.0 153.0 5 2-168.0 138.0 1.75 4 138.0 154.0 1.5 154.0 1.25 107.0 3



1

0.75

0.5

0.25

39.95

40

40.05 40.1

Acquisition Time (min)

107.0

2

1

40

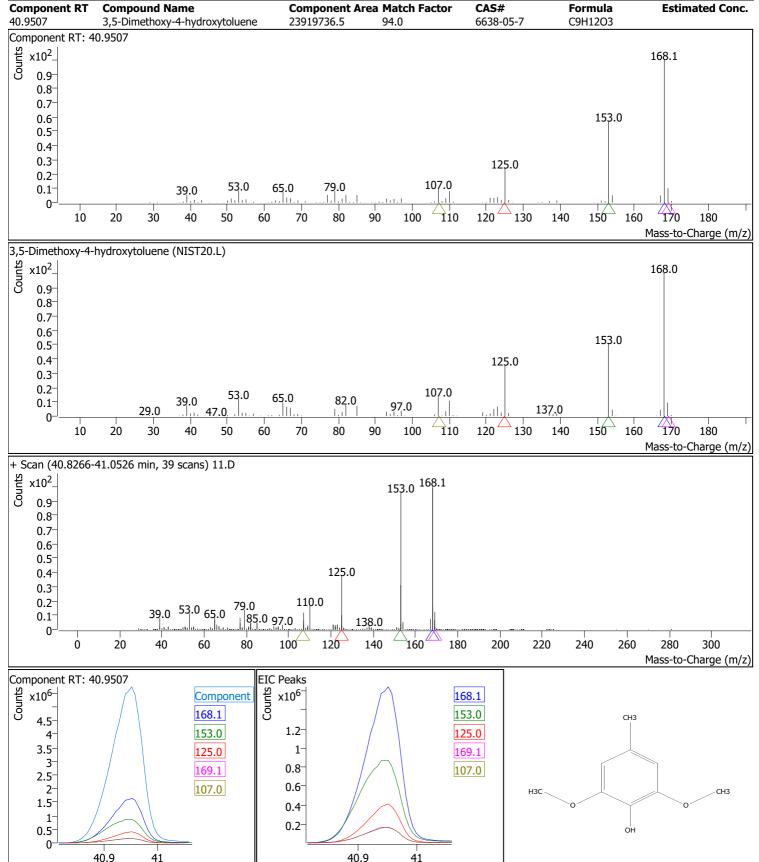
40.1

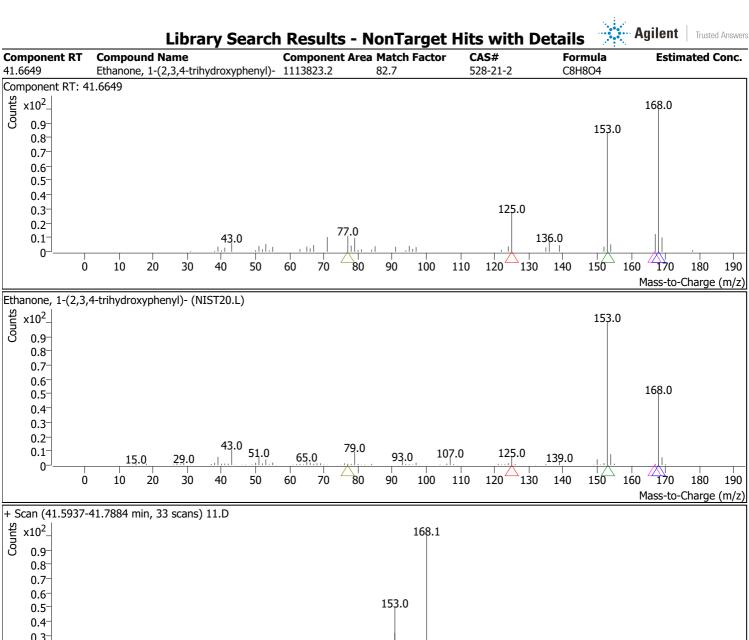
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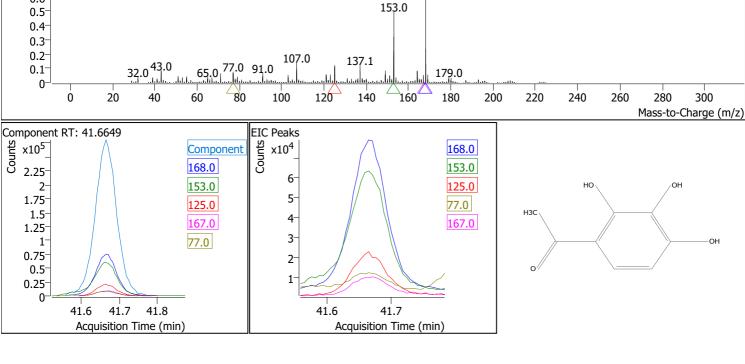
нзс











--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 41.8055 Eugenol 1556733.5 81.9 97-53-0 C10H12O2 Component RT: 41.8055 $x10^{2}$ 164.0 0.9 137.0 149.0 0.8 0.7^{-} 0.6 0.5 0.4 0.3 121.0 91.0 180.0 77.0 103.0 0.2 0.1 150 90 10 20 30 40 50 60 70 80 100 110 120 130 170 180 Mass-to-Charge (m/z) Eugenol (NIST20.L) st x10²_ 0.9-164.0 0.8 0.7 0.6 0.5 0.4 149.0 0.3 131.0 0.2 77.0 103.0 91.0 55.0 121.0 0.1 39.0 65.0 27.0 115.0 74.0 [∠]140 150 10 20 30 40 50 60 70 80 90 100 110 120 130 170 180 Mass-to-Charge (m/z) + Scan (41.6472-41.9365 min, 49 scans) 11.D st x10² 0.9 168.1 0.8 0.7 0.6 137.0 71.0 0.5 0.4 0.3 176.1 91.0103.0 121.0 0.2 77.0 55.0 0.1 140 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 41.8055 Counts Counts x10⁴ 164.0 Component 164.0 137.0 5 3 137.0 149.0 2.5 149.0 91.0



41.8

Acquisition Time (min)

41.9

121.0

3

2-

41.7

121.0

91.0

2

1.5

0.5

41.7

41.8

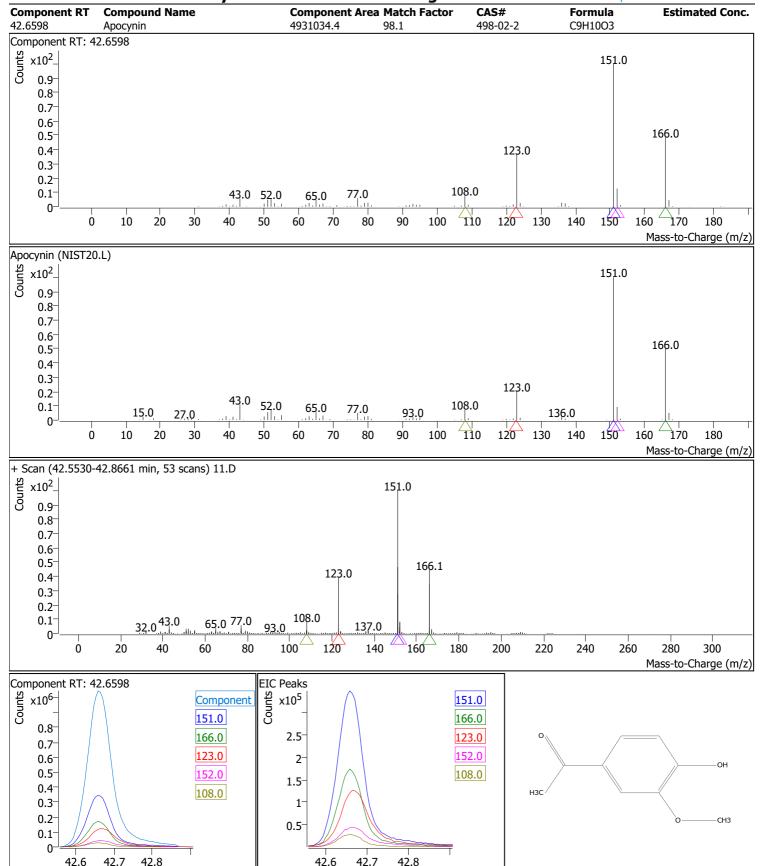
Acquisition Time (min)

41.9

CH2

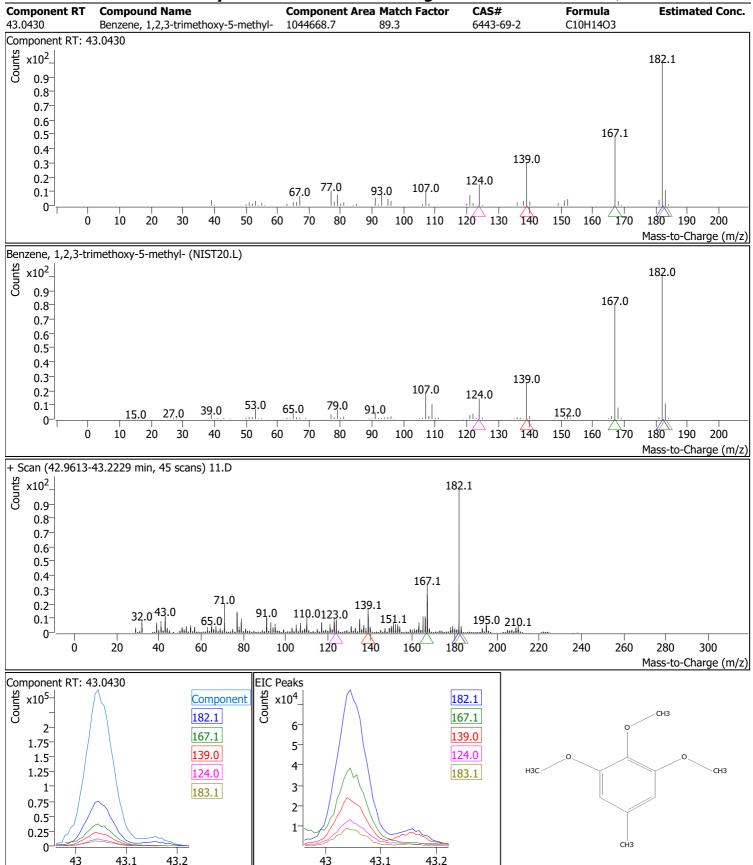






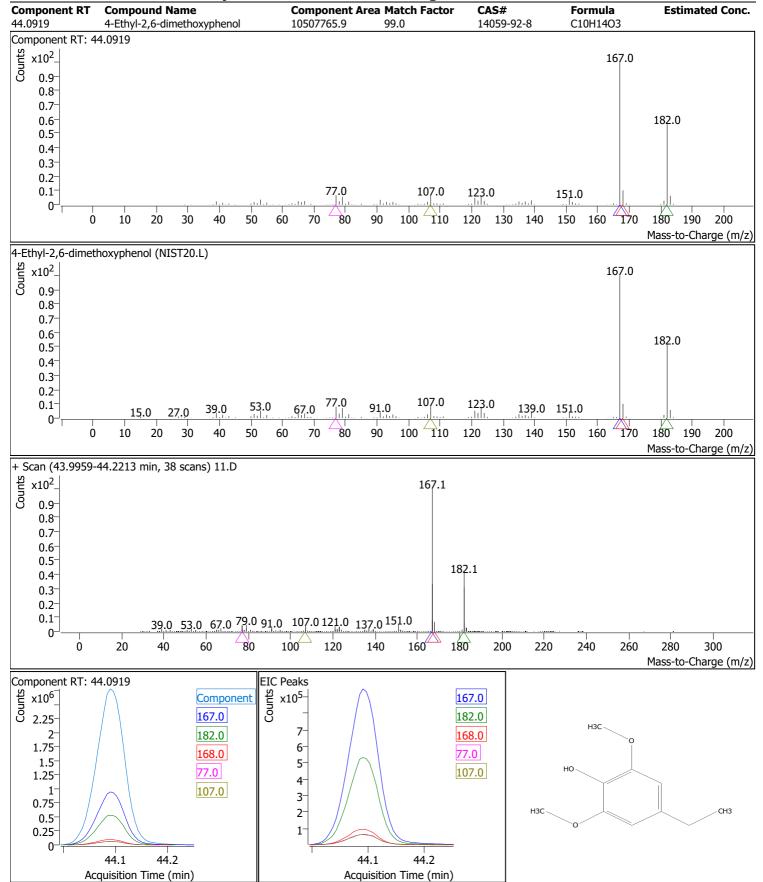




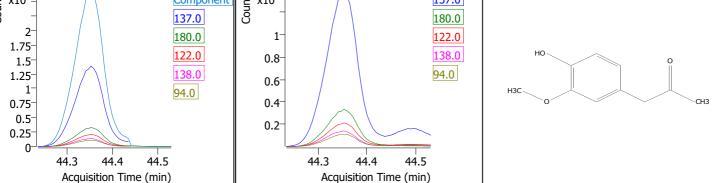


Library Search Results - NonTarget Hits with Details



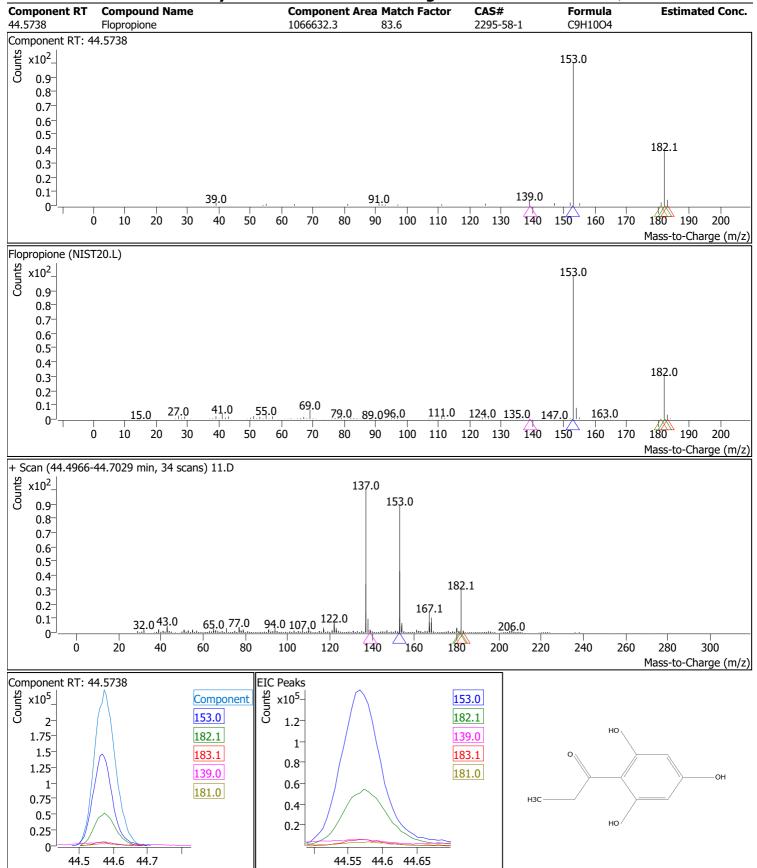


··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 44.3530 2-Propanone, 1-(4-hydroxy-3-12225428.5 88.4 2503-46-0 C10H12O3 methoxyphenyl) Component RT: 44.3530 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 122.0 0.1 51.0 66.0 39.0 120 180 20 30 40 50 60 70 80 90 100 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 66.0 85.0⁹1.0 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 90 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2281-44.4359 min, 35 scans) 11.D x10². 137.1 0.9 0.8 0.7^{-} 0.6 0.5 0.4 180.1 0.3 74.0 0.2 122.0 87.0 43.0 0.1 55.0 115.0 171.1 0 100 140 180 Ó 20 40 60 80 120 160 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 44.3530 **EIC Peaks** Counts Counts x10⁶x10⁶ 137.0 Component 180.0 137.0 2 180.0 1 122.0 1.75



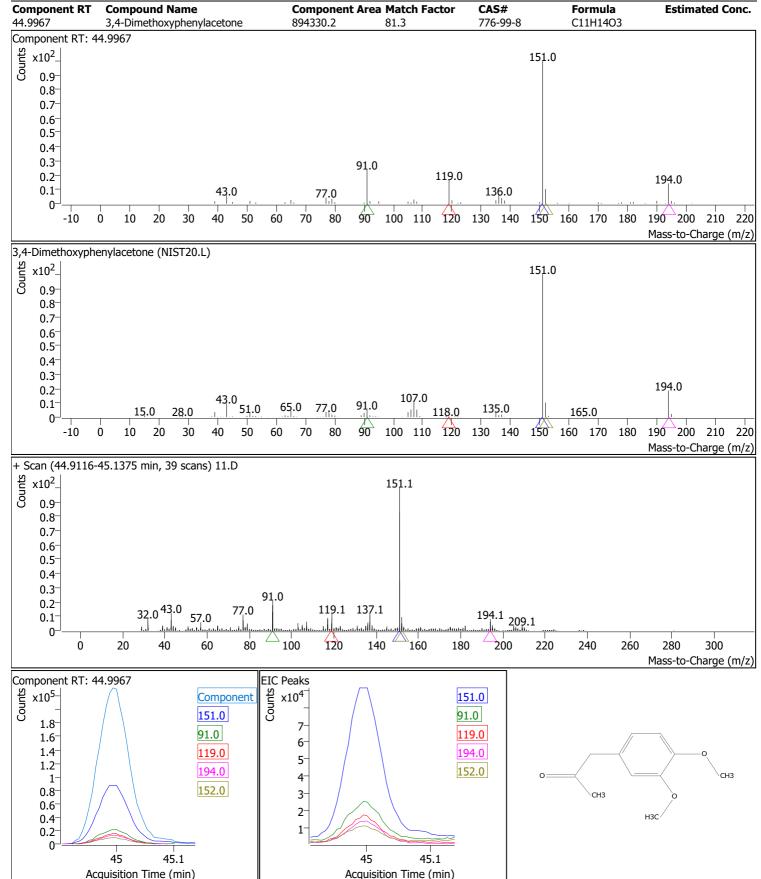






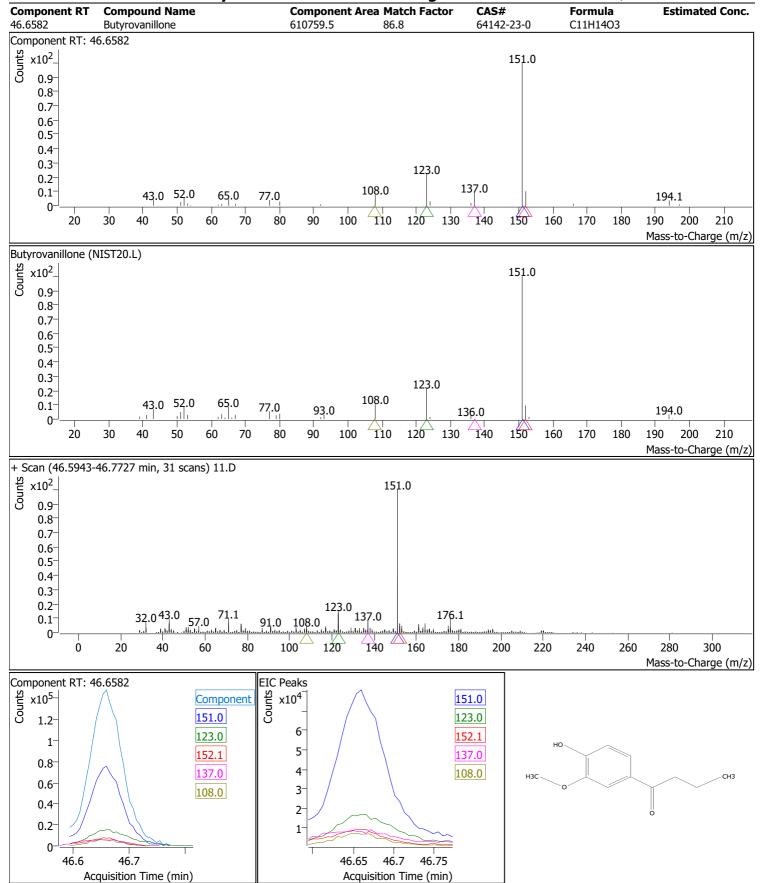


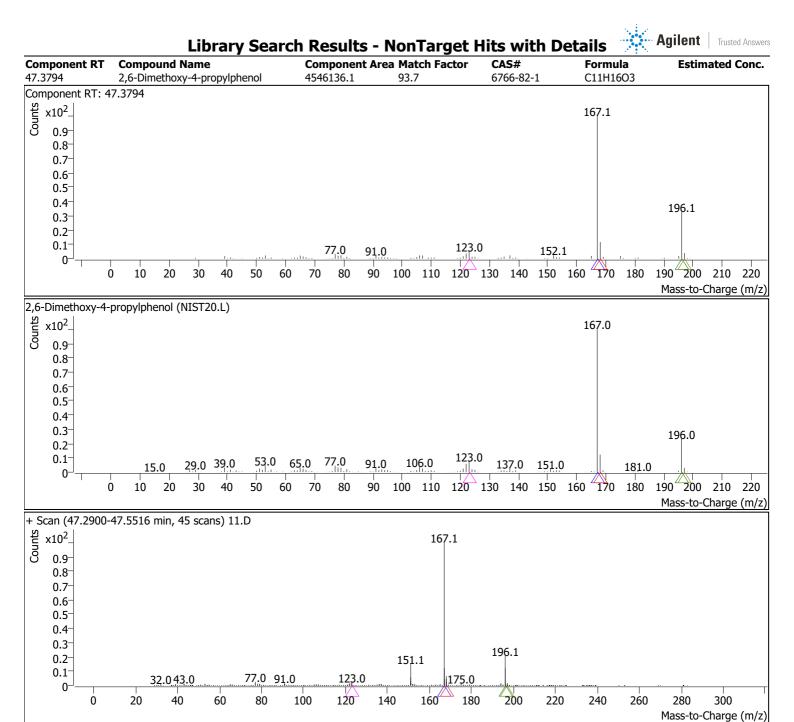


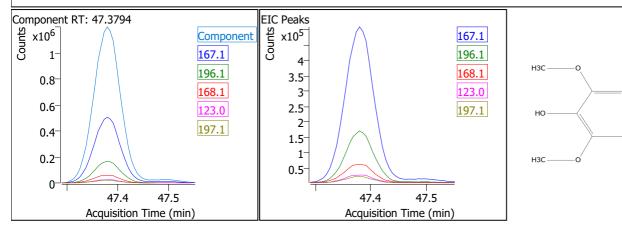






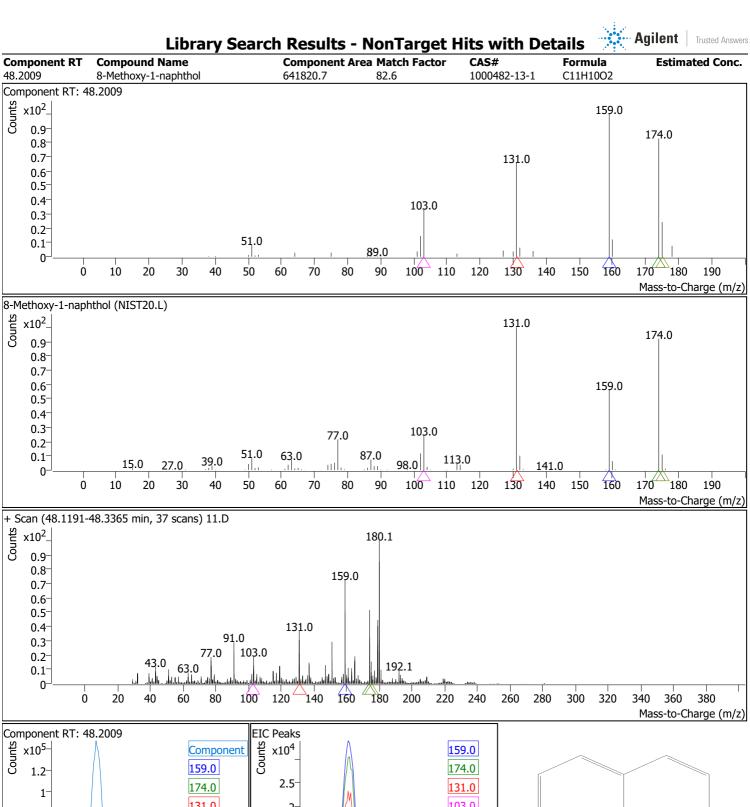


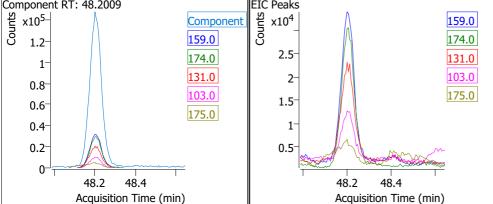


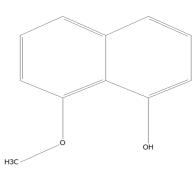


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-CH3







--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2305-13-7 49.0032 Benzenepropanol, 4-hydroxy-3-3980098.9 87.4 C10H14O3 methoxy-Component RT: 49.0032 x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 182.0 0.4 0.3 0.2^{-} 158.0 122.0 77.0 91.0 107.0 0.1 0-140 10 20 30 40 50 60 70 80 90 100 110 120 130 150 160 170 180 190 200 Mass-to-Charge (m/z) Benzenepropanol, 4-hydroxy-3-methoxy- (NIST20.L) $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 0.5 182.0 0.4 0.3 122.0 0.2 77.0 91.0 65.0 106.0 0.1 31.0 39.0 53.0 149.0 164.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (48.9090-49.1333 min, 38 scans) 11.D x10². 137.0 0.9 0.8 0.7^{-} 0.6 0.5 182.1 0.4 0.3 0.2 158.1 65.0 77.0 91.0 _{107.0} 122.0 0.1 32.043.0 0 40 120 140 180 0 20 60 80 100 160 200 220 240 260 280 300 320 Mass-to-Charge (m/z) Component RT: 49.0032 **EIC Peaks** Counts Counts x10⁵ x10⁵ 137.0 Component 182.0 137.0 1.8 6 182.0 138.0 1.6 5 1.4 138.0 158.0 1.2

49

49.1

Acquisition Time (min)

122.0

4

3

2

1

48.9

49

49.1

Acquisition Time (min)

158.0

122.0

1

0.8⁻

0.4

0.2

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49.4

49.5

Acquisition Time (min)

2-

1

1.5

0.5

183.0

49.5

0.6

0.4

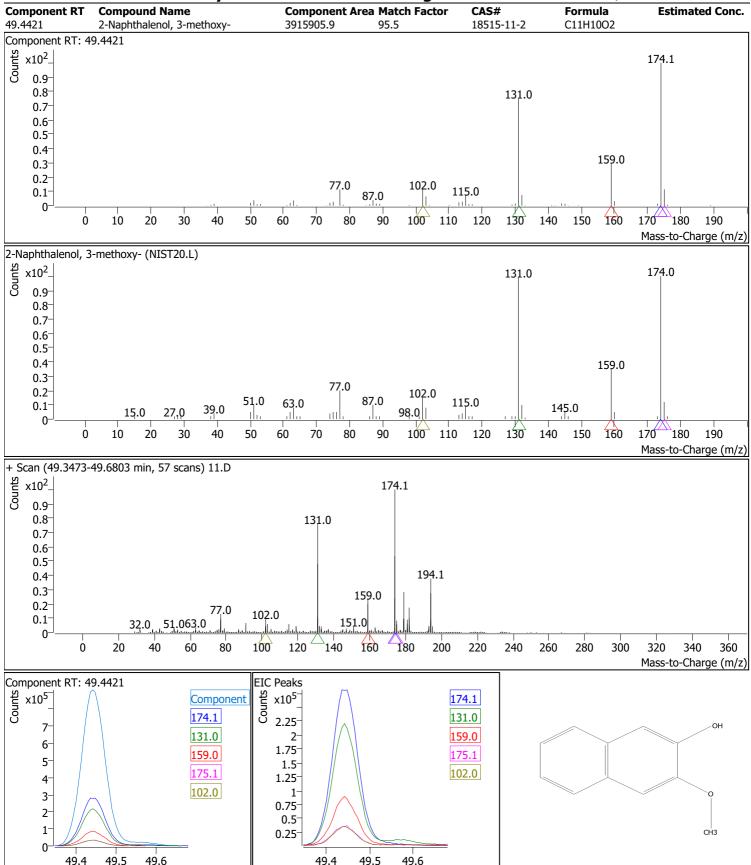
0.2

49.4

Acquisition Time (min)

ОΉ





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49.55

49.6

Acquisition Time (min)

0.4

 0.2^{-1}

49.5

1.5

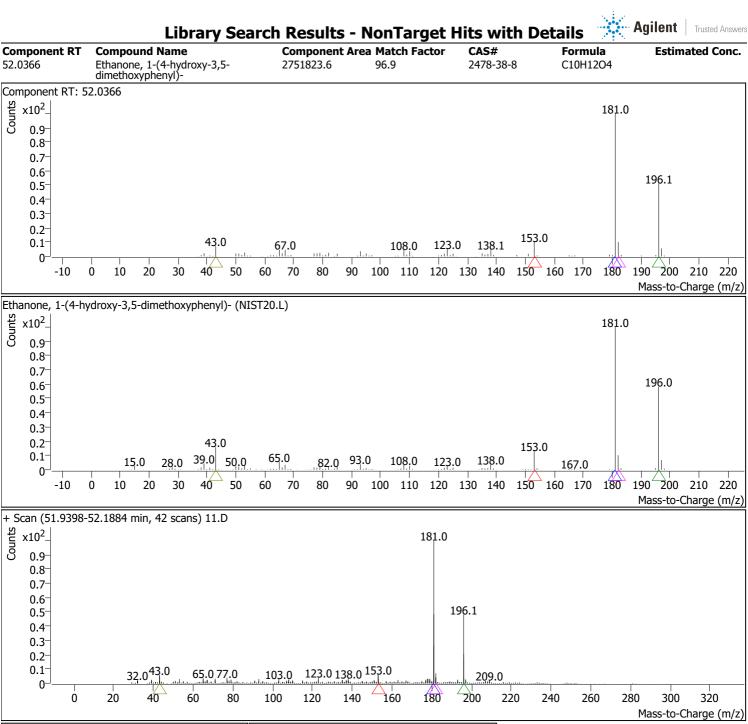
0.5

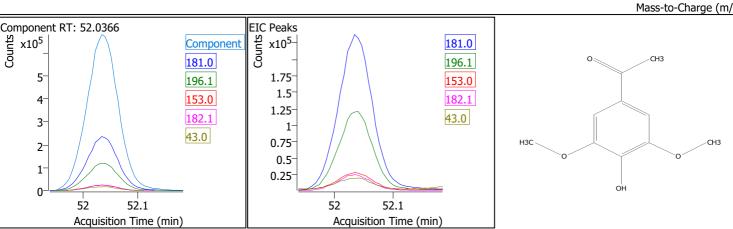
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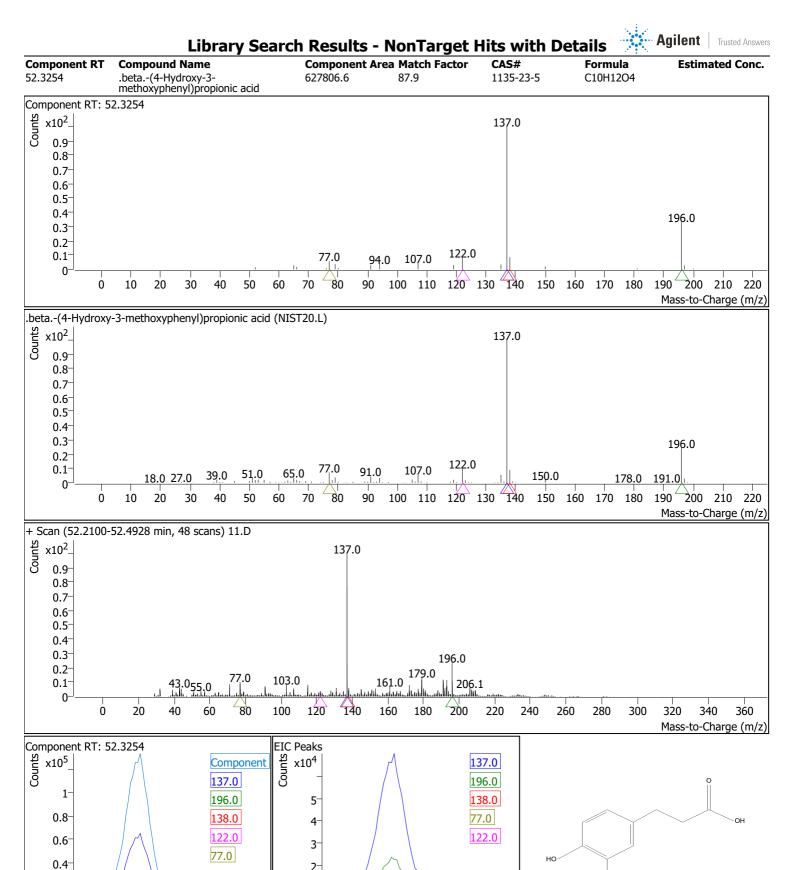
49.6

Acquisition Time (min)

НЗС







52.3

52.4

Acquisition Time (min)

2-

1

0.2

52.2

52.3

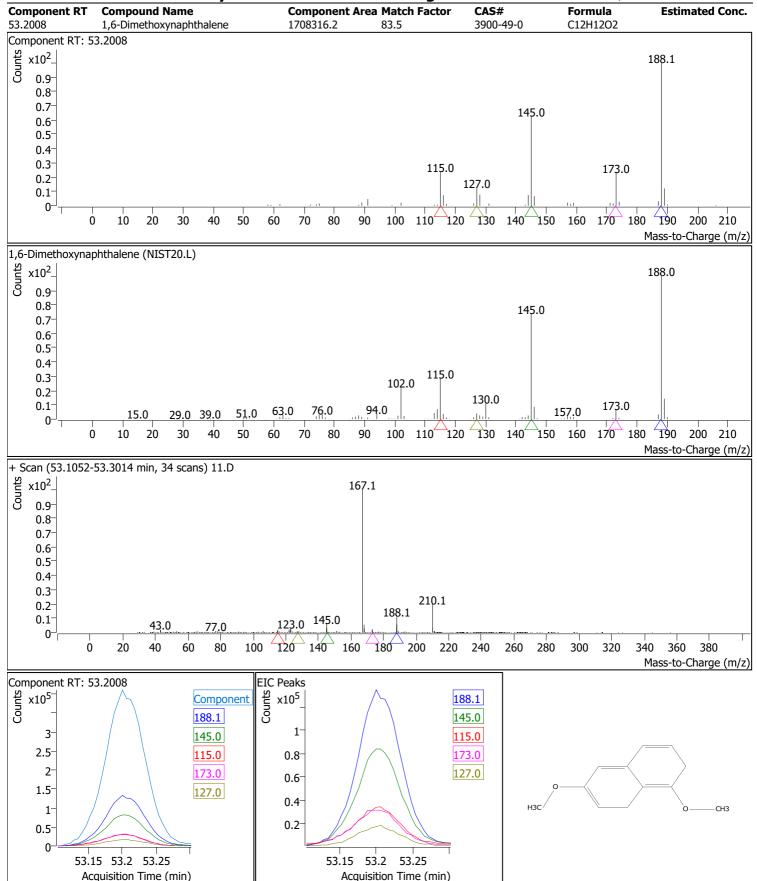
52.4

Acquisition Time (min)

СНЗ

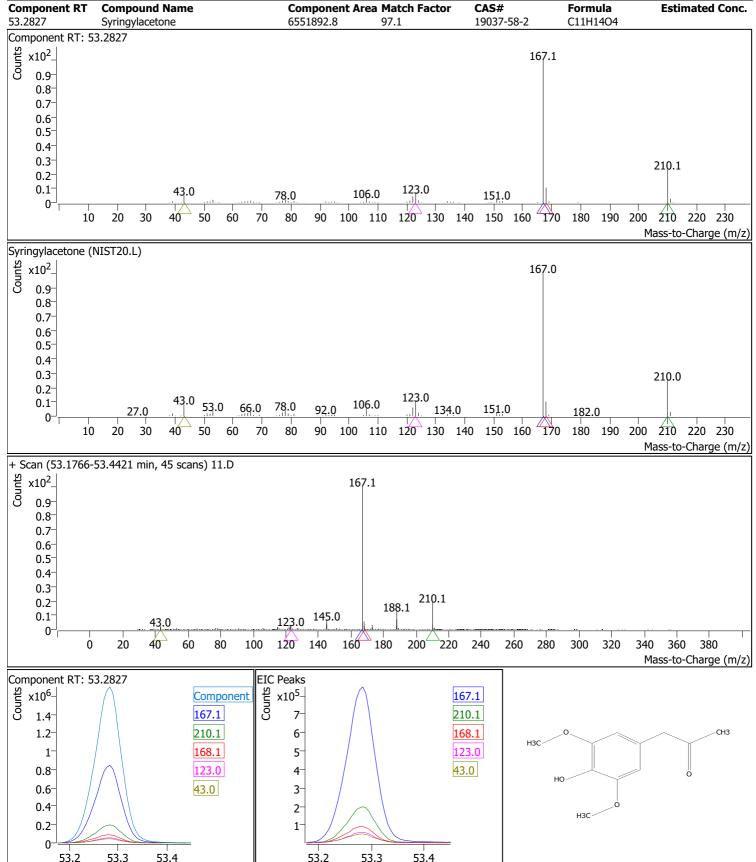


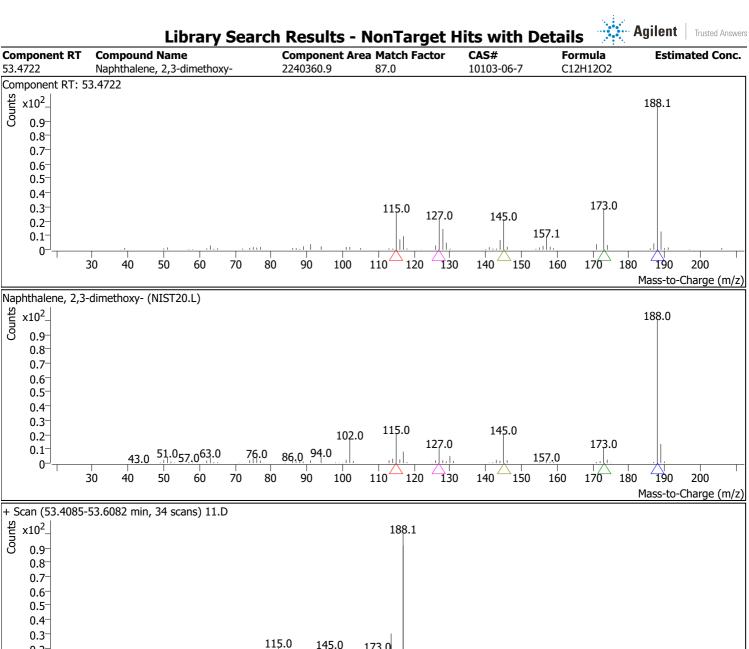








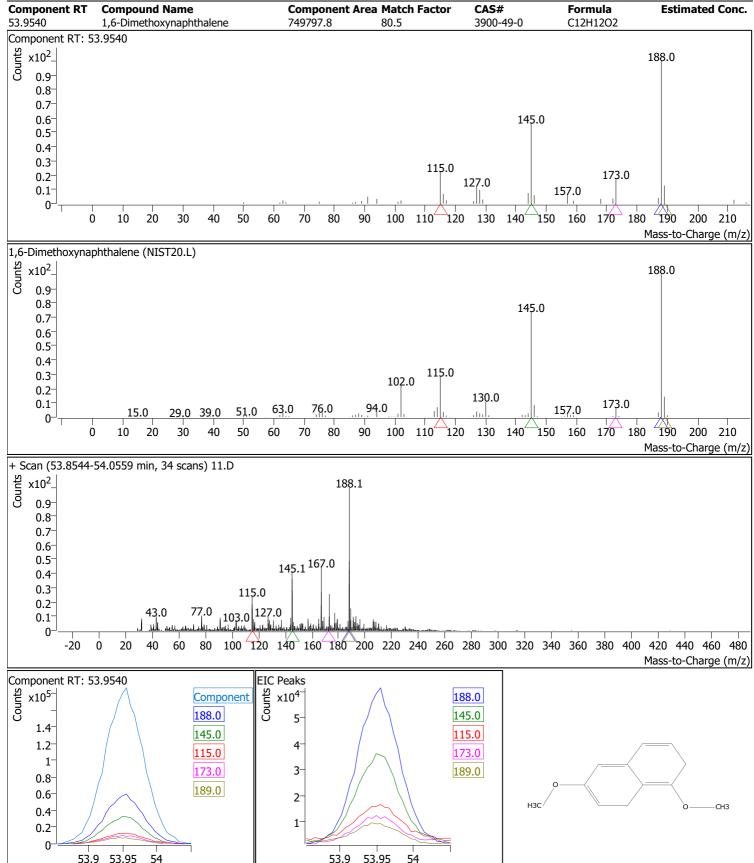




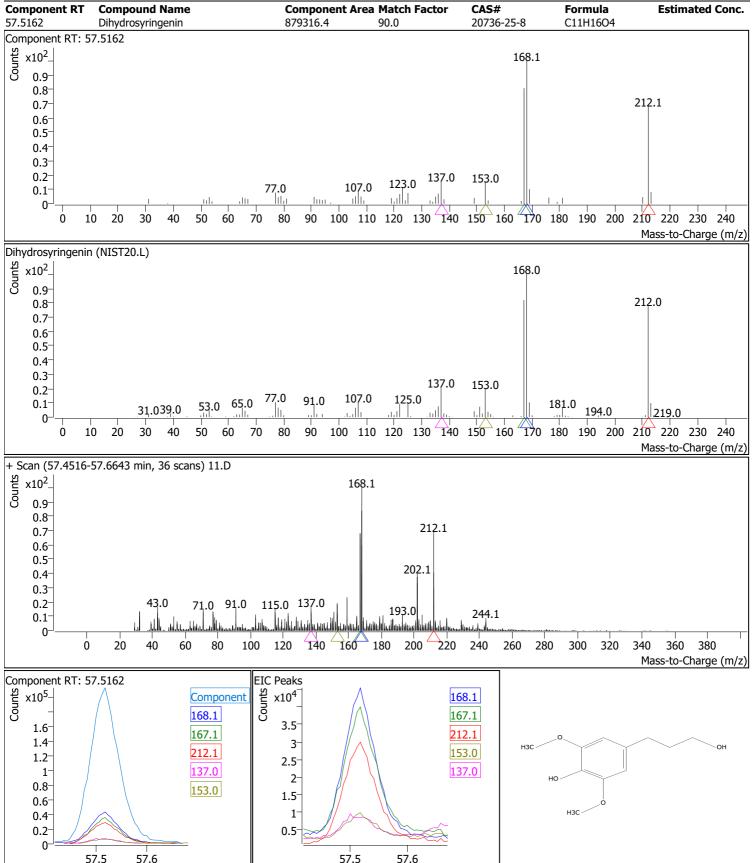
380

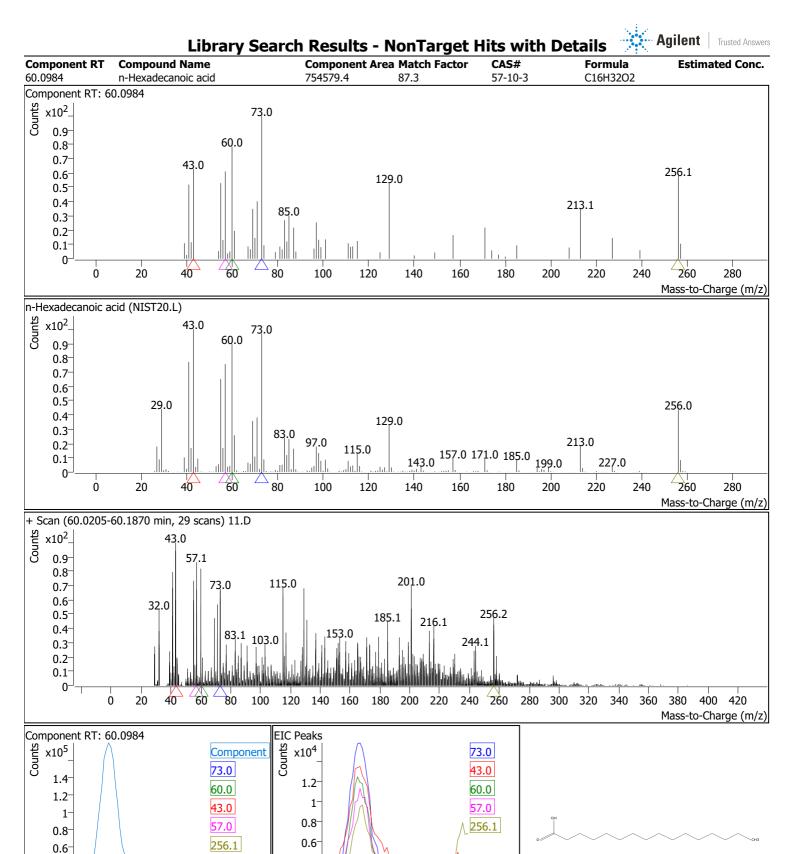












0.4

0.2

60.1

60.2

Acquisition Time (min)

60.3

0.4

60.1

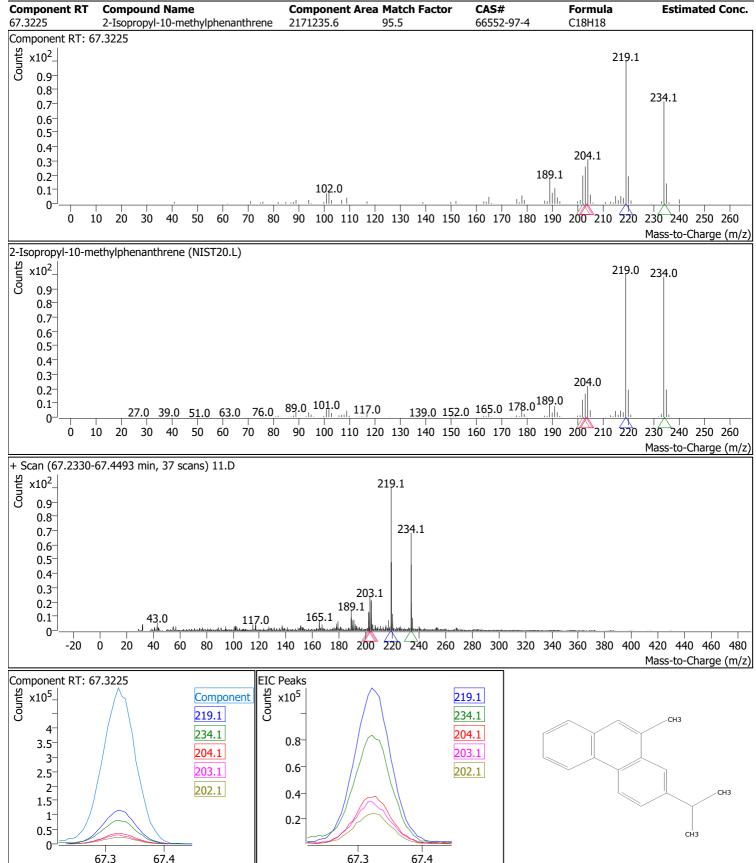
60.2

Acquisition Time (min)

60.3

Library Search Results - NonTarget Hits with Details

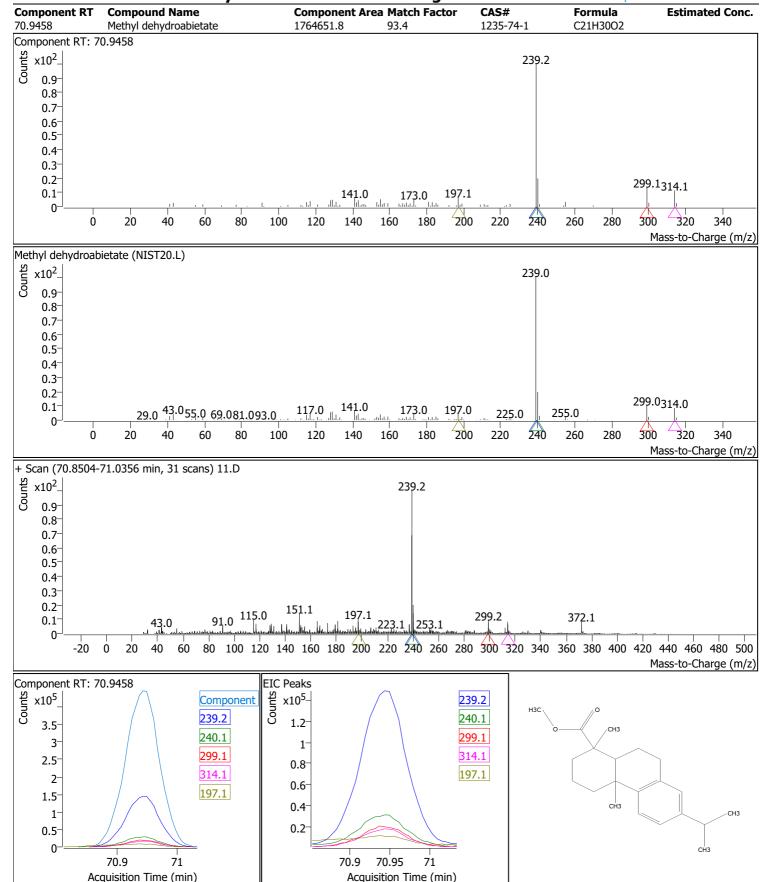




Acquisition Time (min)







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.)]-73.6655 8672669.1 93.4 5155-70-4 C20H28O2 Component RT: 73.6655 $x10^{2}$ 285.2 239.2 0.9 0.8 0.7 0.6 0.5 197.1 0.4^{-} 300.1 0.3 141.0 0.2 0.1 300 200 240 280 320 0 20 40 60 80 100 120 140 160 180 220 260 Mass-to-Charge (m/z) 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L) Counts x10²_ 285.0 0.9 0.8 239.0 0.7° 0.6 0.5 0.4 300.0 0.3 197.0 43.0 0.2 141.0 117.0 55.0 _{69.0} 91.0 183.0 0.1 225.0 255.0 240 280 300 0 20 40 60 80 100 120 140 160 180 200 220 260 320 Mass-to-Charge (m/z) + Scan (73.5358-73.8450 min, 53 scans) 11.D 돌 x10². 285.2 239.2 0.9 0.8 0.7 0.6 0.5 0.4 300.2 197.1 0.3 0.2 129.1 155.1 43.0 0.1 91.0 253.1 250 275 300 325 350 375 400 425 450 475 500 525 550 200 225 25 50 75 100 125 175 -25 0 150 Mass-to-Charge (m/z) Component RT: 73.6655 EIC Peaks x10⁶ x10⁵ 285.2 Component 285.2 239.2 1.8 СНЗ 1.2 1.6 239.2 197.1 1.4 1 197.1 300.1 1.2

73.7

73.8

Acquisition Time (min)

141.0

0.8

0.6

0.4

 0.2^{-}

73.7

73.6

73.8

Acquisition Time (min)

300.1

141.0

1

0.8⁻ 0.6⁻

0.4

73.6

СНЗ

