Library Search Results - NonTarget Hits with Details



D:\MassHunter\GCMS\1\data\RBEL\240503 scan **Batch Path**

240503 report_2.uaf **Analysis File Name**

Analyst Name admin **Analysis Time** 5/7/2024 12:37:54 PM

D:\MassHunter\GCMS\1\data\RBEL\240503 scan **File Name** 16_2.D **Path Name** 16_2 240503 scan **Sample Name Sample Type** Sample Acq. Method Path Acq. Operator Acq. Method File D:\MassHunter\GCMS\1\methods\RBEL\ Acq. Date-Time

5/3/2024 4:25:30 PM **Instrument Name** GCMSD Dil. 1

Section Case	Instrument Na	inc GCFI3D	Diii.	-			
3,9812	Component RT	Compound Name	CAS#	Formula		Match Factor	
3,9812	3.3163	Propanoic acid	79-09-4	C3H6O2		98.3	
Submorle acid 107-92-6 C4H802 1832380.1 89.3 11.3217 1.3-Proparediol, 3-methoxy- 623-39-2 C4H1003 12570584 87.3 11.3217 1.3-Proparediol, 3-methoxy- 1207-56 C5H805 711137.2 92.4 12.3814 Butyrolatene 110-19-1 C4H805 711137.2 92.4 12.3814 Butyrolatene 110-19-1 C4H805 711137.2 92.4 12.3814 Butyrolatene 110-19-1 C4H805 77128739.2 93.8 12.3814 12.3814 Butyrolatene 110-19-1 C4H805 77128739.2 93.8 12.3814		•	57-55-6	C3H8O2	784529.3	91.1	
11.3217 1.2-Propanediol, 3-methosy-	5.8016	Butanoic acid	107-92-6	C4H8O2	1832380.1	89.3	
11.7887 2-Cyclopenten-1-one, 2-methyl- 1120-73-6 C6H8C0 711137 29.4		1,3-Propanediol	504-63-2	C3H8O2			
11.7887 2-Cyclopenten-1-one, 2-methyl- 1120-73-6 C6H8C0 711137 29.4	11.3217	1,2-Propanediol, 3-methoxy-	623-39-2	C4H10O3	1257058.4	87.3	
12.3814 Butyroisctone 96-48-0 C41602 7729739.2 93.8 15.2236 2(3H)-Furanone, dihydro-5-methyl- 109-29-2 C51802 C5125.2.1 95.0 15.2236 2(2H)-Furanone, dihydro-5-methyl- 108-29-2 C51802 C5125.1 95.0 15.2236 2(2H)-Furanone, dihydro-5-methyl- 178-818-1 C6180 C6125.1 95.0 17.9321 Phenol 18.839 Phenol 2-dhyl- 18.839	11.7387		1120-73-6	C6H8O	711137.2	92.4	
15.2236	12.3814		96-48-0	C4H6O2	7728739.2		
16.0102 2-Cyclopenters-In-one, 3-methyl- 2788-18-1 C6H8O 2805949.0 97.7	13.6103	2,5-Hexanedione	110-13-4	C6H10O2	2154342.0	95.6	
17.9521	15.2236	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	C5H8O2	621252.1	95.0	
18.1809 2-Cyclopenters—In-one, 2,3-dimethyl- 1121-05-7 C7H100 408237.0 89.5	16.0102	2-Cyclopenten-1-one, 3-methyl-	2758-18-1	C6H8O	2805949.0	97.7	
18.699		Phenol	108-95-2			92.8	
18.699	18.1809	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	408237.0	89.5	
19.7605 2-Cyclopenten-1-one, 3,4-dimethyl- 3043-64-1 C7H100 827759.2 91.0 19.8195 1,3-Dioxolane-4-methanol, 2-ethyl- 53951-44-3 C6H1203 2330259.4 93.8 20.1325 3,6-Heptanedione 1703-51-1 C7H1202 1092763.8 90.9 20.6287 2-Cyclopenten-1-one, 2,3-dimethyl- 55683-21-1 C8H120 1445938.0 93.3 22.9075 2-Cyclopenten-1-one, 3,4-5-trimethyl- 55683-21-1 C8H120 1445938.0 93.3 22.5015 Pentanoic acid, 4-toxor, ethyl ester 539-88-8 C7H1203 991155.7 93.7 23.6209 Pentanoic acid, 4-toxor, ethyl ester 539-88-8 C7H1203 991155.7 93.7 23.6209 Phenol, 2-methoxy- 20.05-1 C7H802 29117845.3 97.7 23.6209 Phenol, 2-methoxy- 20.05-1 C7H802 29137845.3 97.7 23.8309 Ethanone, 1-(2-thientyl-) 88-15-3 C6H60S 1143988.5 89.9 24.3368 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 139537.5 96.6 24.9402 Phenol, 2,6-dimethyl- 576-26-1 C8H100 1395537.5 96.9 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8 25.8444 Phenol, 2-tylinentyl- 90-00-6 C8H100 1595524.1 93.0 27.3792 Phenol, 2,4-dimethyl- 105-67-9 C8H100 4052045.8 98.5 28.8430 Phenol, 2,2-dimethyl- 105-67-9 C8H100 4052045.8 98.5 28.8430 Phenol, 2,2-dimethyl- 105-67-9 C8H100 4184009.0 94.5 28.8431 Phenol, 2,3-dimethyl- 195-87-4 C8H100 119597.9 97.9 28.8460 Z-Methoxy-5-methylphenol 1195-90-1 C8H100 4184009.0 94.5 28.8370 Phenol, 2,3-dimethyl- 95-87-6 C8H100 119388.9 99.3 29.2072 Crosol 2-dimethyl- 95-87-6 C8H100 119388.9 99.3 29.2073 Z-Methoxy-5-methylphenol 1195-90-1 C8H100 4184009.0 94.5 29.2072 Phenol, 3,4-dimethyl- 95-88-8 C8H100 119388.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-90-1 C8H100 4184009.0 94.5 29.2073 2-Methoxy-5-methylphenol 195-90-1 C8H100 119388.9 99.3 29.2073 2-Methoxy-5-methylphenol 195-90-1 C8H100	18.6599		544-01-4	C10H22O	3196448.9	86.7	
19.8195	18.8487	Pentanoic acid	109-52-4	C5H10O2	1166461.0	85.7	
20.1325 3,6-Heptanecione 1703-51-1 C7H1202 1092763.8 90.9 20.08267 C2-Volopenten-1-one, 2,3-dimethyl- 1521-05-7 C7H100 4944028.4 95.7 22.0975 2-Cyclopenten-1-one, 3,45-trimethyl- 55683-21-1 C8H120 145938.0 93.3 22.29.15 Pentanoic acid, 4-cxor, ethyl ester 539-88-8 C7H1203 991155.7 93.7 23.0976 1-Octanol 111-87-5 C8H180 4768450.2 94.1 23.6209 Phenol, 2-methoxy- 90-05-1 C7H802 29117845.3 97.7 23.6209 Phenol, 2-methoxy- 90-05-1 C7H802 29117845.3 97.7 23.8339 Ethanone, 1-(2-thienyl)- 88-15-3 C6H605 1143988.5 89.9 24.3368 2-Ethyl-3-methylcyclopent-2-en-1-one 100423-46-8 C8H120 1395373.8 86.6 24.9402 Phenol, 2,5-dimethyl- 576-26-1 C8H1100 1395537.5 96.9 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 100423-46-8 C8H120 1692432.9 89.8 27.3792 Phenol, 2,4-dimethyl- 90-00-6 C8H100 1585624.1 93.0 27.3792 Phenol, 2,4-dimethyl- 105-67-9 C8H1100 4184009.0 94.5 28.8610 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 4184009.0 94.5 28.8701 Phenol, 2,3-dimethyl- 526-75-0 C8H1100 4184009.0 94.5 28.8730 Phenol, 2,3-dimethyl- 526-75-0 C8H1100 119398.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 1113938.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 1113938.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 1113938.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 2430431.3 98.0 20.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1100 2430431.3 99.3 20.2074 2-Methoxy-5-meth	19.7605	2-Cyclopenten-1-one, 3,4-dimethyl-	30434-64-1	C7H10O	827759.2	91.0	
20.6887 2-Cyctopenten-1-one, 2,3-d-imethy 112-105-7 CPH100 4844028.4 95.7	19.8195	1,3-Dioxolane-4-methanol, 2-ethyl-	53951-44-3	C6H12O3	2530259.4	93.8	
22,0975 2-Cyclopenten-1-one, 34,5-trimethy 55683-21-1	20.1325	3,6-Heptanedione	1703-51-1	C7H12O2	1092763.8	90.9	
22.4211	20.6287	2-Cyclopenten-1-one, 2,3-dimethyl-	1121-05-7	C7H10O	4844028.4	95.7	
22.5015	22.0975	2-Cyclopenten-1-one, 3,4,5-trimethyl-	55683-21-1	C8H12O	1445938.0	93.3	
11.87-5	22.2421	Phenol, 2-methyl-	95-48-7	C7H8O	6805836.6	97.6	
23.6209	22.5015	Pentanoic acid, 4-oxo-, ethyl ester	539-88-8	C7H12O3	991155.7	93.7	
23.7337 2-Cyclopenten-1-one, 2,3,4-trimethyl- 28790-86-5 C8H120 2551710.6 89.8 23.8309 Ethanone, 1,C-thienyl)- 88-15-3 C6H6C5 1143988.5 89.9 24.3368 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1034733.8 86.6 24.9402 Phenol, 2,6-dimethyl- 95-67-4 C8H100 1397981.9 96.9 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H100 1397981.9 96.9 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H100 1585624.1 93.0 27.3792 Phenol, 2,4-dimethyl- 105-67-9 C8H100 4052045.8 98.5 27.3792 Phenol, 2,4-dimethyl- 95-87-4 C8H100 1585624.1 93.0 27.3792 Phenol, 2,5-dimethyl- 95-87-4 C8H100 4052045.8 98.5 27.5117 Phenol, 2,5-dimethyl- 95-87-4 C8H100 497612.3 87.5 28.8370 Phenol, 2,3-dimethyl- 29.2072 Cressol 93-51-6 C8H100 942992.8 92.8 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H100 942992.8 99.2 29.30337 Phenol, 2,3-dimethyl- 95-65-8 C8H100	23.0976	1-Octanol	111-87-5	C8H18O	4768450.2	94.1	
23.8399 Ethanone, 1-(2-thienyl)- 24.3368 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 (BH120 1395337.5 96.6 24.9402 Phenol, 2,6-dimethyl- 576-26-1 C8H100 1395337.5 96.6 24.9402 Phenol, 2,6-dimethyl- 95-87-4 C8H100 1395337.5 96.6 25.9577 2-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8 26.8444 Phenol, 2-ethyl- 105-67-9 C8H100 1585624.1 93.0 1585624.1 93.0 1585624.1 93.0 1585624.1 93.0 1585624.1 93.0 1585624.1 93.0 1585624.1 93.0 1585627.3 159.0 159.0 159.0 159.0 1585624.1 93.0 1585624.1 93.0 159.0 159.0 159.0 159.0 159.0 159.0 159.0 159.0 1585624.1 93.0 159.0 1	23.6209	Phenol, 2-methoxy-	90-05-1	C7H8O2		97.7	
24.3486 2-Ethyl-3-methylcydopent-2-en-1-one 1000423-46-8 C8H120 1034733.8 86.6 24.9402 Phenol, 2,5-6-dimethyl- 576-6-1 C8H100 1397881.9 96.9 24.9405 Phenol, 2,5-6-dimethyl- 95-87-4 C8H100 1397881.9 96.9 25.9577 2-Ethyl-3-methylcydopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8 26.8444 Phenol, 2-ethyl- 90-00-6 C8H100 1585524.1 93.0 27.3792 Phenol, 2,4-6-dimethyl- 105-67-9 C8H100 4052045.8 98.5 27.3792 Phenol, 2,4-6-dimethyl- 95-87-4 C8H100 1585524.1 93.0 27.3792 Phenol, 2,4-6-dimethyl- 95-87-4 C8H100 4186090.0 94.5 28.7618 Naphthalene 91-20-3 C10H8 997612.3 87.5 28.8370 Phenol, 2,3-dimethyl- 526-75-0 C8H100 949292.8 92.8 29.2072 Crossol 93-51-6 C8H100 949292.8 92.8 29.2072 Crossol 93-51-6 C8H100 949292.8 92.8 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 11143988.9 99.3 29.2073 2-Methoxy-5-methylphenol 129-09-1 C8H1002 11143988.9 99.2 29.4375 Octanoic acid 12-407-2 C8H1602 2561653.7 86.2 29.7292 Phenol, 3,3-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.9357 Phenol, 2,3-5-trimethyl- 95-65-8 C8H100 1000220.5 92.0 30.935 Catechol 12-80-9 C8H602 34530431.3 98.0 31.0736 Phenol, 2-propyl- 644-35-9 C8H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2068639.0 95.7 33.0371 3,5-bimethoxytolucne 4179-19-5 C9H1202 7792070.2 88.8 3.35.0 Phenol, 4-ethyl-2-methoxy- 2785-89-9 C9H1202 7577604.5 97.5 57.5 57.5 57.5 C9H100 15000000000000000000000000000000000	23.7337	2-Cyclopenten-1-one, 2,3,4-trimethyl-	28790-86-5	C8H12O	2351710.6	89.8	
24.9402 Phenol, 2,6-dimethyl- Phenol, 2,5-dimethyl- Phenol, 2,5-dimethyl- Phenol, 2,5-dimethyl- Phenol, 2,5-dimethyl- Phenol, 2-ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8 26.8444 Phenol, 2-ethyl- Phenol, 2,4-dimethyl- Phenol, 2,4-dimethyl- Phenol, 2,5-dimethyl- Phenol, 2,5-trimethyl- Phenol, 2,5-trimethyl- Phenol, 2,5-trimethyl- Phenol, 2,5-trimethyl- Phenol, 2,7-brimethyl- Phenol, 2,7-brimethoxy- Phenol, 2,7-brimethoxy- Phenol, 2,7-brimethyl- Phenol, 2,7-bri	23.8309	Ethanone, 1-(2-thienyl)-	88-15-3	C6H6OS	1143988.5	89.9	
24.9405 Phenol, 2,5-dimethyl- 95-87-4 C8H100 1397981.9 96.9	24.3368	2-Ethyl-3-methylcyclopent-2-en-1-one	1000423-46-8	C8H12O	1034733.8	86.6	
25.9577 Z-Ethyl-3-methylcyclopent-2-en-1-one 1000423-46-8 C8H120 1692432.9 89.8	24.9402	Phenol, 2,6-dimethyl-	576-26-1	C8H10O	1395537.5	96.6	
26.8444 Phenol, Z-4thyl- 90-00-6 C8H100 1585624.1 93.0 27.3792 Phenol, Z,4-dimethyl- 105-67-9 C8H100 4052045.8 98.5 27.5117 Phenol, Z,5-dimethyl- 95-87-4 C8H100 1816927.9 97.9 28.4840 2-Methoxy-5-methylphenol 1195-09-1 C8H100 4184009.0 94.5 28.8370 Phenol, Z,3-dimethyl- 526-75-0 C8H100 942992.8 92.8 29.2072 Cressol 93-51-6 C8H1002 11193880.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 11143948.9 99.2 29.4375 Octanoic acid 124-07-2 C8H1602 2561653.7 86.2 29-7292 Phenol, 3,4-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.3845 Catechol 120-80-9 C6H602 34530431.3 98.0 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 506825.0 86.6 31.38145 Benzene, 1-ethyl-4-m	24.9405	Phenol, 2,5-dimethyl-	95-87-4	C8H10O	1397981.9	96.9	
27.3792 Phenol, 2,4-dimethyl- 105-67-9 C8H100 4052045.8 98.5 27.5117 Phenol, 2,5-dimethyl- 95-87-4 C8H100 1816927.9 97.9 28.4840 2-Nethoxy-5-methylphenol 1195-09-1 C8H100 4184009.0 94.5 28.8370 Phenol, 2,3-dimethyl- 526-75-0 C10H8 497612.3 87.5 28.8370 Phenol, 3,3-dimethyl- 526-75-0 C8H100 942992.8 92.8 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 11143948.9 99.2 29.4375 Octanoic acid 124-07-2 C8H1602 2561653.7 86.2 29.7292 Phenol, 3,4-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.0837 Phenol, 2-propyl- 644-35-9 C9H120 967091.5 89.7 31.0736 Phenol, 2-propyl- 644-35-9 C9H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2066639.0 95.7 32.5930 1	25.9577	2-Ethyl-3-methylcyclopent-2-en-1-one	1000423-46-8	C8H12O	1692432.9	89.8	
27.5117	26.8444	Phenol, 2-ethyl-	90-00-6	C8H10O	1585624.1	93.0	
28.48440 2-Methoxy-5-methylphenol 1195-09-1 C10H8 497612.3 87.5 28.7618 Naphthalene 91-20-3 C10H8 497612.3 87.5 28.8370 Phenol, 2,3-dimethyl- 526-75-0 C8H100 942992.8 92.8 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 11193890.9 99.3 29.4375 Octanoic acid 124-07-2 C8H1602 2561653.7 66.2 29.7292 Phenol, 3,4-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.0837 Phenol, 2,3-5-trimethyl- 697-82-5 C9H120 967091.5 89.7 30.3945 Catechol 120-80-9 C6H602 34530431.3 98.0 31.0736 Phenol, 2-propyl- 644-35-9 C9H120 506825.0 66.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 1734327.2 91.8 31.8145 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2068639.0 95.7 33.0527 1,2-Benzenediol, 3-methyl- 488-17-5 C7H802 29042.5 86.6 <	27.3792		105-67-9	C8H10O	4052045.8	98.5	
28.7618 Naphthalene 91-20-3 C10H8 497612.3 87.5 28.8370 Phenol, 2,3-dimethyl- 526-75-0 C8H100 94292.8 92.8 29.2072 Creosol 93-51-6 C8H1002 11193880.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 2561653.7 86.2 29.7292 Phenol, 3,4-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.0837 Phenol, 2,5,5-trimethyl- 697-82-5 C9H120 967091.5 89.7 30.3945 Catechol 120-80-9 C6H602 34530431.3 98.0 31.0736 Phenol, 2-propyl- 644-35-9 C9H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2068639.0 95.7 32.5930 1,2-Benzenediol, 3-methoxy- 934-00-9 C7H803 23431289.9 95.7 33.3627 1,2-Benzenediol, 3-methyl- 488-17-5 C7H802 2757604.5 97.5 33.3628 Phenol, 4-ethyl-	27.5117	Phenol, 2,5-dimethyl-	95-87-4	C8H10O	1816927.9	97.9	
28.8370 Phenol, 2,3-dimethyl- 526-75-0 C8H100 94292.8 92.8 29.2072 Creosol 93-51-6 C8H1002 11198380.9 99.3 29.2073 2-Methoxy-5-methylphenol 1195-09-1 C8H1002 11143948.9 99.2 29.4375 Octanoic acid 124-07-2 C8H1602 2561653.7 86.2 29.7292 Phenol, 3,4-dimethyl- 697-82-5 C8H100 1000220.5 92.0 30.0837 Phenol, 2,3,5-trimethyl- 697-82-5 C9H120 967091.5 89.7 30.3945 Catechol 120-80-9 C6H602 34530431.3 98.0 31.0736 Phenol, 2-propyl- 644-35-9 C9H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 1734327.2 91.8 31.8145 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2068639.0 95.7 32.5930 1,2-Benzenedol, 3-methoxy- 934-00-9 C7H803 23431289.9 95.7 33.0371 3,5-Dim	28.4840	2-Methoxy-5-methylphenol	1195-09-1	C8H10O2	4184009.0	94.5	
29.2072 Creoso 93-51-6 C8H1002 11198380.9 99.3 29.2073 2. Methoxy-5-methylphenol 1195-09-1 C8H1002 11143948.9 99.2 29.7375 Octanoic acid 124-07-2 C8H1602 2561653.7 86.2 29.7292 Phenol, 3,4-dimethyl- 95-65-8 C8H100 1000220.5 92.0 30.0837 Phenol, 2-propyl- 644-35-9 C6H602 34530431.3 98.0 31.0736 Phenol, 2-propyl- 644-35-9 C9H120 506825.0 86.6 31.3726 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 1734327.2 91.8 31.8145 Benzene, 1-ethyl-4-methoxy- 1515-95-3 C9H120 2068639.0 95.7 32.5930 1,2-Benzenediol, 3-methoxy- 934-00-9 C7H803 23431289.9 95.7 33.0371 3,5-Dimethoxytoluene 4179-19-5 C9H120 802942.5 86.6 33.2627 1,2-Benzenediol, 3-methyl- 488-17-5 C7H802 27577604.5 97.5 33.3820							
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40.8429 1,4-Benzenediol, 2,3,5-trimethyl- 700-13-0 C9H12O2 15103226.8 85.9 41.2785 3-Isopropyl-1,2-benzenediol 2138-48-9 C9H12O2 10708557.2 91.1	40.6665	•	2431-91-6	C9H12O2	7991285.2	87.6	
41.2785 3-Isopropyl-1,2-benzenediol 2138-48-9 C9H12O2 10708557.2 91.1	40.8429			C9H12O2	15103226.8		
	41.2785	3-Isopropyl-1,2-benzenediol	2138-48-9	C9H12O2			

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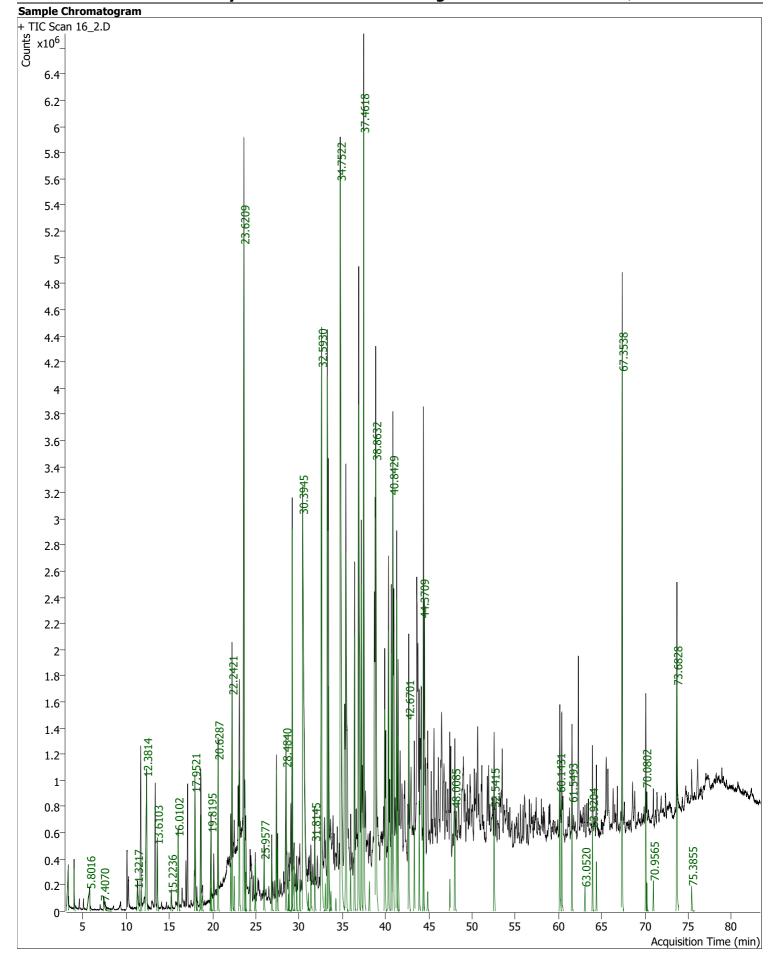
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Library Search Results - NonTarget Hits with Details

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Trusted Answers

Component	RT Compound Name	CAS#	Formula	Component Area	Match Factor	Estimated Conc.
41.4376	5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-, hydrate	62732-46-1	C10H14N2	5961511.5	86.5	
42.6701	1,3-Benzenediol, 4-propyl-	18979-60-7	C9H12O2	6500553.0	87.2	
43.3174	3-Isopropyl-1,2-benzenediol	2138-48-9	C9H12O2	2659046.6	85.8	
43.8823	3-Isopropyl-1,2-benzenediol	2138-48-9	C9H12O2	3406173.7	87.9	
44.3709	Dodecanoic acid, methyl ester	111-82-0	C13H26O2	7669325.3	93.5	
44.3939	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	2503-46-0	C10H12O3	4704510.9	87.0	
44.8750	Benzeneethanethioic acid, S-methyl ester	5925-74-6	C9H10OS	678705.3	86.6	
47.4329	Pyrolo[3,2-d]pyrimidin-2,4(1H,3H)-dione	65996-50-1	C6H5N3O2	945353.0	88.8	
48.0085	1-Methyl-2-naphthol	1076-26-2	C11H10O	3797502.6	96.7	
52.5415	1-Naphthol, 6,7-dimethyl-	31776-14-4	C12H12O	3585147.1	88.5	
60.1431	n-Hexadecanoic acid	57-10-3	C16H32O2	3965245.8	89.7	
60.3688	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	3482413.0	89.0	
61.5493	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	1000197-14-1	C19H28	3227440.2	91.4	
63.0520	Anthracene, 9-(1-methylethyl)-	1498-80-2	C17H16	759878.8	87.3	
63.9204	3,4'-Diisopropylbiphenyl	61434-46-6	C18H22	2653635.6	85.7	
64.3744	Nonane, 3-methyl-5-propyl-	31081-18-2	C13H28	1408141.2	89.8	
67.3538	Retene	483-65-8	C18H18	17373414.7	96.6	
70.0802	8-Isopropyl-1,3-dimethylphenanthrene	135886-06-5	C19H20	4015475.8	92.1	
70.2004	Hexadecane	544-76-3	C16H34	833510.0	85.9	
70.2010	Nonadecane	629-92-5	C19H40	833627.5	85.7	
70.9565	Methyl dehydroabietate	1235-74-1	C21H30O2	941584.5	90.6	
73.6828	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	8770907.8	94.8	
75.3855	1-Tetradecanol	112-72-1	C14H30O	866216.8	86.6	



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 3.3163 Propanoic acid 1926119.2 98.3 Component RT: 3.3163 y x10² 0.9 74.0 0.8 0.7 45.0 29.0 0.6 0.5 0.4 57.0 0.3 55.0 0.2 42.1 0.1 15 20 25 35 45 55 70 10 30 40 50 65 80 Mass-to-Charge (m/z) Propanoic acid (NIST20.L) Square x10² 0.9 28.0 0.8 74.0 0.7 0.6 45.0 0.5 0.4 0.3 57.0 0.2 55.0 0.1 15.0 42.0 53.0 15 10 20 25 30 35 40 45 50 55 60 65 70 80 Mass-to-Charge (m/z) + Scan (3.0968-3.3606 min, 45 scans) 16_2.D st x10² 0.9 45.0 74.0 0.8 0.7 29.1 0.6 0.5 0.4 57.0 0.3 0.2 0.1 40 20 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) EIC Peaks Component RT: 3.3163 Counts Counts x10⁵ x10⁴_ Component 74.0 74.0 29.0 6 2.5 ОН 73.0 45.0 5 2 45.0 73.0 57.0 29.0 1.5

3.2 3.25 3.3

Acquisition Time (min)

3

2-

3.15

57.0

1

3.2

3.3

Acquisition Time (min)

0.5

CH3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 3.9825 Propylene Glycol 784529.3 91.1 57-55-6 C3H8O2 Component RT: 3.9825 y x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 43.0 0.2 31.0 61.0 0.1 29.0 33.0 15 25 30 35 70 75 5 10 20 40 50 55 60 65 80 Mass-to-Charge (m/z) Propylene Glycol (NIST20.L) Square x10² 0.9 45.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 43.0 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 (3.9553-4.1336 min, 30 scans) 16_2.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 0.3 0.2 29.0 0.1 61.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 3.9825 EIC Peaks Counts Counts x10⁵ x10⁵ 45.0 Component 45.0 43.0 2.5 1.6 43.0 31.0 1.4 2 61.0 31.0 1.2

4.05

Acquisition Time (min)

4.1

42.1

61.0

42.1

1.5

1

4.05

Acquisition Time (min)

4.1

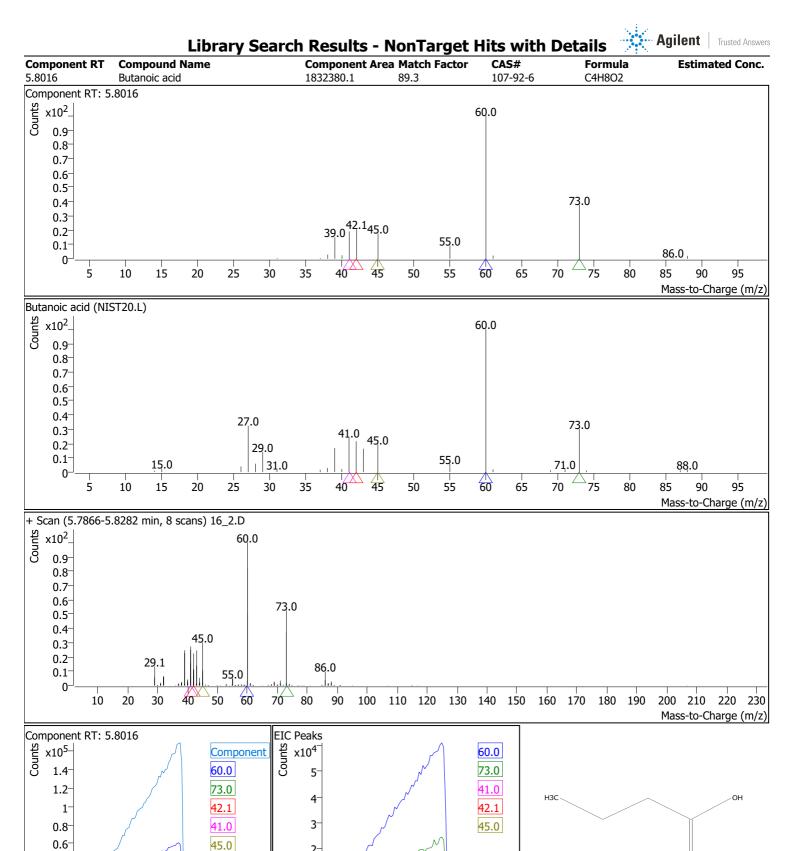
0.5

1

0.8

0.6⁻ 0.4⁻

0.2



2

1

5.5

5.6

5.7

Acquisition Time (min)

5.8

0.4

0.2

5.5

5.6 5.7 5.8

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0.75

0.5

0.25

7.6

7.4

7.8

8.2

8

Acquisition Time (min)

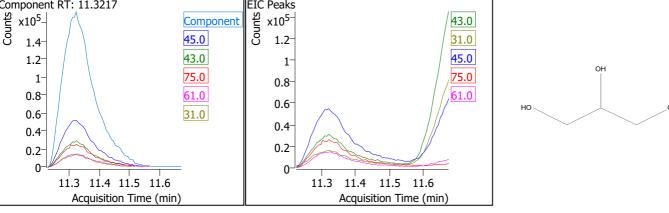
2

1

7.4 7.6 7.8

8

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CH3

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11.7

11.8

Acquisition Time (min)

68.0

0.8

0.6

0.4

0.2

0-

11.7

11.8

Acquisition Time (min)

39.0

68.0

2

1.5

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.** 96-48-0 12.3814 Butyrolactone 7728739.2 93.8 C4H6O2 Component RT: 12.3814 v10² 0.9 42.1 0.8 0.7^{-} 0.6 0.5 86.0 0.4 29.0 56.0 0.3 39.0 0.2 60.0 0.1 10 15 20 25 30 35 40 50 55 60 65 70 75 85 90 95 Mass-to-Charge (m/z) Butyrolactone (NIST20.L) st x10²_ 0.9-42.0 28.0 0.8 0.7 0.6 0.5 0.4 56.0 86.0 0.3 0.2 39.0 0.1 15.0_{18.0} 31.034 53.0 67.0 71.0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (12.1732-12.5532 min, 64 scans) 16_2.D St x10² 0.9 0.8 0.7 0.6 0.5 29.0 0.4^{-} 86.0 0.3 56.0 0.2 60.0 0.1 73.0 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) Component RT: 12.3814 **EIC Peaks** Counts Counts x10⁵-42.1 Component 42.1 41.0 0.8 2.25 41.0 86.0 0.7 2 29.0 86.0 1.75 0.6



12.3

12.4

Acquisition Time (min)

12.5

56.0

1.5

1.25

0.75

0.5

0.25

1

29.0

56.0

0.5

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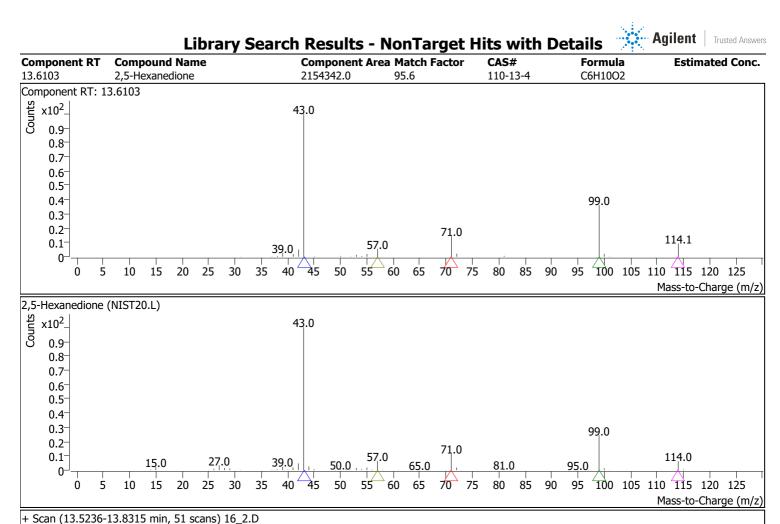
0.1

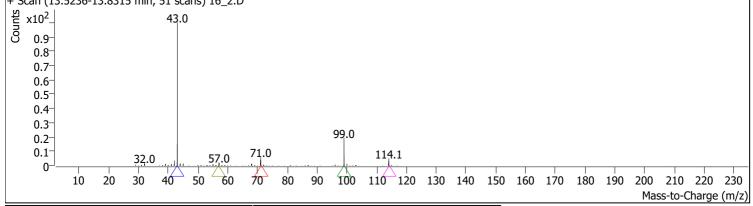
12.3

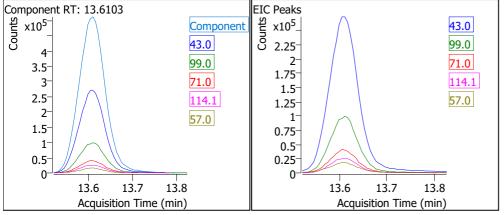
12.4

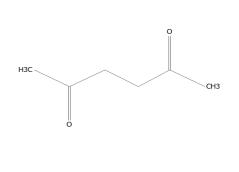
Acquisition Time (min)

12.5



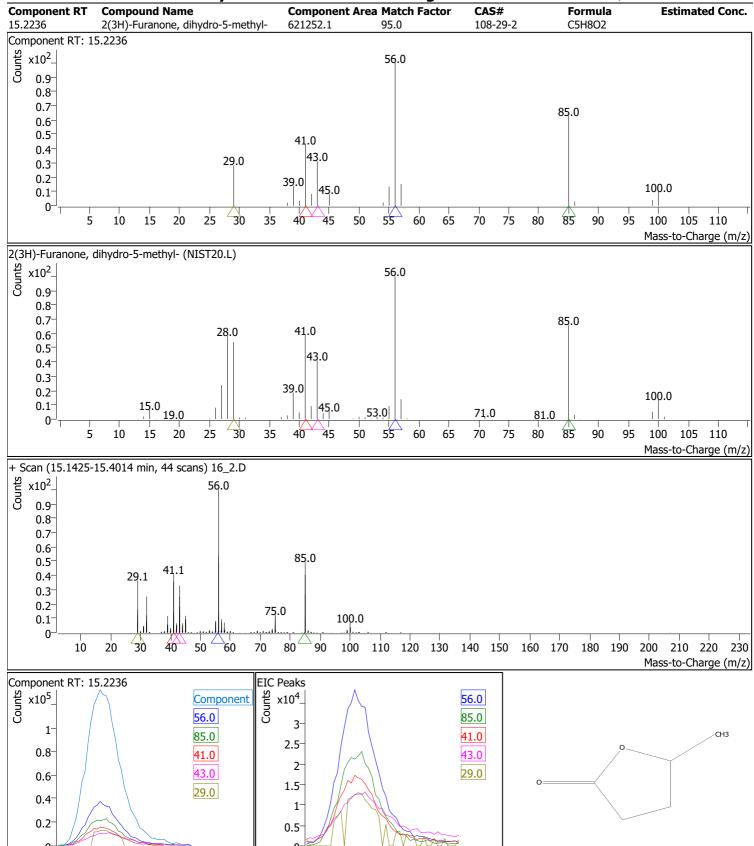










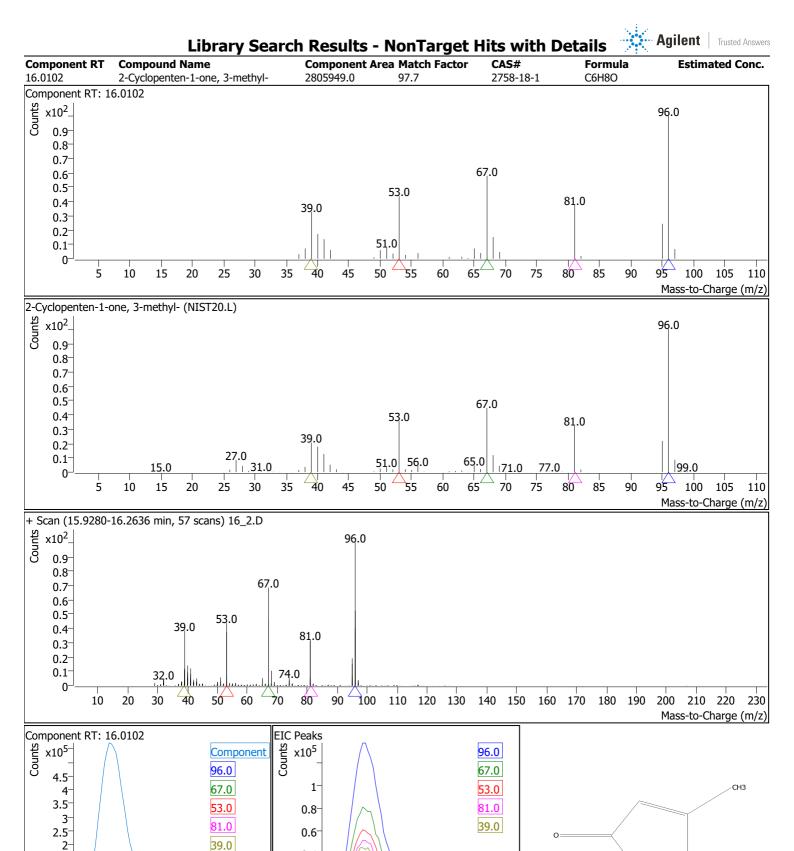


15.2

2 15.3 Acquisition Time (min)

15.2

15.3





16.1

Acquisition Time (min)

16.2

0.4

0.2

16

1.5⁻

0.5

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.** 108-95-2 17.9521 Phenol 4443750.1 92.8 C6H6O Component RT: 17.9521 v10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4 66.0 0.3 39.0 0.2 0.1 55.0 63.0 50.0 -95 50 65 20 25 30 35 40 45 55 60 75 80 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 66.0 0.3 39.0 0.2 0.1 47.050.0 63.0 31.0 74.0 79.0 295 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 100 105 Mass-to-Charge (m/z) + Scan (17.8868-18.2674 min, 65 scans) 16_2.D st x10² 0.9 94.0 0.8 0.7 0.6 0.5 0.4^{-} 66.0 0.3 0.2 39.0 110.1 0.1 55.0 32.0 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: 17.9521 **EIC Peaks** Counts Counts x10⁵ 94.0 Component 94.0 66.0 7 3 66.0 65.0 6 2.5 39.0 65.0 5 2 39.0 40.0

18

18.1

Acquisition Time (min)

18.2

1.5

1

0.5

40.0

4

3

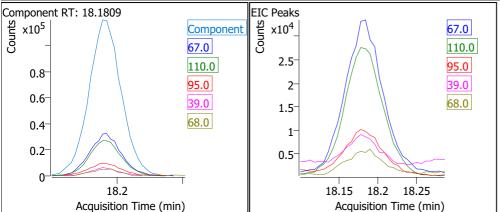
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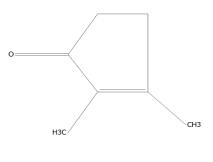
1

18

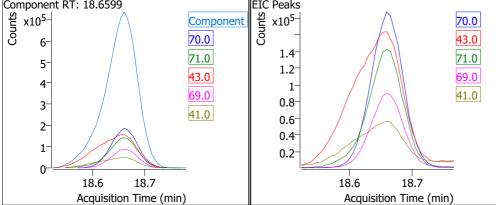
18.1 18.2

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 18.1809 2-Cyclopenten-1-one, 2,3-dimethyl-408237.0 89.5 1121-05-7 C7H10O Component RT: 18.1809 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 0.3 39.0 0.2 53.0 81.0 0.1 110 115 120 125 10 25 30 35 40 50 55 65 80 85 100 105 15 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 110.0 67.0 0.8 0.7 0.6 0.5 0.4 82.0 95.0 0.3 54.0 39.0 0.2 27.0 0.1 51.0 65.0 79.0 99.0 91.0 10 15 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (18.1009-18.2852 min, 32 scans) 16_2.D St x10² 0.9 67.0 0.8 0.7^{-} 0.6 110.0 0.5 0.4^{-} 94.0 0.3 0.2 53.0 79.0 0.1 103.0 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) EIC Peaks Component RT: 18.1809 Counts Counts x10⁴ 67.0 Component 67.0 110.0 2.5 110.0 95.0 0.8





-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 544-01-4 18.6599 Diisoamyl ether 3196448.9 86.7 C10H22O Component RT: 18.6599 v10² 0.9 70.0 0.8 43.0 0.7^{-} 0.6 0.5 0.4 0.3 41.0 55.0 0.2 39.0 0.1 87.0 20 25 30 35 40 50 55 60 65 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) Diisoamyl ether (NIST20.L) Counts x10²_ 0.9 43.0 70.0 0.8 0.7 0.6 0.5 0.4 0.3 41.0 55.0 0.2 101.0 29.0 39.0 45.0 0.1 31.0 53.0 20 25 30 35 40 45 50 55 60 65 75 80 85 90 95 100 105 110 Mass-to-Charge (m/z) + Scan (18.5706-18.7668 min, 34 scans) 16_2.D St x10² 0.9 103.0 57.0 70.1 0.8 0.7 0.6 0.5 0.4^{-} 0.3 29.1 0.2 0.1 87.0 131.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 18.6599 **EIC Peaks** Counts x10⁵ x10⁵ 70.0 Component 70.0 43.0 6 1.4 71.0 71.0 5 1.2



-- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 109-52-4 18.8487 Pentanoic acid 1166461.0 85.7 C5H10O2 Component RT: 18.8487 v10² 0.9 60.0 0.8 0.7^{-} 0.6 73.0 0.5 0.4 0.3 87.0 0.2 45.0 39.0 56.0 0.1 95.0 40 25 85 90 95 10 15 20 30 35 45 50 55 65 70 80 Mass-to-Charge (m/z) Pentanoic acid (NIST20.L) st x10²_ 0.9-60.0 0.8 0.7 0.6 0.5 0.4 73.0 0.3 27.0 0.2 45.0 39.0 55.0 0.1 15.018.0 31.0 87.0 40 60 85 10 15 20 25 30 35 45 50 55 65 70 75 80 90 95 Mass-to-Charge (m/z) + Scan (18.4364-18.9382 min, 84 scans) 16_2.D St x10² 57.0 103.0 70.1 0.8 0.7 0.6 0.5 0.4^{-} 29.1 0.3 0.2 0.1 87.0 131.0 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 18.8487 EIC Peaks Counts Counts x10⁴-60.0 Component 45.0 60.0 0.9 3 8.0 73.0 73.0 2.5 0.7 87.0 39.0 0.6 2

18.5 18.6 18.7 18.8 18.9

Acquisition Time (min)

87.0

Н3С -

45.0

39.0

1.5

1

0.5

0.5

0.4⁻ 0.3⁻

0.2

18.6

18.8

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 19.7605 2-Cyclopenten-1-one, 3,4-dimethyl-827759.2 91.0 30434-64-1 C7H10O Component RT: 19.7605 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| 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 (19.6790-19.8665 min, 31 scans) 16_2.D St x10² 0.9 57.0 103.0 0.8 0.7 0.6 0.5 43.0 0.4^{-} 0.3 29.0 0.2 61.0 95.0 110.1 72.1 0.1 117.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 19.7605 x10⁵ Counts x10⁴ 95.0 Component 95.0 110.0 1.4 3.5 110.0 67.0 1.2 3 67.0 39.0 1 2.5

19.8

Acquisition Time (min)

19.9

65.0

НЗС

39.0

65.0

2

1

19.7

1.5

0.5

0.8

0.6

0.4

0.2

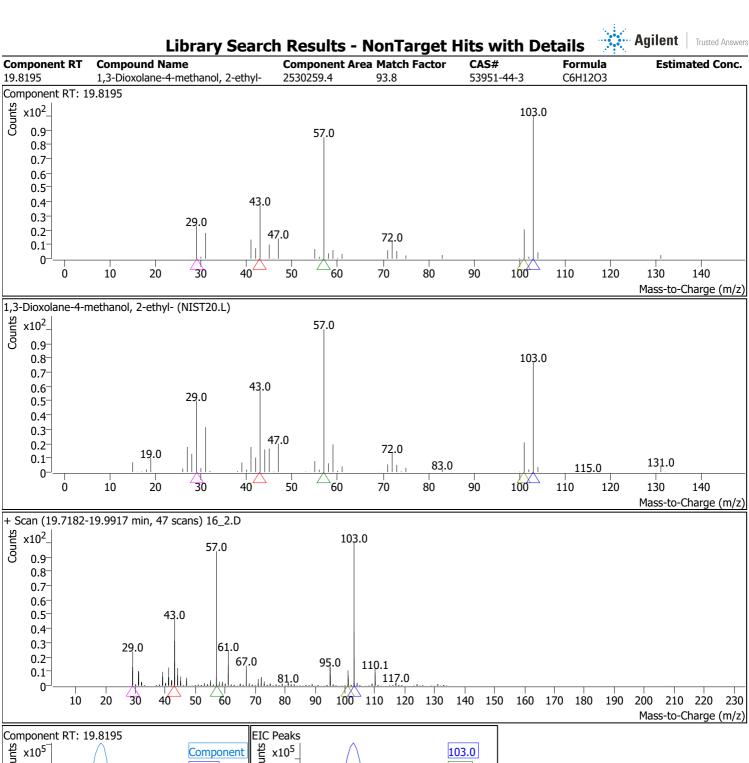
19.7

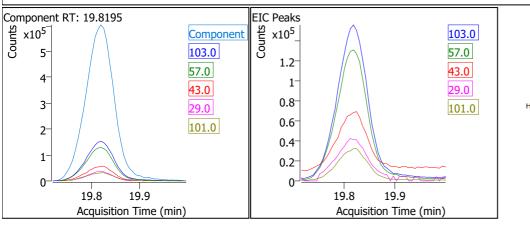
19.8

Acquisition Time (min)

19.9

CH3





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20.2

Acquisition Time (min)

71.0

5

4

3

2

1

20.1

71.0

29.0

1.5

1

1.25

 0.75^{-}

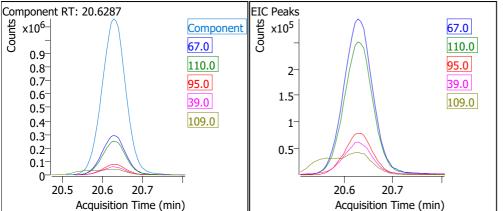
0.25

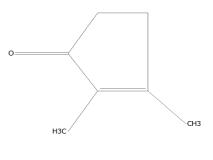
0.5

20.1

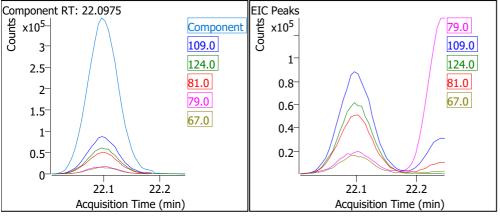
20.2

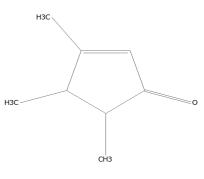
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 20.6287 2-Cyclopenten-1-one, 2,3-dimethyl-4844028.4 95.7 1121-05-7 C7H10O Component RT: 20.6287 v10² 0.9 67.0 110.0 0.8 0.7^{-} 0.6 0.5 0.4 95.0 0.3 39.0 0.2 54.0 41.0 81.0 0.1 105 110 115 120 125 10 25 30 35 40 50 55 65 80 85 90 100 15 75 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 110.0 67.0 0.8 0.7 0.6 0.5 0.4 82.0 95.0 0.3 54.0 39.0 0.2 27.0 0.1 51.0 65.0 79.0 99.0 91.0 100 105 110 115 120 125 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 Mass-to-Charge (m/z) + Scan (20.5271-20.8122 min, 47 scans) 16_2.D St x10² 0.9 67.0 110.1 0.8 0.7^{-} 0.6 0.5 0.4^{-} 61.0 0.3 43.0 0.2 95.0 31.0 53.0 81.1 0.1 124.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 20.6287 Counts Counts x10⁵ 67.0 Component 67.0 110.0 0.9 110.0 95.0 0.8 2





··· 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 2-Cyclopenten-1-one, 3,4,5-trimethyl-1445938.0 C8H12O Component RT: 22.0975 $x10^{2}$ 109.0 0.9 0.8 124.0 0.7^{-} 81.0 0.6 0.5 0.4 0.3 79.0 67.0 0.2 39.0 96.0 53.0 0.1 30 35 40 45 50 55 65 70 75 80 85 95 100 105 110 115 130 Mass-to-Charge (m/z) 2-Cyclopenten-1-one, 3,4,5-trimethyl- (NIST20.L) st x10²_ 0.9-109.0 0.8 0.7 0.6 124.0 0.5 81.0 0.4 0.3 0.2 41.0 53.0 79.0 67.0 0.1 96.0 125 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 130 Mass-to-Charge (m/z) + Scan (22.0116-22.1858 min, 30 scans) 16_2.D st x10² 0.9 0.8 43.0 0.7^{-} 0.6 0.5 0.4^{-} 109.0 0.3 31.0 81.1 0.2 124.1 0.1 55.0 67.0 117.0 96.1 10 20 30 40 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) EIC Peaks Component RT: 22.0975 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 22.2421 Phenol, 2-methyl-6805836.6 97.6 C7H8O Component RT: 22.2421 v10² 0.9 108.0 0.8 0.7 0.6 0.5 0.4 77.0 0.3 90.0 0.2 39.0 51.0 61.0 0.1 90 15 20 25 30 35 40 45 50 55 60 65 75 85 95 100 115 Mass-to-Charge (m/z) Phenol, 2-methyl- (NIST20.L) Counts x10²_ 0.9 108.0 0.8 0.7 0.6 0.5 0.4 79.0 0.3 90.0 0.2 39.0 51.0 27.0 0.1 63.0 43.0 74.0 29.0 68.0 86.0 90 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 95 100 105 110 115 Mass-to-Charge (m/z) + Scan (22.1561-22.4534 min, 51 scans) 16_2.D st x10² 0.9 108.0 43.0 0.8 0.7 0.6 0.5 0.4^{-} 77.0 31.0 0.3 0.2 90.0 51.0 0.1 39.0 117.0 **110** 10 20 30 40 50 60 70 80 90 100 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 22.2421 **EIC Peaks** Counts Counts x10⁵ 108.0 Component 108.0 107.0 3 1.2 107.0 77.0 2.5 1 77.0 79.0 НО



22.3

22.4 Acquisition Time (min)

90.0

2

1 0.5

22.2

1.5

79.0

90.0

0.8

0.6

0.4

0.2

22.2

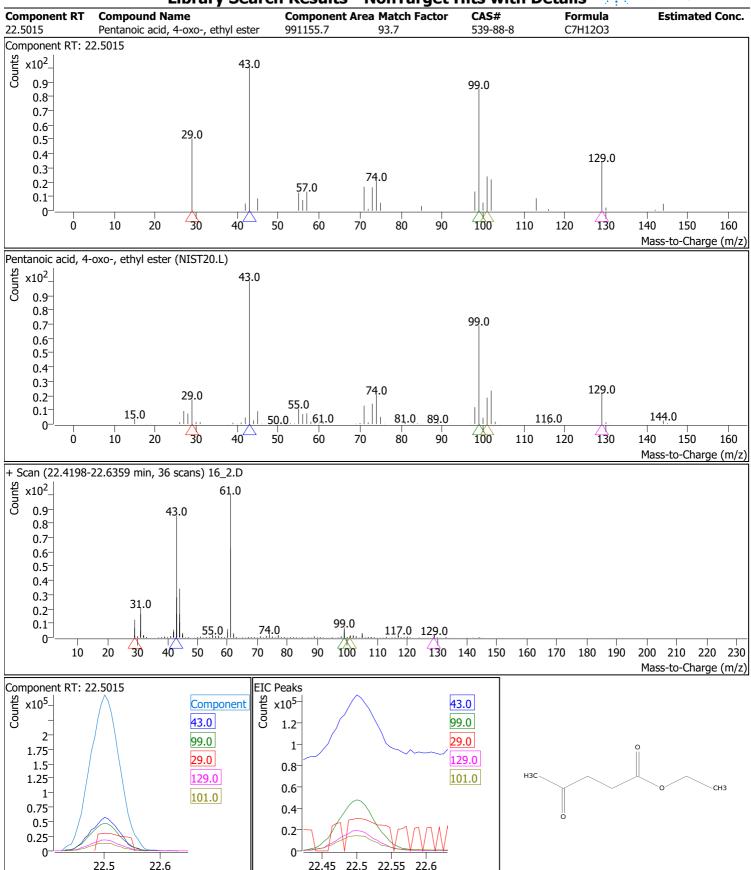
22.3

22.4

Acquisition Time (min)

H3C





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.** 23.0976 1-Octanol 4768450.2 111-87-5 C8H18O Component RT: 23.0976 y x10² 0.9 56.0 41.0 0.8 70.1 0.7 84.1 0.6 0.5 0.4 0.3 0.2 0.1 70 100 105 110 115 120 125 130 135 140 65 75 80 85 Mass-to-Charge (m/z) 1-Octanol (NIST20.L) Counts x10²_ 0.9 56.0 0.8 41.0 70.0 0.7 0.6 84.0 0.5 0.4 29.0 0.3 0.2 0.1 97.0 112.0 70 55 20 25 35 40 45 50 60 65 75 80 85 90 95 100 105 110 115 120 125 130 135 140 Mass-to-Charge (m/z) + Scan (23.0012-23.2516 min, 42 scans) 16_2.D st x10² 0.9 0.8 43.0 0.7 0.6 0.5 0.4^{-} 31.0 0.3 56.1 0.2 69.1 83.1 110.1 0.1 0 504 10 20 30 40 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 Mass-to-Charge (m/z) Component RT: 23.0976 **EIC Peaks** Counts x10⁶ 0.9 Counts x10⁵-56.0 Component 56.0 55.0 8.0 55.0 41.0 0.7^{-} 0.8 41.0 70.1 0.6

23.1

23.2

Acquisition Time (min)

70.1

69.1

23.2

Acquisition Time (min)

23.1

0.5⁻

0.3⁻ 0.2⁻

0.1

23

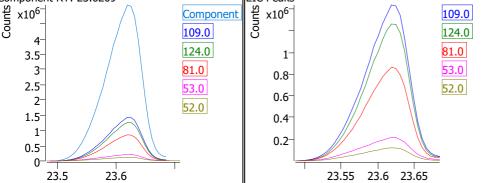
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0.4

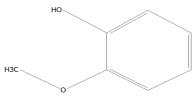
0.2

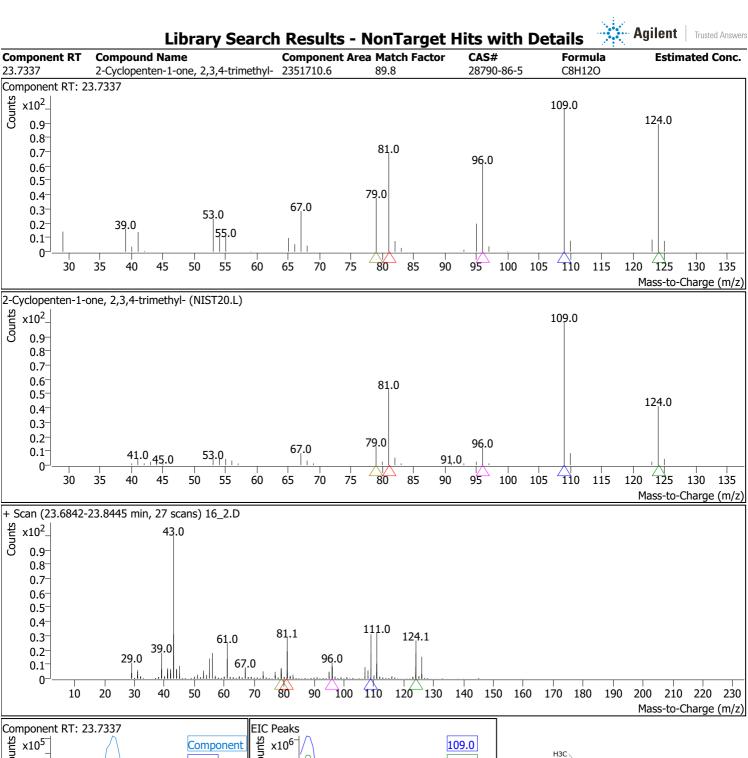
69.1

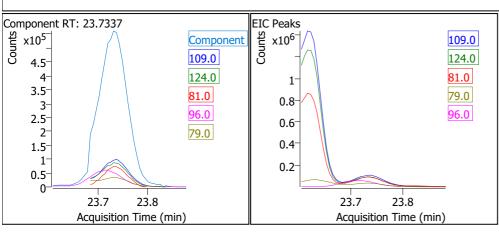
--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 90-05-1 23.6209 Phenol, 2-methoxy-21917845.3 97.7 C7H8O2 Component RT: 23.6209 v10² 0.9 109.0 124.0 0.8 0.7 81.0 0.6 0.5 0.4 0.3 0.2 53.0 39.0 77.0 0.1 50 80 110 10 20 30 40 60 90 100 120 130 140 Mass-to-Charge (m/z) Phenol, 2-methoxy- (NIST20.L) Counts x10²_ 0.9 109.0 124.0 0.8 81.0 0.7 0.6 0.5 0.4 0.3 53.0 0.2 39.0 63.0 0.1 27.0 77.0 95.0 110 10 20 30 40 50 60 70 80 90 100 120 130 140 Mass-to-Charge (m/z) + Scan (23.4898-23.6842 min, 33 scans) 16_2.D st x10² 0.9 109.0 124.0 0.8 0.7 0.6 81.0 0.5 0.4^{-} 0.3 53.0 61.0 0.2 77.0 0.1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.6209 Counts Counts x10⁶ 109.0 Component 109.0 124.0 124.0 81.0 3.5 1

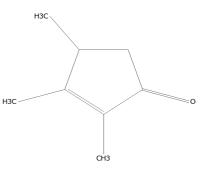


Acquisition Time (min)

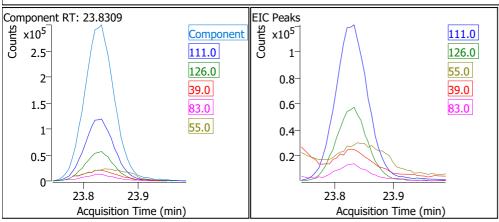


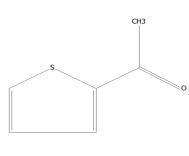


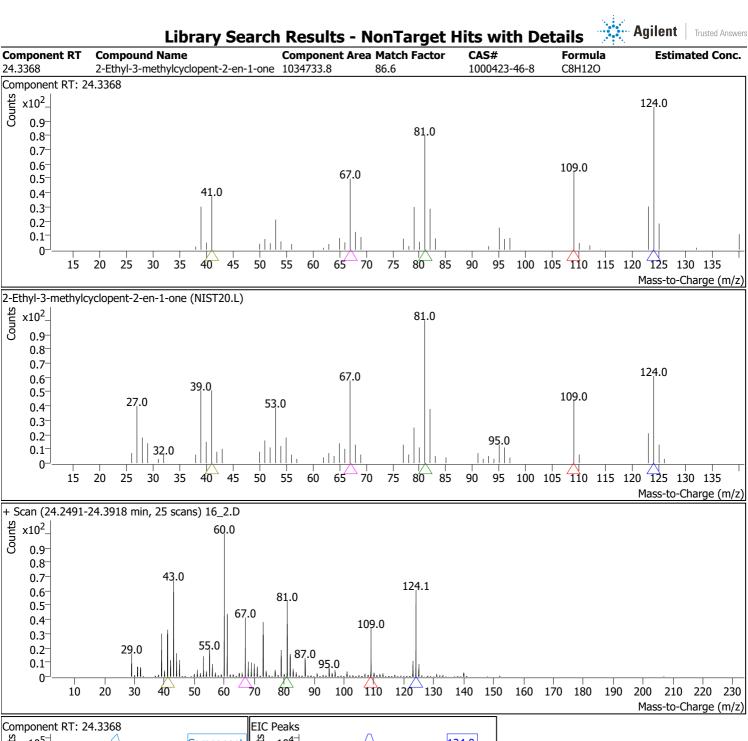


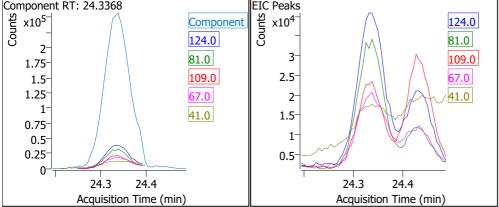


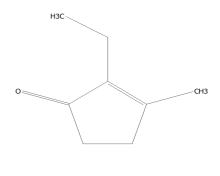
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 88-15-3 23.8309 Ethanone, 1-(2-thienyl)-1143988.5 89.9 C6H6OS Component RT: 23.8309 v10² 0.9 111.0 0.8 0.7 0.6 126.0 0.5 0.4 0.3 0.2 39.0 83.0 55.0 0.1 45.0 40 50 55 60 75 80 85 95 100 105 110 115 130 Mass-to-Charge (m/z) Ethanone, 1-(2-thienyl)- (NIST20.L) st x10² 0.9 111.0 0.8 0.7 126.0 0.6 0.5 39.0 0.4 0.3 43.0 0.2 83.0 0.1 45.0 58.0 98.0 53.0 69.0 35 50 55 65 70 75 80 85 90 95 100 105 110 115 120 125 130 Mass-to-Charge (m/z) + Scan (23.7437-23.9927 min, 42 scans) 16_2.D st x10² 0.9 0.8 0.7 0.6 0.5 0.4^{-} 111.0 0.3 56.0 0.2 126.0 39.0 81.1 29.0 0.1 73.0 96.1 120^{-/} 10 20 30 50 60 70 80 90 100 110 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 23.8309 st x10⁵ 2.5 Counts x10⁵ 111.0 Component 111.0 126.0 1 СНЗ 126.0 55.0

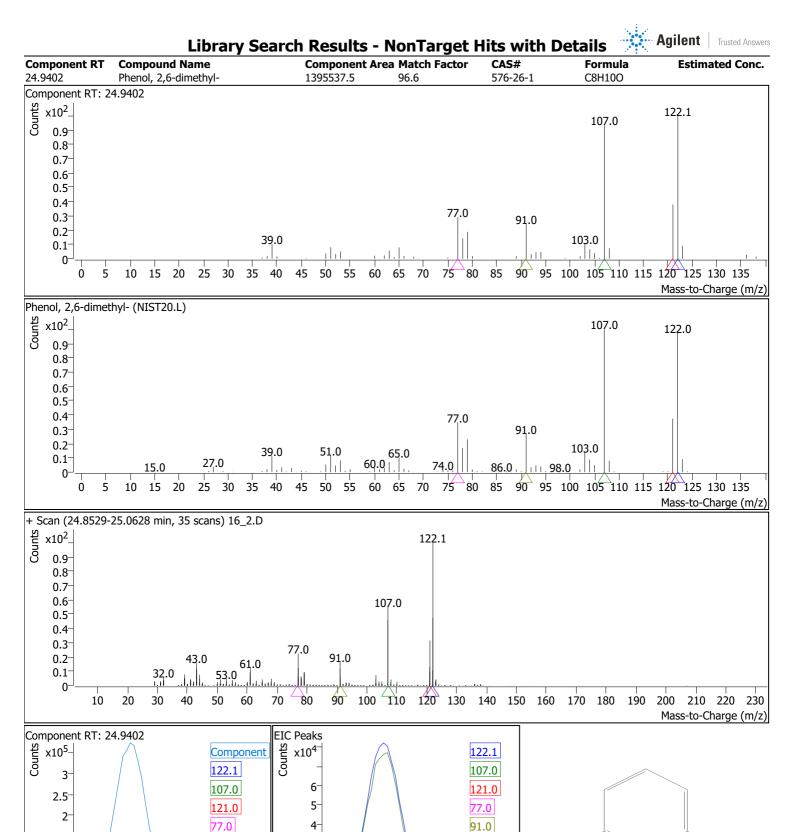














24.95

25

Acquisition Time (min)

77.0

91.0

25

Acquisition Time (min)

3-

2

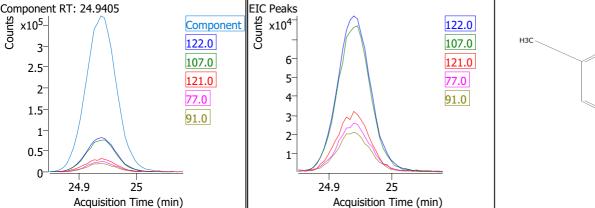
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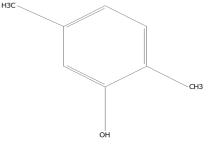
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0.5 0CH3

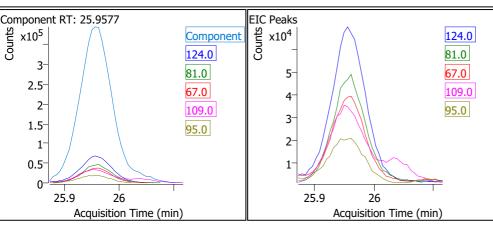
H3C

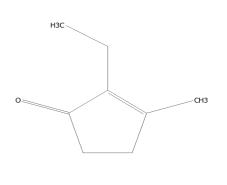
··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** Phenol, 2,5-dimethyl-95-87-4 24.9405 1397981.9 96.9 C8H10O Component RT: 24.9405 v10² 0.9 122.0 107.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 91.0 0.2 39.0 103.0 0.1 35 08 85 95 100 105 110 115 120 125 130 135 75 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 (24.8529-25.0628 min, 35 scans) 16_2.D st x10² 0.9 122.1 0.8 0.7^{-} 0.6 107.0 0.5 0.4^{-} 0.3 77.0 91.0 0.2 61.0 53.0 0.1 100 110 10 20 30 40 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 24.9405 Sin x10⁵-Counts x10⁴ 122.0 Component 122.0 107.0 3 6 107.0 121.0 2.5





--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1000423-46-8 2-Ethyl-3-methylcyclopent-2-en-1-one 1692432.9 89.8 C8H12O Component RT: 25.9577 $x10^{2}$ 124.0 0.9 0.8 81.0 0.7^{-} 0.6 67.0 109.0 0.5 0.4 95.0 0.3 39.0 53.0 0.2 0.1 105 T10 115 120 T25 130 135 20 25 35 40 50 55 65 75 80 85 95 100 60 70 90 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 32.0 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (25.8724-26.1161 min, 42 scans) 16_2.D St x10² 0.9 81.1 124.1 43.0 0.8 0.7^{-} 67.0 109.0 0.6 0.5 0.4^{-} 39.0 0.3 95.0 53.0 ⁶¹.0 91.0 0.2 32.0 73.0 0.1 103.0 10 20 30 40 50 60 70 90 100 110 120 130 140 150 170 180 190 200 210 220 230 160 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.** 90-00-6 26.8444 Phenol, 2-ethyl-1585624.1 93.0 C8H10O Component RT: 26.8444 Counts $x10^{2}$ 107.0 0.9 0.8 0.7^{-} 0.6 0.5 122.0 0.4 77.0 0.3 0.2 91.0 0.1 50 85 90 95 100 105 110 115 55 Mass-to-Charge (m/z) Phenol, 2-ethyl- (NIST20.L) Counts x10²_ 0.9 107.0 0.8 0.7 0.6 122.0 0.5 0.4 0.3 77.0 0.2 0.1 39.0 103.0 27.0 65.0 18.0 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 Mass-to-Charge (m/z) + Scan (26.7524-27.0556 min, 51 scans) 16_2.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 77.0 122.1 0.2 95.0 39.0 117.1 67.0 0.1 51.0 151.0 166.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) Component RT: 26.8444 **EIC Peaks** Counts Counts x10⁵ 107.0 Component 107.0 122.0 3 122.0 77.0 1 2.5 77.0 123.0

26.9

Acquisition Time (min)

79.0

0.8

0.6

0.4

0.2

26.8

123.0

79.0

2

1.5

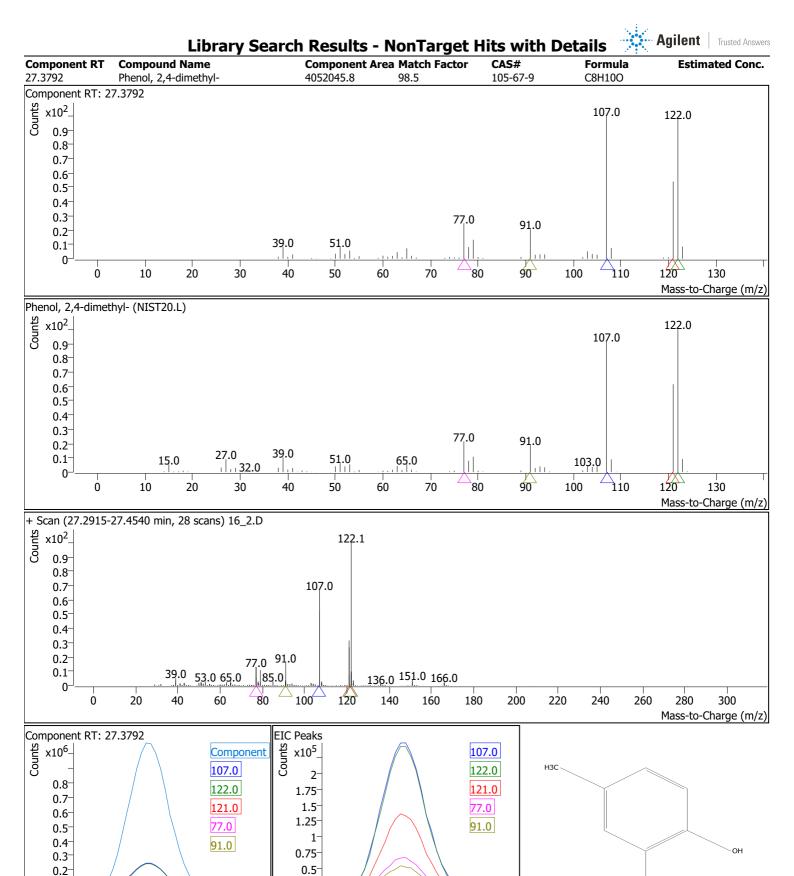
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26.8

26.9

Acquisition Time (min)

0.5



0.25

27.3

27.35

27.4

Acquisition Time (min)

0.1

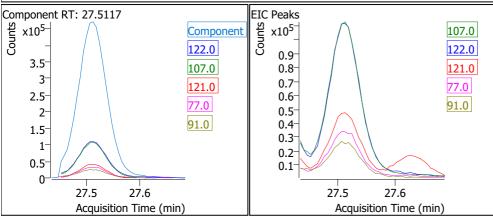
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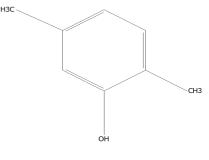
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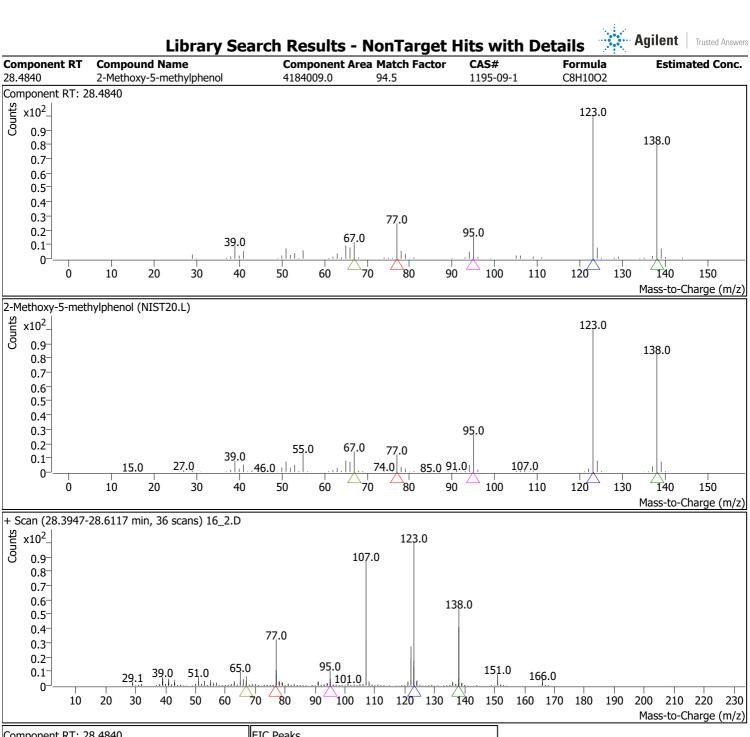
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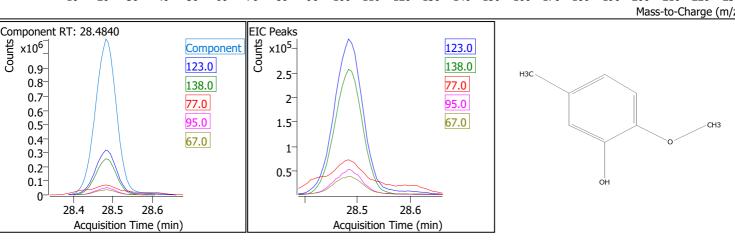
СНЗ

... 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 27.5117 1816927.9 97.9 C8H10O Component RT: 27.5117 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 51.0 104.0 0.1 35 40 50 55 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 90 95 100 105 110 115 120 125 130 135 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 Mass-to-Charge (m/z) + Scan (27.4540-27.6362 min, 31 scans) 16_2.D st x10² 0.9 122.1 107.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 39.0 51.0 _{65.0} 166.0 0.1 136.0 Ó 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 27.5117 EIC Peaks Counts x10⁵⁻ Counts x10⁵ 107.0 Component 122.0 122.0 0.9 3.5 107.0 0.8 121.0 3









--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 91-20-3 28.7618 Naphthalene 497612.3 87.5 C10H8 Component RT: 28.7618 y x10² 0.9 128.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 102.0 0.1 64.0 75.0 75 65 45 50 55 60 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 (28.6794-28.8632 min, 31 scans) 16_2.D st x10² 0.9 128.0 0.8 107.0 0.7 0.6 122.1 0.5 151.0 0.4^{-} 166.0 0.3 0.2 91.0 55.0 69.0 136.0 0.1 <u>փաժարատակութի</u> <u>ىلىنىلىلىلىنىنىل</u> 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: 28.7618 Counts Counts x10⁴ 128.0 Component 128.0 127.0 1 6 127.0 129.0 5 0.8 129.0 102.0 4

126.0

102.0

126.0

3

2

1

28.7

28.75

28.8 Acquisition Time (min)

0.6

0.4

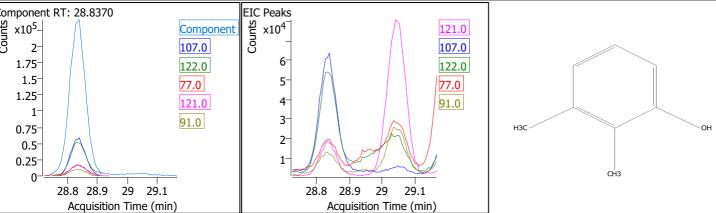
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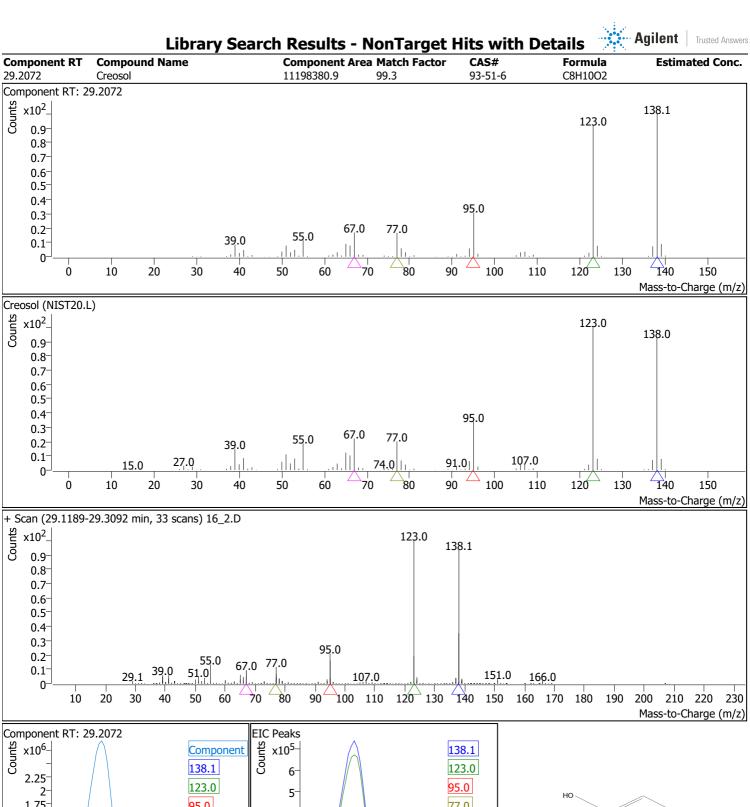
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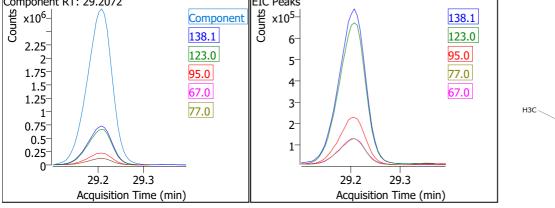
28.7

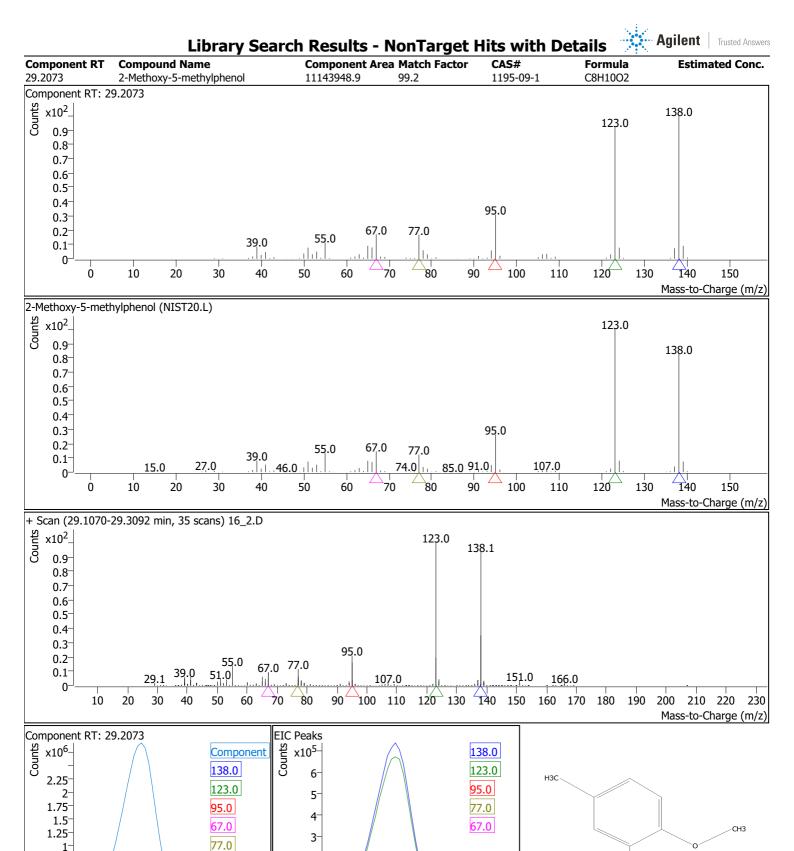
28.8

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 28.8370 Phenol, 2,3-dimethyl-942992.8 92.8 526-75-0 C8H10O Component RT: 28.8370 v10² 0.9 107.0 122.0 0.8 0.7^{-} 0.6 0.5 0.4 77.0 0.3 91.0 0.2 79.0 103.0 39.0 55.0 0.1 50 55 75 100 105 110 115 Mass-to-Charge (m/z) Phenol, 2,3-dimethyl- (NIST20.L) Counts x10²_ 0.9 122.0 0.8 107.0 0.7 0.6 0.5 0.4 0.3 77.0 0.2 0.1 89.093.0 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 (28.7709-28.9108 min, 24 scans) 16_2.D st x10² 0.9 107.0 122.1 0.8 0.7^{-} 0.6 0.5 151.0 0.4^{-} 166.0 0.3 0.2 91.0 69.0 136.0 0.1 تلتبا للحد عباياته تبيب تنابييا 100 110 10 20 50 60 70 80 90 120 130 140 150 160 170 180 190 200 210 220 230 Mass-to-Charge (m/z) EIC Peaks Component RT: 28.8370 strucy x10⁵-Counts x10⁴ 121.0 Component 107.0 107.0 6 1.75 122.0 122.0









29.15 29.2 29.25 29.3

Acquisition Time (min)

2-

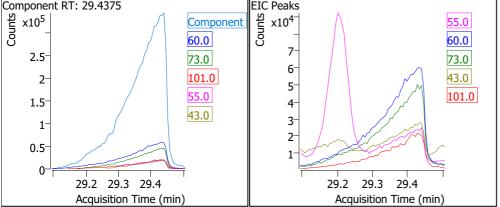
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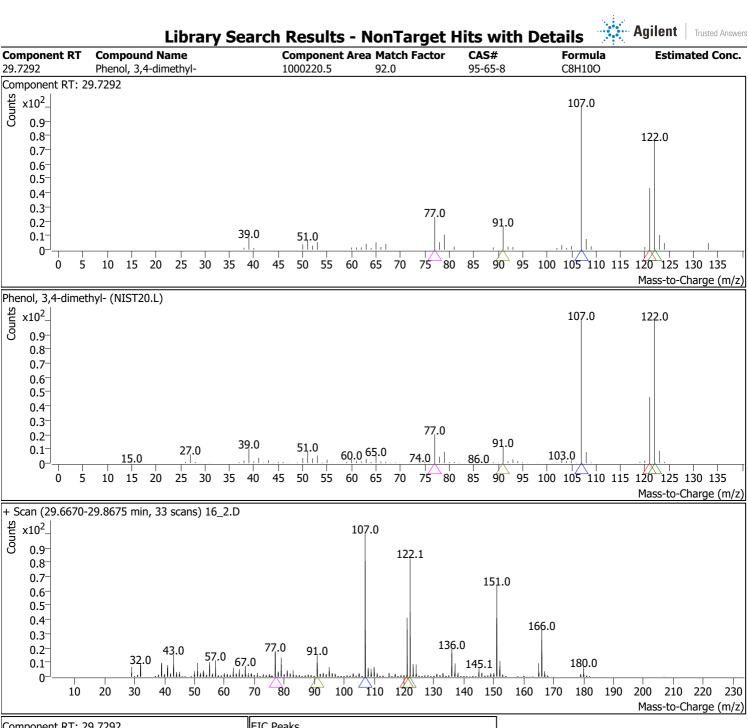
29.2

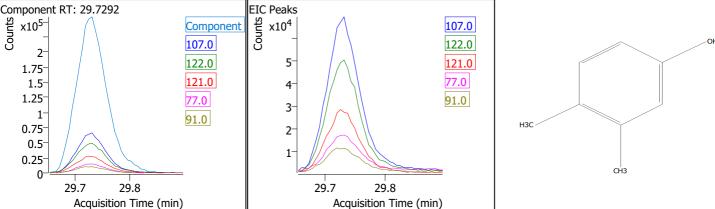
Acquisition Time (min)

0.75 0.5 0.25

--- 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 29.4375 Octanoic acid 2561653.7 86.2 C8H16O2 Component RT: 29.4375 v10² 0.9 60.0 0.8 73.0 0.7 0.6 0.5 0.4 101.0 55.0 43.0 0.3 85.0 29.0 0.2 110.0 0.1 0 10 20 30 40 50 60 80 100 110 120 130 140 150 160 Mass-to-Charge (m/z) Octanoic acid (NIST20.L) Counts x10²_ 0.9 60.0 0.8 0.7 73.0 0.6 0.5 43.0 0.4 0.3 55.0 85.0 29.0 101.0 0.2 69.0 115.0 0.1 144.0 18.0 ||32.0 98.0 129.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 Mass-to-Charge (m/z) + Scan (29.1773-29.4876 min, 53 scans) 16_2.D st x10² 0.9 123.0 138.1 0.8 0.7 0.6 0.5 0.4^{-} 0.3 95.0 0.2 67.0 77.0 0.1 151.0 29.1 101.0 10 20 30 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: 29.4375 Counts Counts x10⁴ Component 55.0 60.0 60.0 7 2.5 73.0 73.0 6







... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 697-82-5 30.0837 Phenol, 2,3,5-trimethyl-967091.5 89.7 C9H12O Component RT: 30.0837 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 39.0 145.0 0.1 0 [∠]80 20 30 40 50 60 70 90 100 110 120 130 140 150 Mass-to-Charge (m/z) Phenol, 2,3,5-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 39.0 77.0 0.1 27.0 65.0 51.0 105.0 115.0 58.0 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (29.9970-30.2222 min, 38 scans) 16_2.D st x10² 0.9 57.0 136.1 121.0 0.8 0.7^{-} 0.6 0.5 151.0 131.0 0.4^{-} 166.0 29.1 0.3 43.0 91.0 77.0 0.2 146.0 110.0 65.0 0.1 51.0 سبليل استبسانات بباللابيانات آثاب 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) EIC Peaks Component RT: 30.0837 Counts stuno x10⁵x10⁴ 121.0 Component НЗС 121.0 136.0 1.75 136.0 5 135.1 1.5 135.1 91.0

30.1

Acquisition Time (min)

77.0

30.2

H3C

1.25

0.75

0.5

0.25

1

91.0

77.0

30.1

Acquisition Time (min)

3

2-

1

30

-CH3

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 120-80-9 30.3945 Catechol 34530431.3 98.0 C6H6O2 Component RT: 30.3945 v10² 0.9 110.0 0.8 0.7 0.6 0.5 0.4 0.3 64.0 0.2 81.0 92.0 53.0 0.1 10 35 50 55 75 80 85 95 100 105 60 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 45 50 55 60 70 75 80 85 90 95 100 105 110 115 120 125 Mass-to-Charge (m/z) + Scan (30.3616-31.2297 min, 147 scans) 16_2.D st x10² 0.9 110.0 0.8 0.7^{-} 0.6 0.5 0.4^{-} 0.3 0.2 81.0 92.0 0.1 53.0 29.0 39.0 20 30 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 10 Mass-to-Charge (m/z) EIC Peaks Component RT: 30.3945 x10⁶ 2.5 Counts x10⁶-110.0 Component 110.0 64.0 2.5 1 64.0 63.0 2 0.8 63.0 81.0

30.6 30.8

31

Acquisition Time (min)

92.0

1.5

1

0.5

0-

30.6 30.8

31 Acquisition Time (min)

81.0

92.0

0.6

0.4

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 31.0736 Phenol, 2-propyl-506825.0 86.6 644-35-9 C9H12O Component RT: 31.0736 v10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 0.4 136.0 0.3 77.0 0.2 79.0 0.1 131.0 100 105 110 115 120 125 130 135 140 145 150 35 65 75 80 95 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 (30.9951-31.1926 min, 33 scans) 16_2.D st x10² 0.9 107.0 0.8 0.7^{-} 0.6 0.5 180.0 125.0 136.1 0.4^{-} 81.0 165.0 0.3 97.0 29.0 39.0 0.2 64.0 91.0 154.0 117.0 0.1 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 20 30 60 70 80 90 10 Mass-to-Charge (m/z) EIC Peaks Component RT: 31.0736 Counts Counts x10⁴ 107.0 Component 107.0 136.0 6 1 136.0 77.0 НО 5 77.0 79.0 0.8



31.05 31.1 31.15

Acquisition Time (min)

108.0

4

3-

2

79.0

108.0

0.6

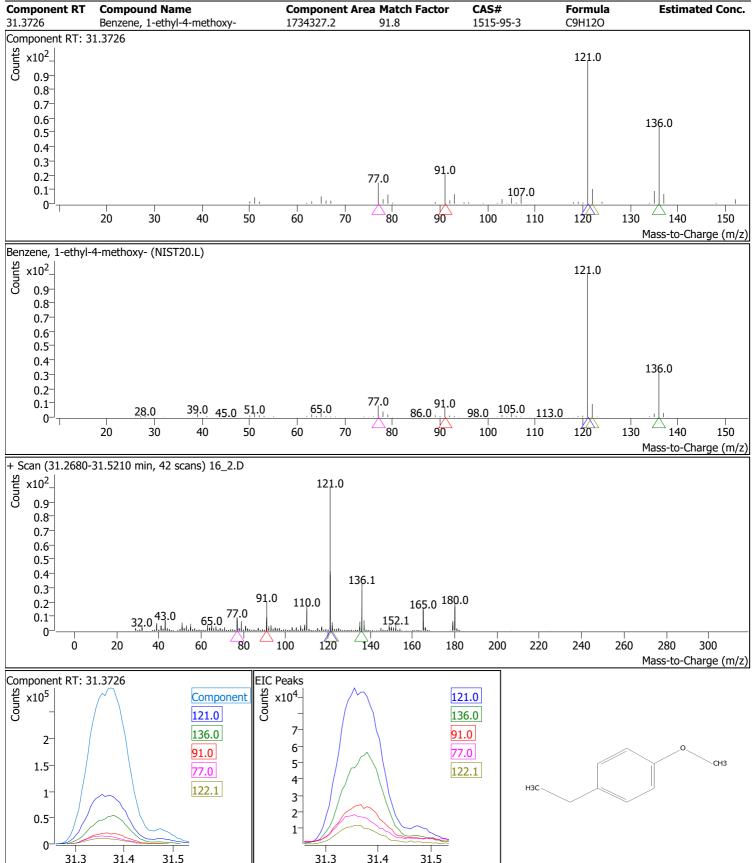
0.4

0.2

31.05 31.1 31.15



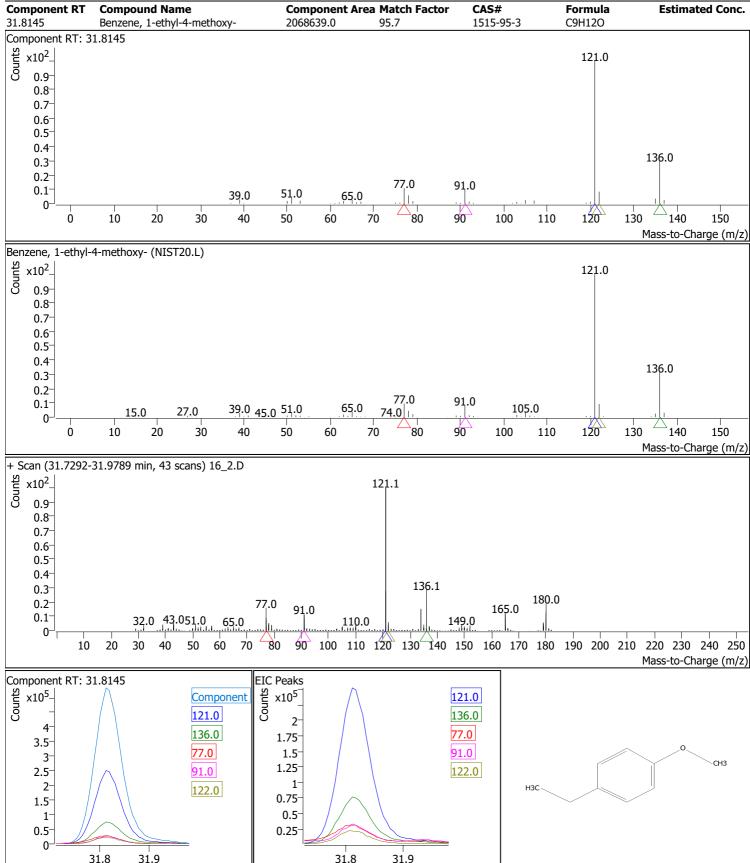




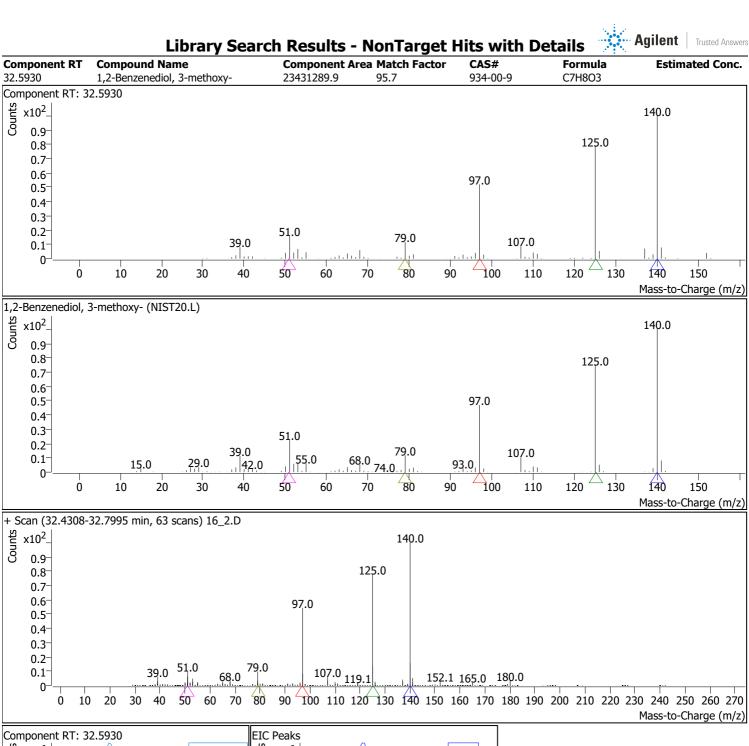
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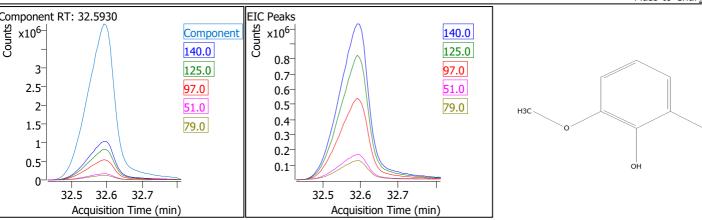


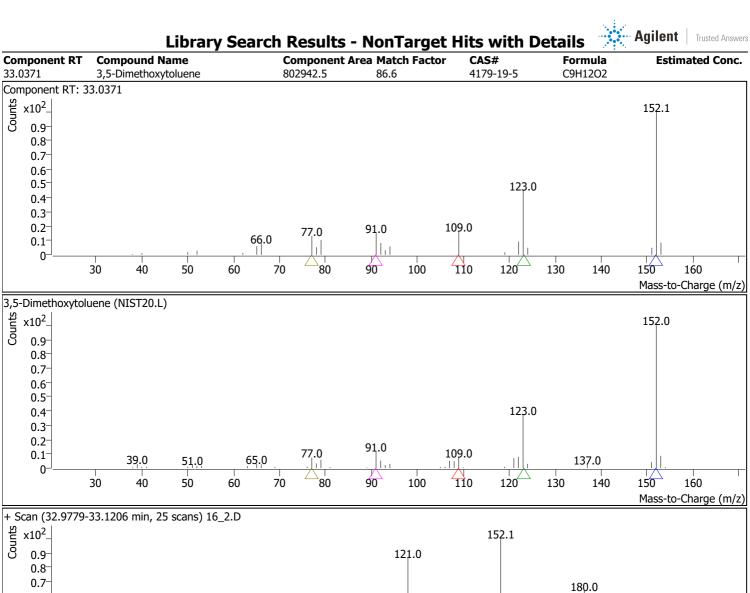


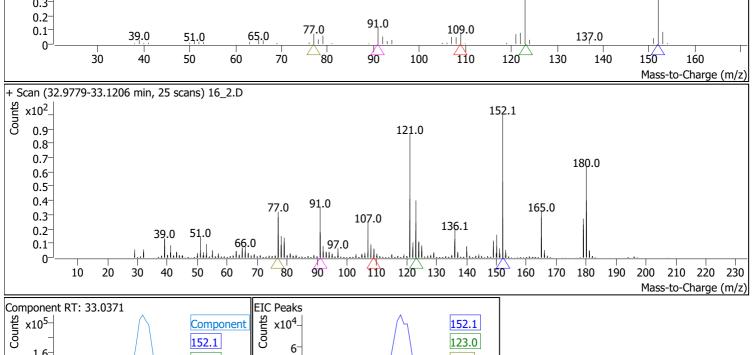


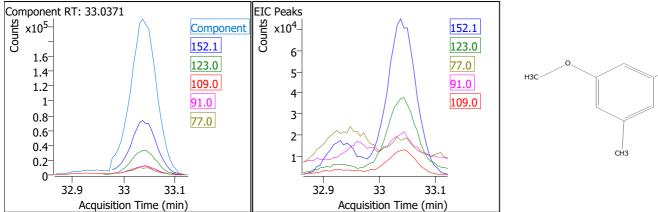
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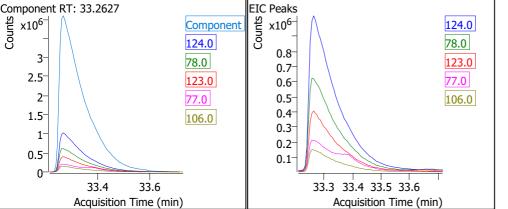


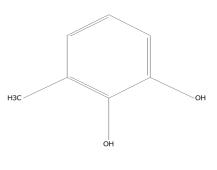


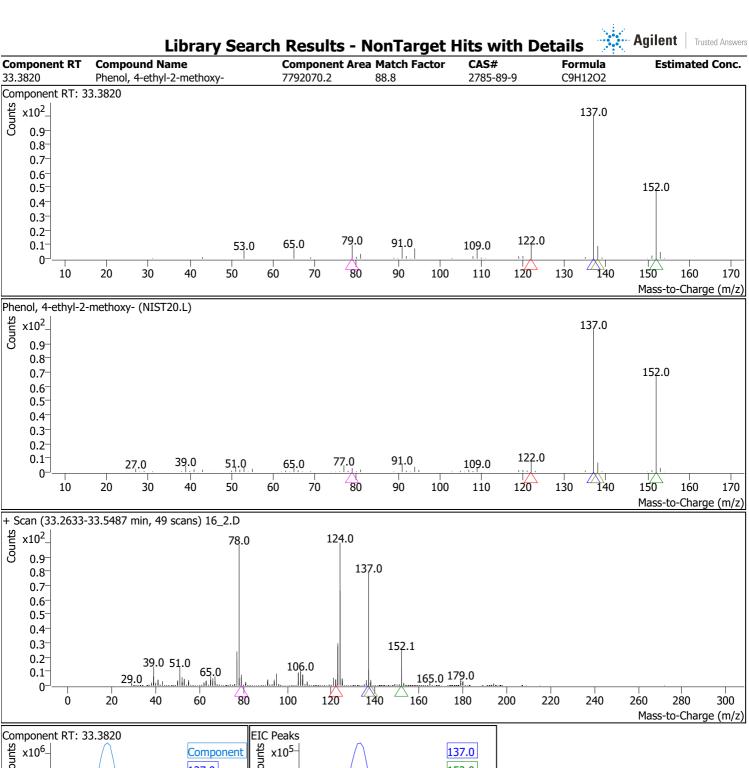


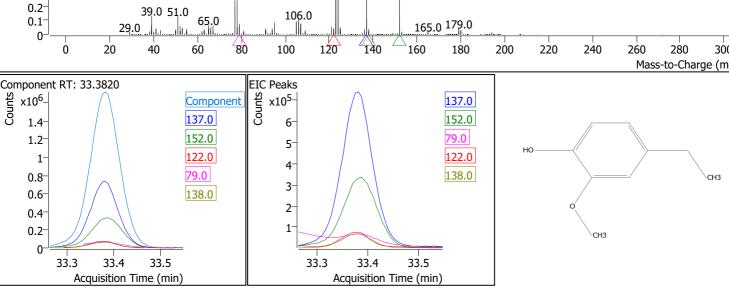


- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 488-17-5 33.2627 1,2-Benzenediol, 3-methyl-27577604.5 97.5 C7H8O2 Component RT: 33.2627 v10² 0.9 124.0 0.8 0.7 78.0 0.6 0.5 0.4 0.3 0.2 106.0 39.0 51.0 95.0 0.1 10 20 30 40 50 60 70 90 100 110 130 140 Mass-to-Charge (m/z) 1,2-Benzenediol, 3-methyl- (NIST20.L) Counts x10²_ 0.9 124.0 0.8 0.7 0.6 0.5 0.4 78.0 0.3 0.2 106.0 39.0 51.0 0.1 62.0 67.0 27.0 18.0 80 10 20 30 40 50 60 70 90 100 110 120 130 140 Mass-to-Charge (m/z) + Scan (33.2157-33.7152 min, 85 scans) 16_2.D st x10² 0.9 78.0 124.0 0.8 137.0 0.7 0.6 0.5 0.4 0.3 152.1 0.2 39.0 51.0 106.0 165.0 179.0 194.1 67.0 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 33.2627 EIC Peaks Counts Counts x10⁶ 124.0 Component 124.0 78.0 0.8 3 78.0 123.0 0.7

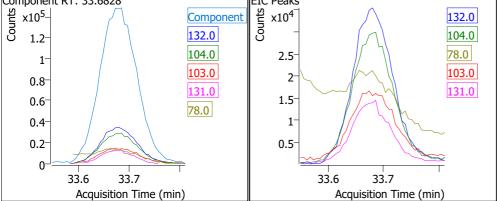


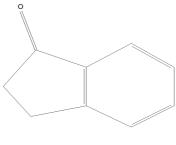


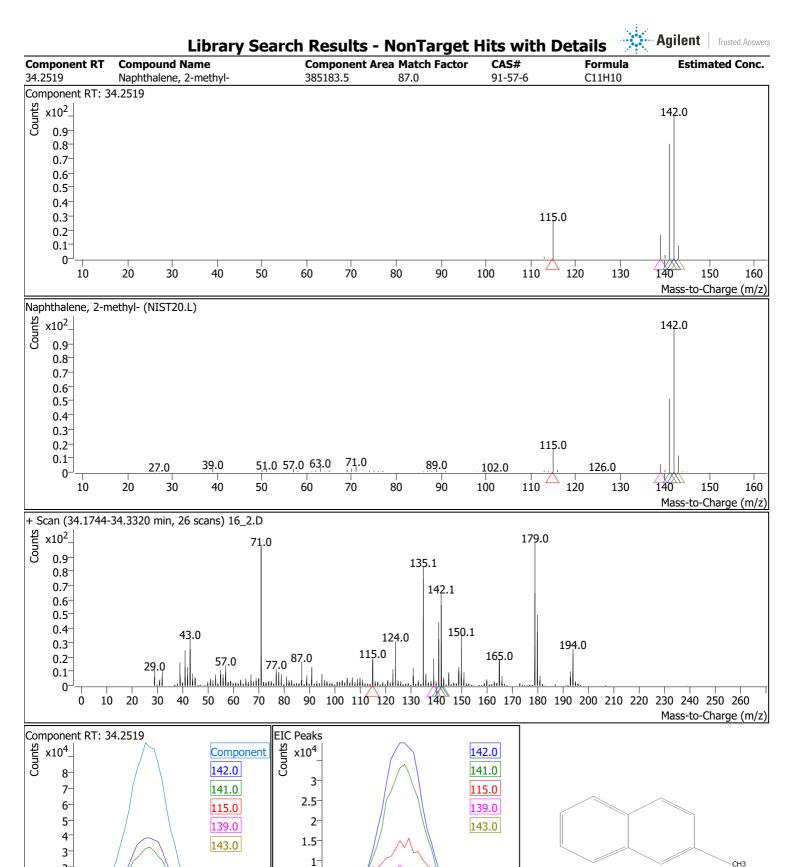




--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 83-33-0 C9H8O 33.6828 1H-Inden-1-one, 2,3-dihydro-760442.2 87.6 Component RT: 33.6828 v10² 0.9 132.0 104.0 0.8 0.7^{-} 0.6 0.5 0.4 78.0 0.3 0.2 51.0 0.1 100 Ó 10 20 30 40 50 60 70 90 110 120 130 140 150 Mass-to-Charge (m/z) 1H-Inden-1-one, 2,3-dihydro- (NIST20.L) Counts x10²_ 0.9 104.0 132.0 0.8 0.7 0.6 0.5 0.4 78.0 0.3 51.0 0.2 63.0 39.0 0.1 27.0 89.0 98.0 115.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 Mass-to-Charge (m/z) + Scan (33.5903-33.8103 min, 38 scans) 16_2.D st x10² 0.9 179.0 0.8 0.7^{-} 194.0 0.6 0.5 91.0 104.0 121.0 135.1 0.4^{-} 0.3 39.0 165.0 0.2 60.0 150.1 32.0 0.1 <u>ռեհհեր հավկերու պատուրդիկանը.</u> 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 10 20 Mass-to-Charge (m/z) EIC Peaks Component RT: 33.6828 stuno x10⁵-Counts x10⁴ 132.0 Component 132.0 104.0 1.2 104.0 78.0 2.5 1







34.2

34.25

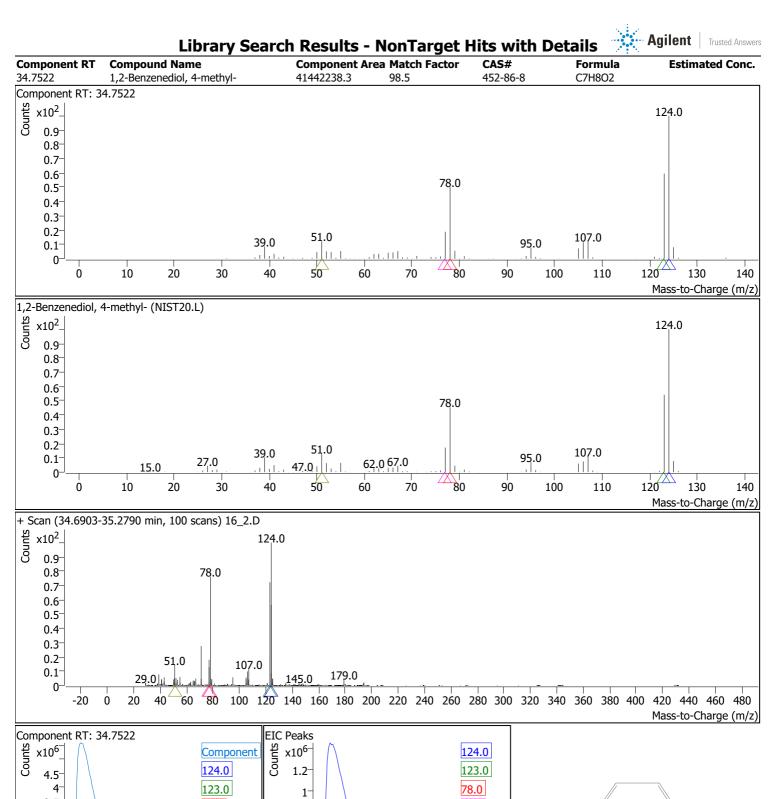
Acquisition Time (min)

34.3

2

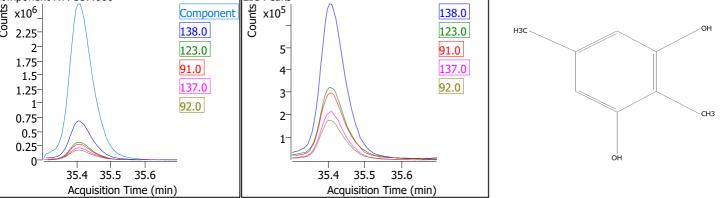
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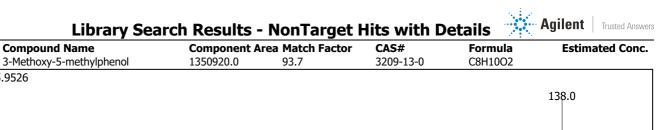
34.2 34.25 34.3

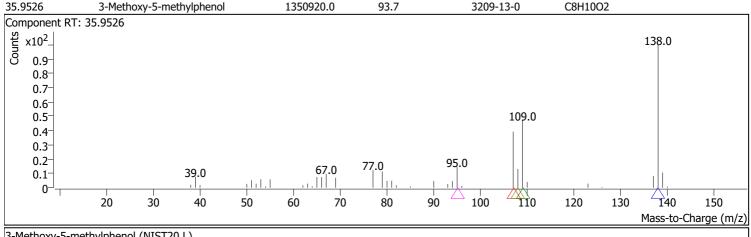


СНЗ

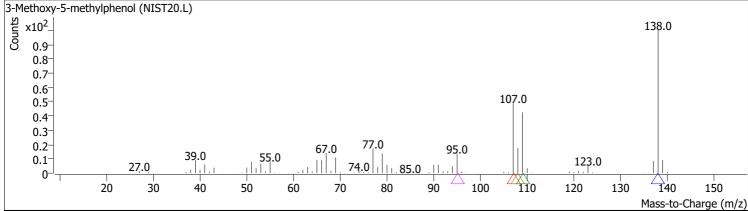
- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 1,3-Benzenediol, 2,5-dimethyl-488-87-9 35.4066 13804273.8 91.9 C8H10O2 Component RT: 35.4066 v10² 0.9 138.0 0.8 0.7 0.6 0.5 123.0 91.0 0.4 0.3 0.2 120.0 65.0 77.0 0.1 120 20 30 40 50 60 70 80 100 110 130 140 150 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 (35.3087-35.6952 min, 66 scans) 16_2.D st x10² 0.9 0.8 0.7 0.6 138.1 0.5 0.4^{-} 123.0 0.3 91.0 43.1 0.2 0.1 29.0 51.0 65.0 77.0 179.0 194.0 107.0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 35.4066 Counts st x10⁶. 2.25 x10⁵ 138.0 Component 138.0 123.0 2.25 нзс 2 123.0 5 91.0 1.75

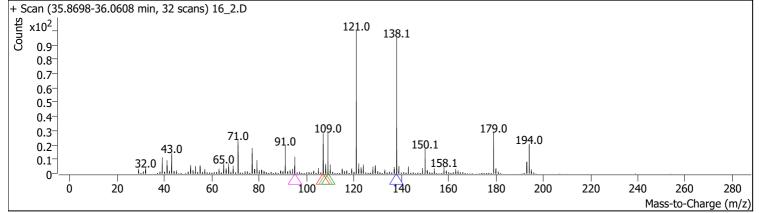


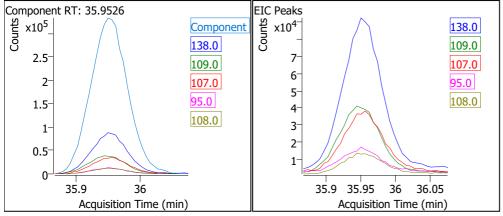


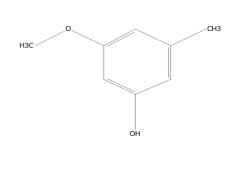


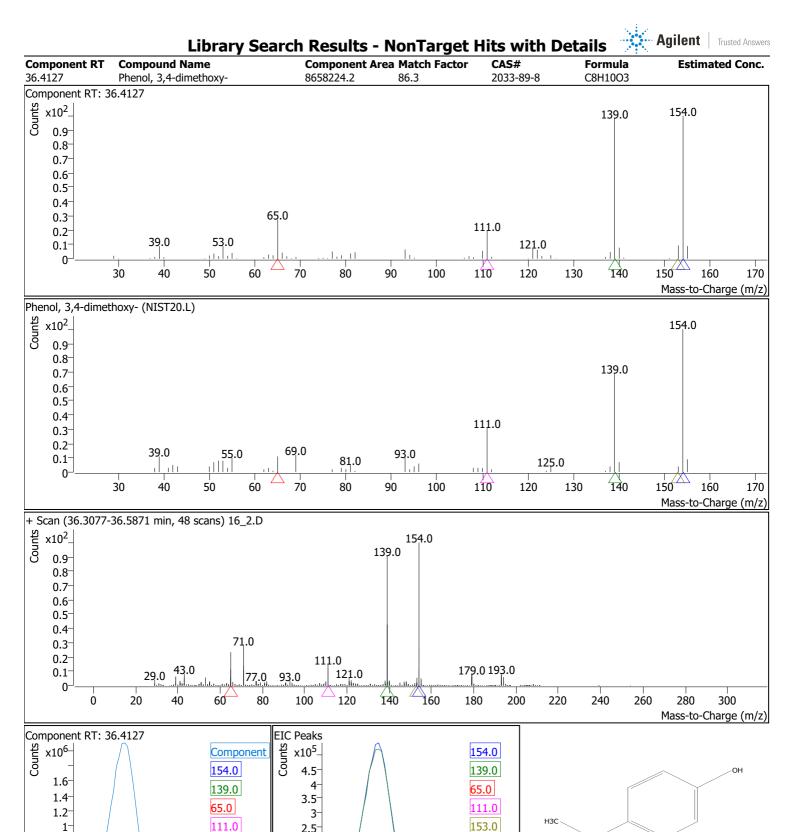
Component RT











36.5

Acquisition Time (min)

111.0

153.0

0.8

0.6

0.4

0.2

36.4

36.5

Acquisition Time (min)

2.5

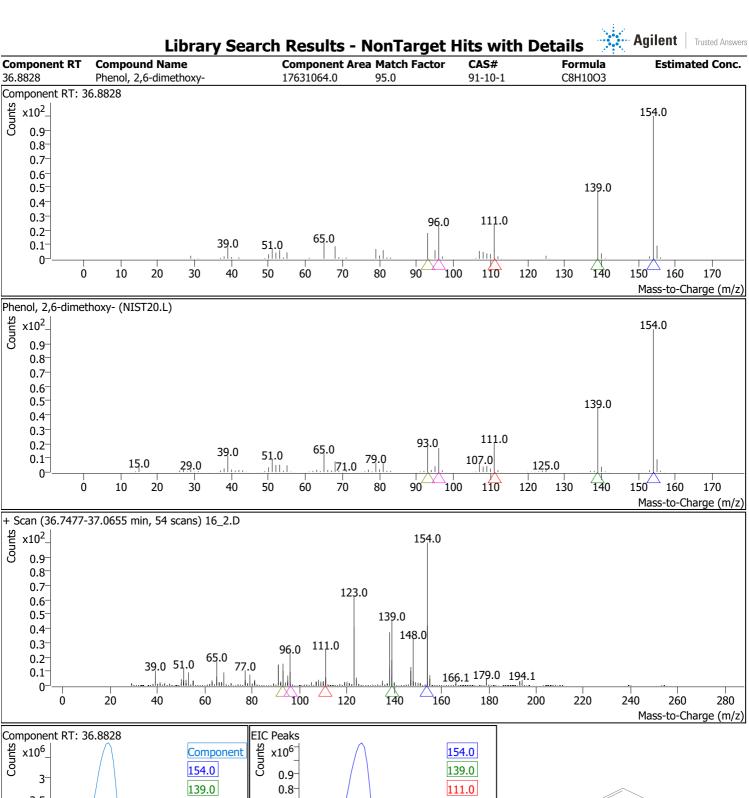
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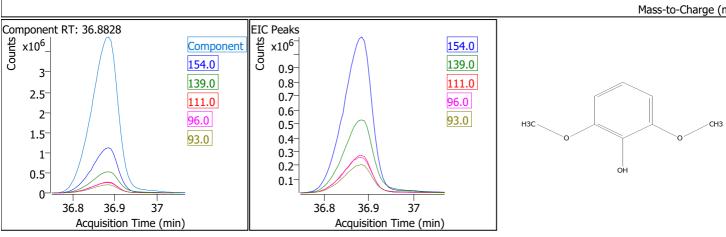
0.5

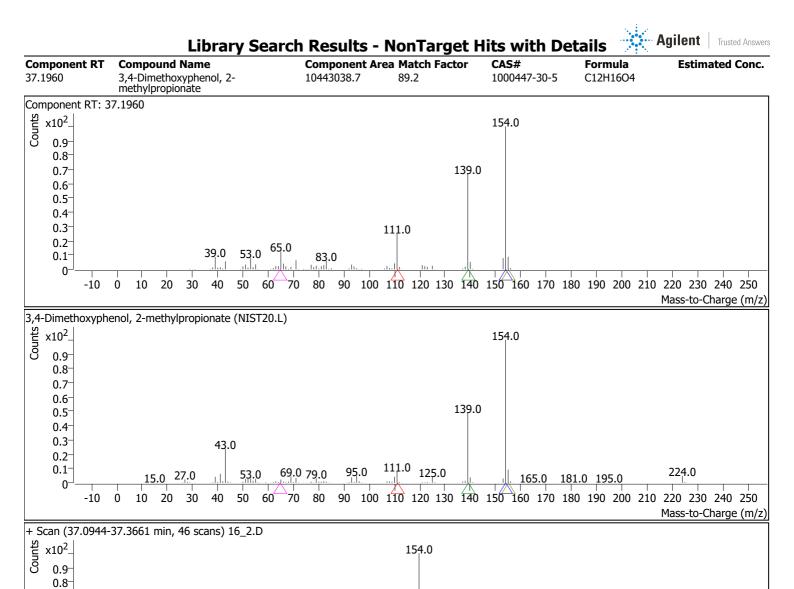
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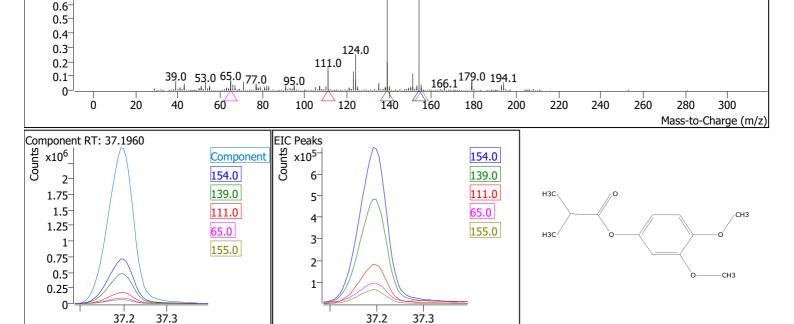
1

CH3









0.7

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, 4,5-dimethyl-527-55-9 37.4618 26210898.9 C8H10O2 Component RT: 37.4618 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 39.0 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 69.0 79.0 0.1 53.0 0 10 20 30 40 50 60 70 80 90 100 110 120 130 150 Mass-to-Charge (m/z) + Scan (37.3780-37.7169 min, 57 scans) 16_2.D st x10² 0.9 138.1 0.8 0.7 0.6 0.5 0.4 123.0 0.3 91.0 0.2 $^{39.0}$ $_{53.0}$ $^{65.0}$ $^{77.0}$ 0.1 162.0 179.0193.1 109.0 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: 37.4618 EIC Peaks Counts Counts x10⁶ x10⁶ 138.1 Component НЗС 138.1 137.0 137.0 123.0 1 123.0 91.0 0.8 3

91.0

92.0

2

1

37.4

37.5

37.6

Acquisition Time (min)

0.6

0.4

0.2

37.4

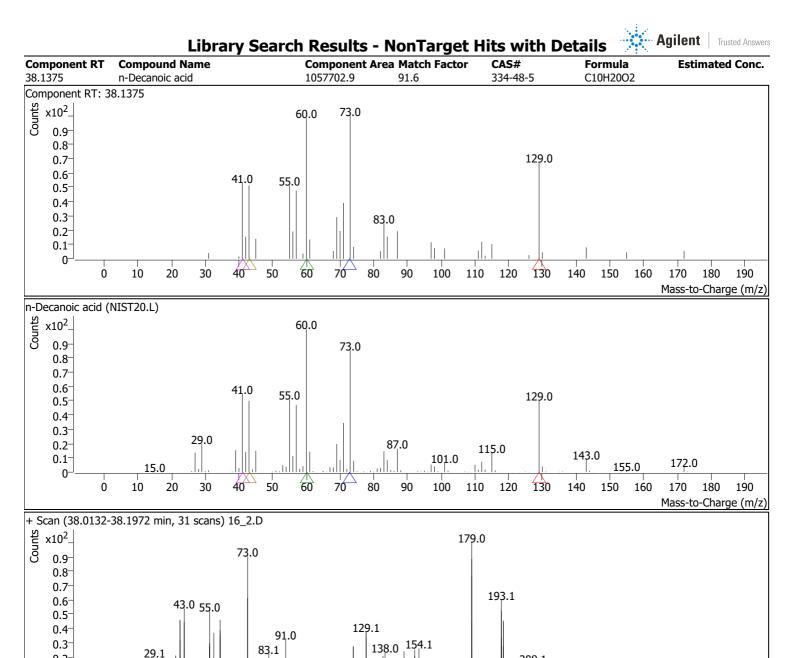
37.5

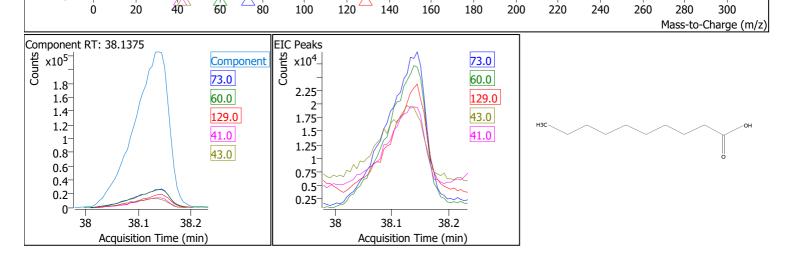
37.6

Acquisition Time (min)

92.0

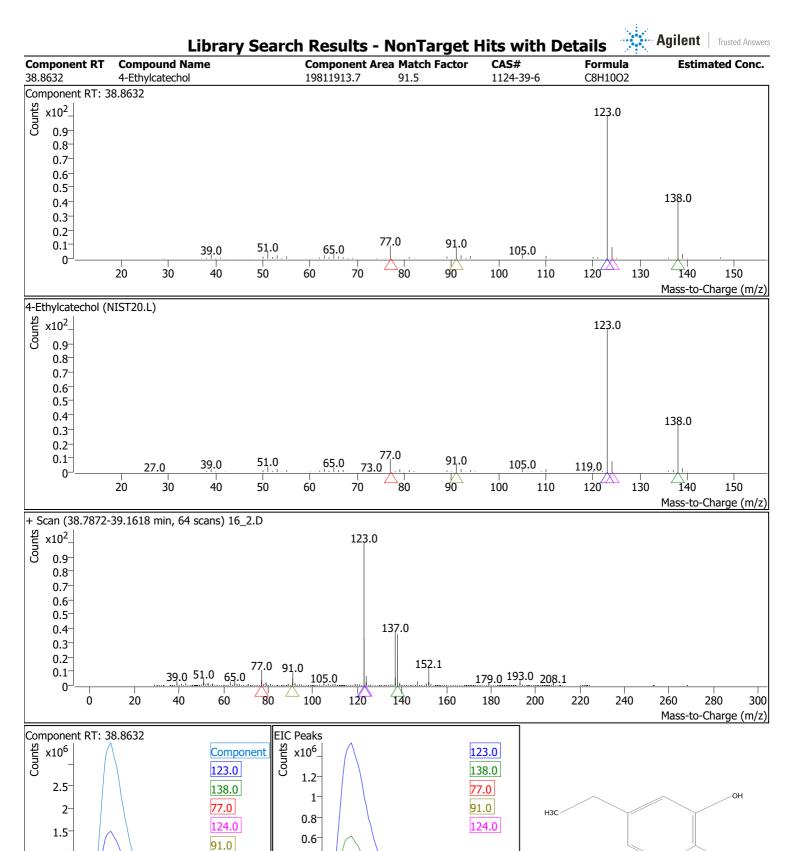
H3C





208.1

0.2





39

Acquisition Time (min)

39.1

0.4

0.2

1

0.5

38.8 38.9

39

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 39.8985 1,3-Benzenediol, 4,5-dimethyl-7537401.8 90.0 C8H10O2 Component RT: 39.8985 v10² 0.9 138.0 123.0 0.8 0.7 0.6 0.5 0.4 0.3 91.0 0.2 39.0 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 79.0 109.0 69.0 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 (39.8039-39.9883 min, 32 scans) 16_2.D st x10² 0.9 123.0 138.0 0.8 0.7 0.6 0.5 0.4 91.0 0.3 193.0 0.2 39.0 53.0 153,0 208.1 0.1 180.1 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 39.8985 Counts x10⁶ x10⁵ 138.0 Component НЗС 138.0 123.0 1.2 2.5 123.0 137.0 1 137.0 2 91.0

39.9

40

Acquisition Time (min)

40.1

92.0

H3C

0.8

0.6

0.4

0.2

39.9

40

Acquisition Time (min)

40.1

91.0

92.0

1.5

1

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 40.3364 5H-1-Pyrindine, 6,7-dihydro-4-amino-8467813.4 89.1 62732-46-1 C10H14N2 2,3-dimethyl-, hydrate Component RT: 40.3364 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 0.1 54.0 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 (40.2380-40.5234 min, 49 scans) 16_2.D st x10² 161.0 0.8 0.7^{-} 0.6 123.0 0.5 0.4 147.0 0.3 0.2 $39.0\ 51.0\ 65.0\ {\overset{77.0}{|}}\ {\overset{91.0}{|}}\ 105.0$ 193.0 138.0 0.1 208.1 0 60 80 100 160 Ó 20 40 120 140 180 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 40.3364 Counts Counts x10⁶x10⁵ 161.0 Component 162.0 161.0 **Н3С** 4 1.6 162.0 147.0 3.5 1.4 147.0 145.0 3 1.2 145.0 2.5 77.0

40.4

Acquisition Time (min)

40.5

2-

1 0.5

40.3

1.5

77.0

0.8

0.6 0.4

0.2

40.3

40.4

Acquisition Time (min)

нзс

NH2

- 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 40.6665 4-Methoxy-2,6-dimethylphenol 7991285.2 87.6 C9H12O2 Component RT: 40.6665 v10² 0.9 137.0 0.8 0.7 152.1 0.6 0.5 0.4 0.3 123.0 0.2 91.0 109.0 65.0 0.1 150 10 20 30 40 50 60 70 90 100 110 120 130 160 170 Mass-to-Charge (m/z) 4-Methoxy-2,6-dimethylphenol (NIST20.L) st x10²_ 0.9-137.0 152.0 0.8 0.7 0.6 0.5 0.4 0.3 0.2 81.0 91.0 109.0 39.0 53.0 67.0 0.1 123.0 0 10 20 30 40 50 60 70 80 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (40.5769-40.7553 min, 31 scans) 16_2.D st x10² 0.9 137.0 0.8 152.1 0.7^{-} 0.6 0.5 0.4 0.3 0.2 123.0 39.0 51.0 65.0 77.0 91.0 0.1 109.0 179.0 193.0 208.1 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 40.6665 EIC Peaks Counts x10⁶_ 1.6 x10⁵-137.0 Component нзс 137.0 152.1 1.6 1.4 152.1 123.0 3.5 1.2 138.1 123.0



77.0

H₃C

3

2

1

40.6

40.65

40.7

Acquisition Time (min)

2.5

1.5

0.5

138.1

77.0

1

0.8

0.6

0.4

0.2

40.6

40.65

40.7

Acquisition Time (min)

-CH3

- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details** CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 700-13-0 40.8429 1,4-Benzenediol, 2,3,5-trimethyl-15103226.8 85.9 C9H12O2 Component RT: 40.8429 Counts $x10^{2}$ 152.1 0.9 137.0 0.8 0.7 0.6 0.5 0.4 0.3 91.0 0.2 77.0 106.0 0.1 10 20 30 50 60 70 90 100 110 120 130 150 160 170 Mass-to-Charge (m/z) 1,4-Benzenediol, 2,3,5-trimethyl- (NIST20.L) Counts x10²_ 0.9 152.0 0.8 0.7 0.6 137.0 0.5 0.4 0.3 0.2 109.0 43.0 0.1 91.0 123.0 27.0 53.0 67.0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (40.7553-41.0229 min, 46 scans) 16_2.D st x10² 0.9 152.1 137.0 0.8 0.7 0.6 0.5 168.1 0.4 0.3 0.2 107.0 125.0 39.0 53.0 65.0 0.1 179.0 193.1 140 Ó 20 40 60 80 100 120 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) EIC Peaks Component RT: 40.8429 Counts x10⁶ Counts x10⁵ 152.1 Component 152.1 137.0 нзс 2.5 6 137.0 151.1 5



40.9

Acquisition Time (min)

41

91.0

77.0

2

1.5

1

0.5

40.8

40.9

Acquisition Time (min)

41

151.1

91.0

77.0

4

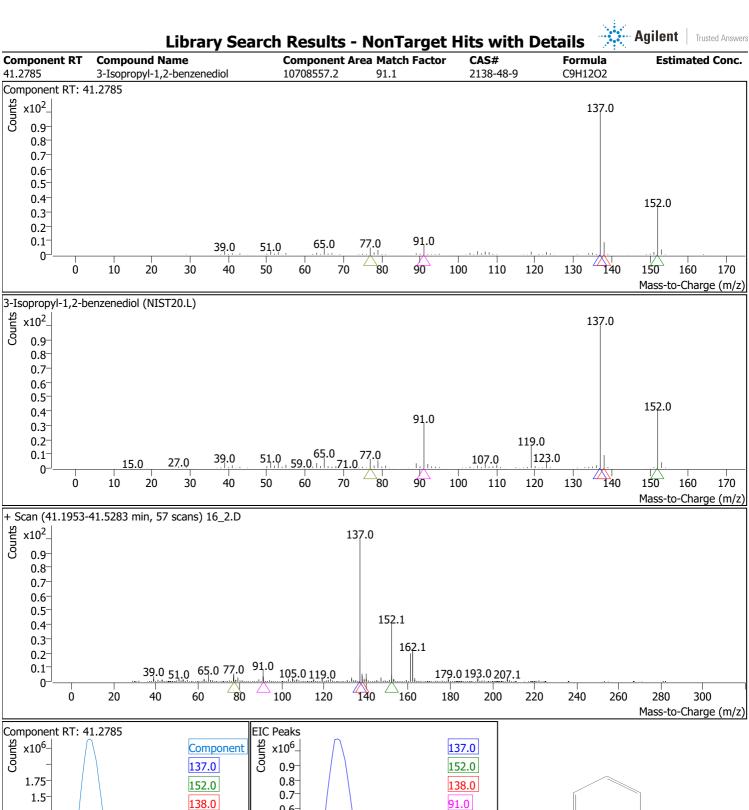
3-

2

40.8

CH3

CH3



0.5

0.4

0.3

91.0

77.0

1.25

0.75

0.5

0.25

1-

--- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 5H-1-Pyrindine, 6,7-dihydro-4-amino-2,3-dimethyl-, hydrate 41.4376 5961511.5 86.5 62732-46-1 C10H14N2 Component RT: 41.4376 Counts x10²_ 162.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 0.2^{-} 147.0 119.0 133.0 0.1 105.0 0-150 10 20 30 40 50 60 100 110 120 130 140 160 170 180 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 (41.3321-41.6041 min, 46 scans) 16_2.D st x10² 0.9 162.1 0.8 0.7 0.6 137.0 0.5 0.4 0.3 152.1 0.2 $39.0_{11.51.0}$ $65.0_{11.0}$ $91.0_{11.0}$ 179.0 193.0 207.1 0.1 0 60 120 Ó 20 40 80 100 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 41.4376 Counts Counts x10⁶ x10⁵-162.0 Component 161.0 162.0 **Н3С** 3-1 161.0 147.0 2.5 8.0 147.0 163.0 2-163.0 91.0

41.5

Acquisition Time (min)

1.5

1

41.4

0.5

91.0

0.6

0.4

0.2

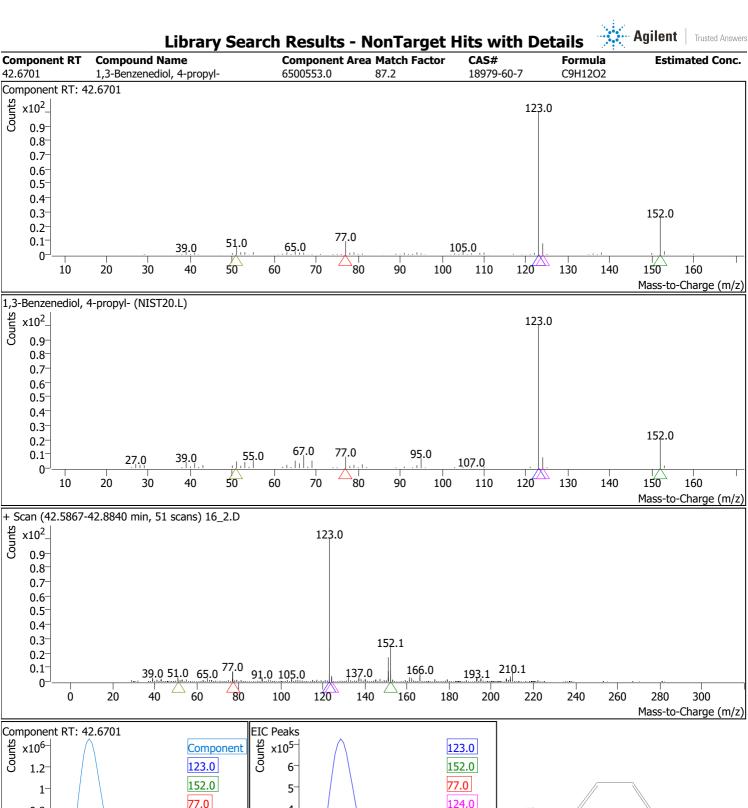
41.4

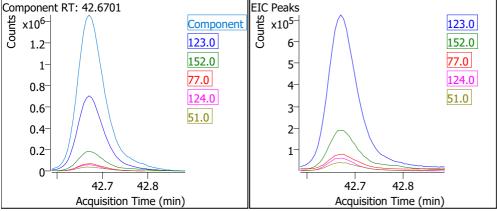
41.5

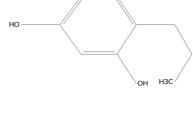
Acquisition Time (min)

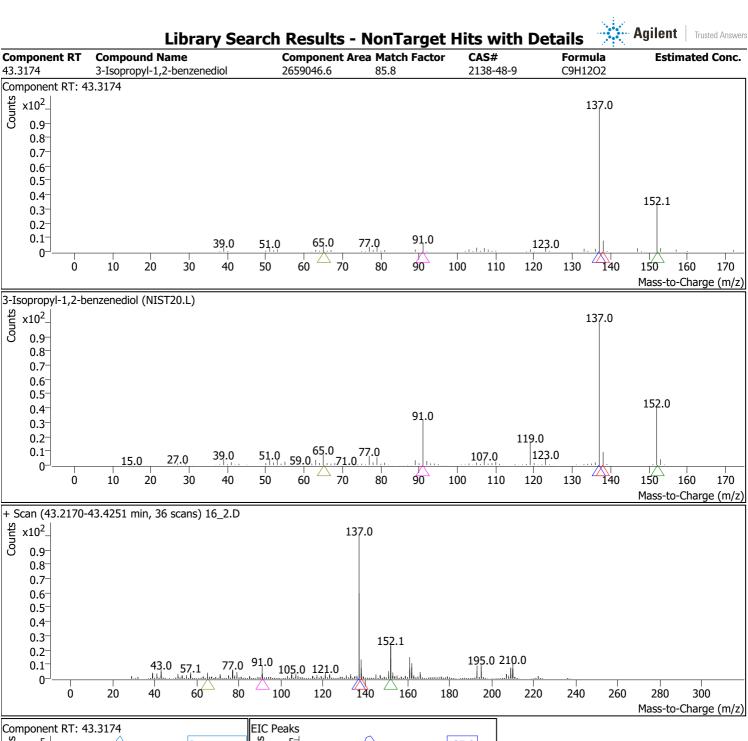
нзс

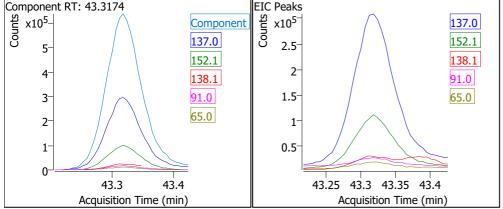
NH2

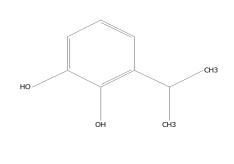












- Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 2138-48-9 43.8823 3-Isopropyl-1,2-benzenediol 3406173.7 87.9 C9H12O2 Component RT: 43.8823 v10² 0.9 137.0 0.8 0.7 0.6 152.1 0.5 0.4 0.3 0.2 91.0 0.1 65.0 106.0 90 150 10 20 30 40 50 60 70 100 110 120 130 160 170 Mass-to-Charge (m/z) 3-Isopropyl-1,2-benzenediol (NIST20.L) Counts x10²_ 0.9 137.0 0.8 0.7 0.6 0.5 152.0 0.4 91.0 0.3 0.2 119.0 0.1 123.0 39.0 107.0 0 10 20 30 60 70 90 100 110 120 130 140 150 160 170 Mass-to-Charge (m/z) + Scan (43.8116-43.9483 min, 24 scans) 16_2.D st x10² 0.9 137.0 0.8 152.1 0.7 0.6 0.5 0.4 0.3 0.2 166.1 0.1 107.0 123.0 53.0 65.0 193.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 Mass-to-Charge (m/z) Component RT: 43.8823 **EIC Peaks** st x10⁵ Supply x10⁵-137.0 Component 137.0 152.1 2.5 6 152.1 91.0 2



43.9

Acquisition Time (min)

77.0

138.1

5

4

3

2

1

43.9

Acquisition Time (min)

91.0

138.1

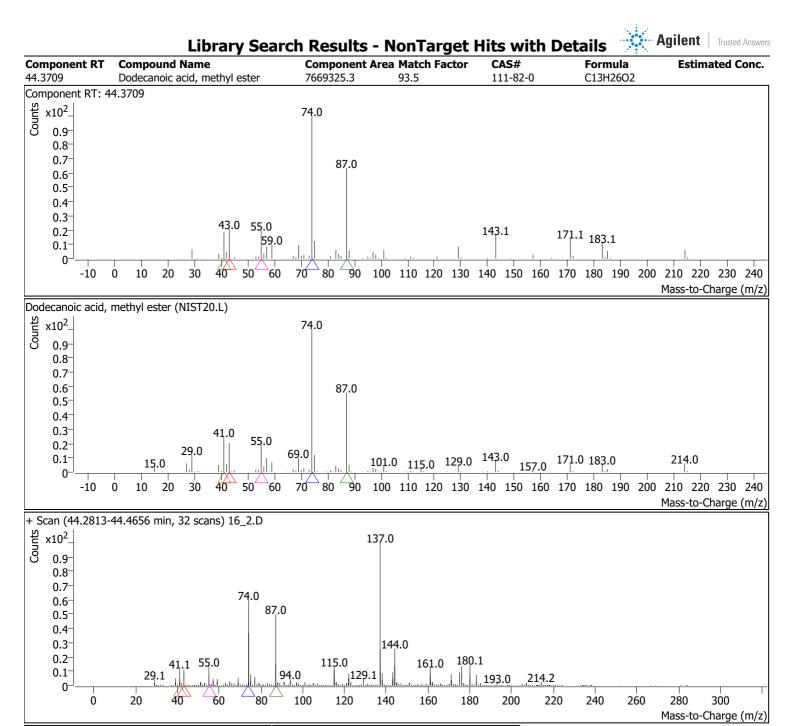
77.0

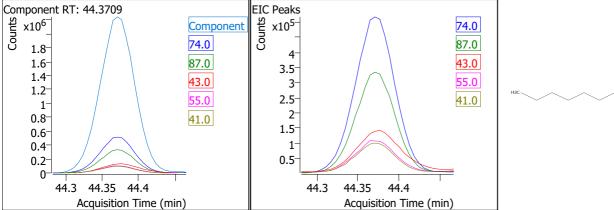
1.5

1

0.5

CH3





... Agilent Trusted Answers **Library Search Results - NonTarget Hits with Details Compound Name Component Area Match Factor** CAS# **Component RT Formula Estimated Conc.** 2-Propanone, 1-(4-hydroxy-3-4704510.9 44.3939 87.0 2503-46-0 C10H12O3 methoxyphenyl)-Component RT: 44.3939 Counts x10²_ 137.0 0.9 8.0 0.7 0.6 0.5 0.4 0.3 180.0 0.2^{-} 122.1 0.1 65.0 51.0 0-120 180 20 30 40 50 60 70 80 100 110 130 140 150 160 170 190 200 Mass-to-Charge (m/z) 2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)- (NIST20.L) Counts $x10^{2}$ 137.0 0.9 0.8 0.7 0.6 180.0 0.5 0.4 122.0 0.3 0.2 0.1 66.0 85.0⁹1.0 99.0 107.0 131.0 147.0 164.0 173.0 0 100 180 20 30 50 60 80 90 110 120 130 140 150 160 170 190 200 Mass-to-Charge (m/z) + Scan (44.2993-44.4954 min, 33 scans) 16_2.D x10². 137.0 0.9 0.8 0.7 0.6 87.0 0.5 161.0 176.1 0.4 144.0 0.3 0.2 115.0 41.1 55.0 0.1 129.1 29.1 94.0 214.2 0 100 140 180 300 0 20 40 60 80 120 160 200 220 240 260 280 Mass-to-Charge (m/z) **EIC Peaks** Component RT: 44.3939 Counts Counts x10⁶ x10⁵ 137.0 Component 180.0 137.0 0.9 4.5 180.0 122.1 0.8 3.5 0.7 122.1 138.1 0.6 3

44.4

Acquisition Time (min)

94.0

44.5

138.1

94.0

0.5⁻ 0.4⁻

0.3

0.2

0.1

44.4

44.5

Acquisition Time (min)

2.5

1.5

0.5

2

1

··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 44.8750 Benzeneethanethioic acid, S-methyl 678705.3 86.6 5925-74-6 C9H10OS ester Component RT: 44.8750 x10²_ 91.0 0.9 8.0 166.1 0.7 0.6 0.5 0.4 119.0 0.3 0.2^{-} 0.1 55 60 65 75 80 85 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 170 175 Mass-to-Charge (m/z) Benzeneethanethioic acid, S-methyl ester (NIST20.L) Counts $x10^{2}$ 91.0 0.9 0.8 0.7 0.6 0.5 166.0 0.4 0.3 0.2 65.0 119.0 0.1 75.0 138.0 100 105 110 115 120 125 130 135 140 145 150 155 160 165 170 175 65 75 80 85 95 Mass-to-Charge (m/z) + Scan (44.7398-45.0186 min, 47 scans) 16_2.D x10². 137.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 161.0 0.2 39.0 51.0 65.0 ^{77.0} 91.0₁03.0 176.1 0.1 123.0 150.1 207.1 n 40 120 300 Ó 20 60 80 100 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) Component RT: 44.8750 **EIC Peaks** Counts Counts 166.1 x10⁵x10⁵-Component 91.0 91.0 1.2 0.8 166.1 119.0 1 0.7 95.0 119.0 0.6 0.8



44.9

Acquisition Time (min)

93.0

93.0

95.0

0.6

0.4

0.2

44.8

44.9

Acquisition Time (min)

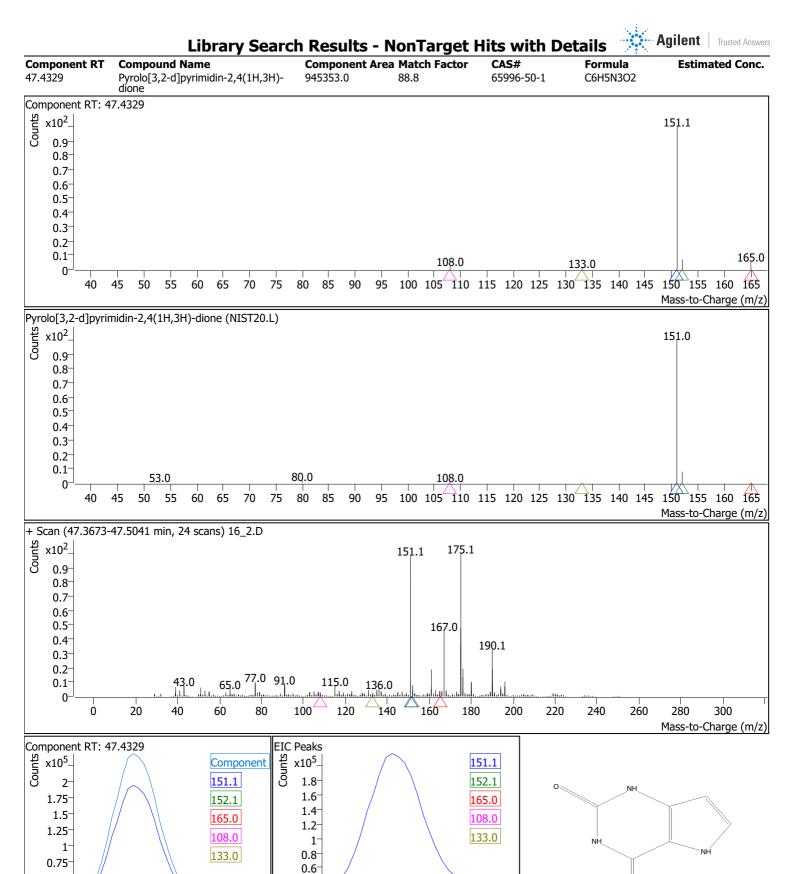
0.5

0.4

0.3

0.1

44.8



47.45

Acquisition Time (min)

0.4

0.2

47.4

0.5

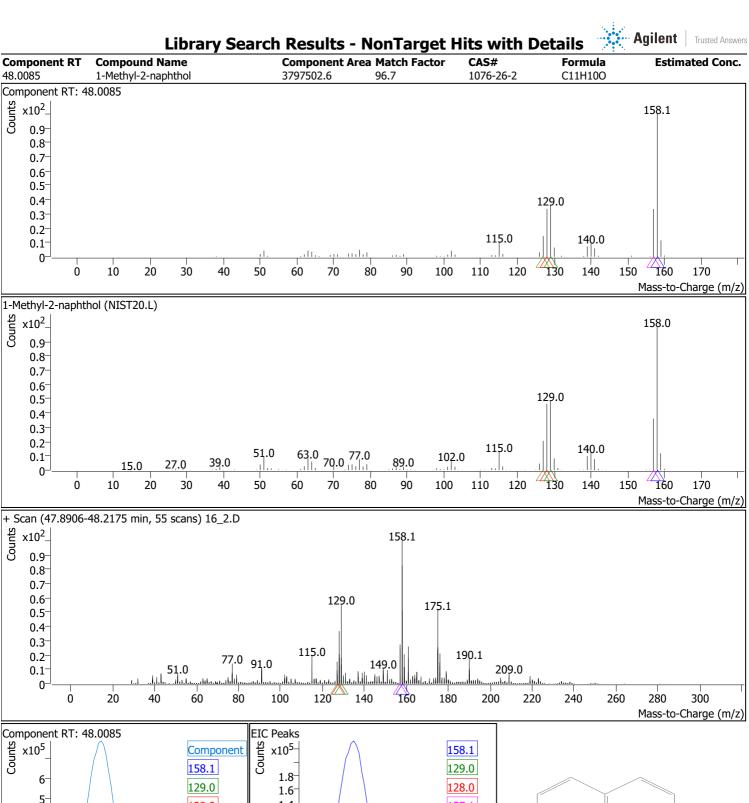
47.4

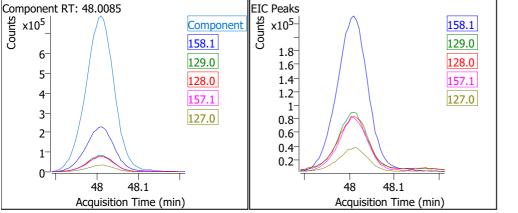
47.45

Acquisition Time (min)

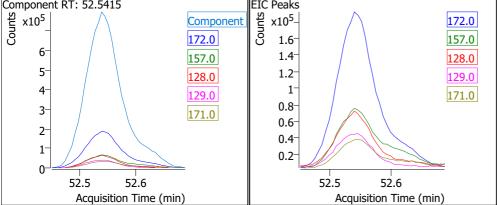
47.5

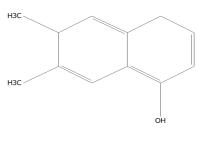
0.25





··· Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 52.5415 1-Naphthol, 6,7-dimethyl-3585147.1 88.5 31776-14-4 C12H12O Component RT: 52.5415 y x10² 0.9 172.0 0.8 0.7 0.6 0.5 0.4 157.0 128.0 0.3 0.2 115.0 141.0 163.0 0.1 0 160 10 20 30 40 50 60 70 80 100 110 120 130 140 150 180 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 (52.4512-52.6890 min, 41 scans) 16_2.D st x10² 0.9 172.1 0.8 0.7^{-} 0.6 0.5 0.4 0.3 137.0 0.2 115.0 65.077.0 189.1 207.1 0.1 39.0 105.0 0 160 Ó 20 40 60 80 100 120 140 180 200 220 240 260 280 300 320 340 Mass-to-Charge (m/z) Component RT: 52.5415 EIC Peaks Counts Counts x10⁵– 172.0 Component 172.0 157.0 1.6 Н3С 6 1.4 157.0 128.0 5 1.2





Library Search Results - NonTarget Hits with Details CAS# **Component Area Match Factor Component RT Compound Name Formula Estimated Conc.** 57-10-3 60.1431 n-Hexadecanoic acid 3965245.8 89.7 C16H32O2 Component RT: 60.1431 v10² 0.9 73.0 0.8 60.0 43.0 0.7^{-} 55.0 129.0 0.6 256.1 0.5 0.4 0.3 0.2 0.1 0 20 40 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) n-Hexadecanoic acid (NIST20.L) st x10²_ 0.9-73.0 0.8 60.0 0.7 43.0 129.0 256.0 0.6 0.5 213.0 0.4 83.0 0.3 97.0 115.0 157.0 171.0 185.0 0.2 29.0 227.0 143.0 199.0 0.1 220.0 239.0 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 Mass-to-Charge (m/z) + Scan (60.0383-60.3297 min, 50 scans) 16_2.D St x10² 0.9 73.0 0.8 43.1 0.7 0.6 129.1 0.5 0.4^{-} 256.2 83.1 0.3 141.1 97.1 199.1 29.1 241.2 0.2 0.1 0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 Mass-to-Charge (m/z) EIC Peaks Component RT: 60.1431 Counts Counts x10⁴ 73.0 Component 73.0 43.0 7 5 60.0 60.0

55.0

57.0

6

5

4

3

2⁻

60.1

60.2

Acquisition Time (min)

60.3

43.0

55.0

57.0

3

2-

60.1

60.2

Acquisition Time (min)

60.3

--- Agilent | Trusted Answers **Library Search Results - NonTarget Hits with Details Component Area Match Factor** CAS# **Component RT Compound Name Formula Estimated Conc.** 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-60.3688 3482413.0 89.0 1000197-14-1 C19H28 Component RT: 60.3688 $x10^{2}$ 159.0 241.0 0.9 0.8 0.7 0.6 0.5 0.4 185.0 256.0 0.3 117.0 0.2 143.0 0.1 0 40 140 160 180 200 220 240 260 0 20 60 80 100 120 280 Mass-to-Charge (m/z) 4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro- (NIST20.L) $x10^{2}$ 241.0 0.9 0.8 0.7 159.0 0.6 0.5 0.4 256.0 185.0 0.3 0.2-213.0 129.0 143.0 199.0 0.1 55.0 91.0 115.0 171.0 69.0 225.0 0 240 20 100 140 220 60 80 120 160 180 200 260 280 Mass-to-Charge (m/z) + Scan (60.2821-60.4579 min, 30 scans) 16_2.D Counts x10²_ 241.2 0.9 159.1 0.8 0.7 0.6 0.5 0.4 185.1 0.3 256.2 115.0 199.1 0.2 141.0 43.0 213.1 0.1 91.0 160 180 240 260 340 360 380 0 20 40 60 80 100 120 140 200 220 280 300 320 400 Mass-to-Charge (m/z) Component RT: 60.3688 EIC Peaks Counts x10⁵x10⁵ 159.0 Component СНЗ 159.0 241.0 1.2 241.0 185.0 6 1 5 185.0 256.0 0.8 242.0 256.0 4

60.4

Acquisition Time (min)

60.5

0.6

0.4

0.2

242.0

3

2

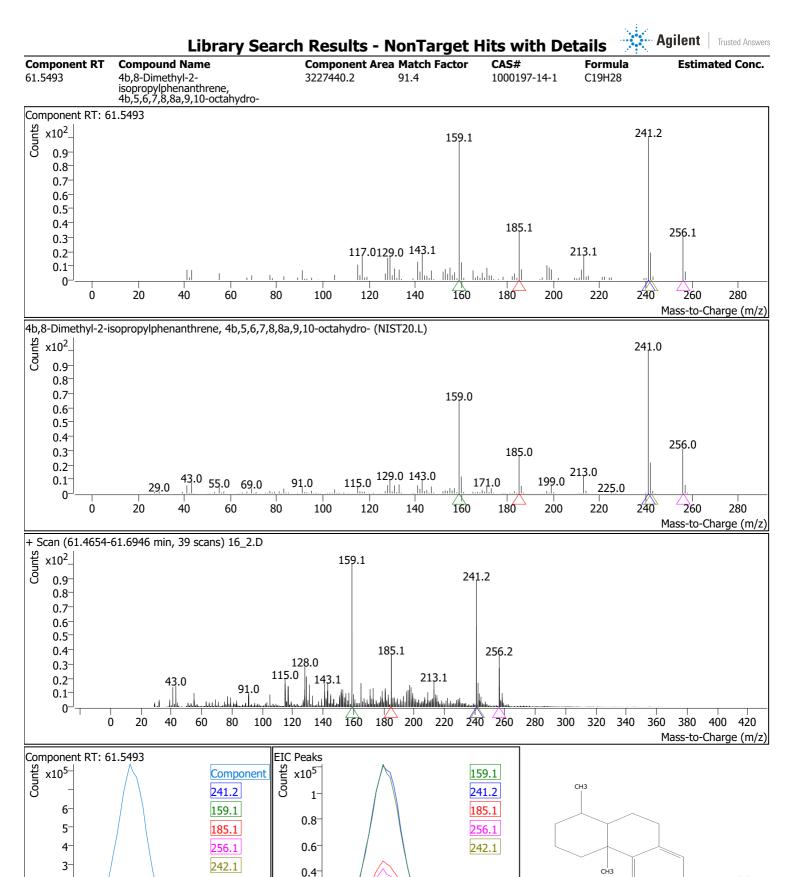
1

60.4

Acquisition Time (min)

60.5

СНЗ



Acquisition Time (min)

0.2

61.5

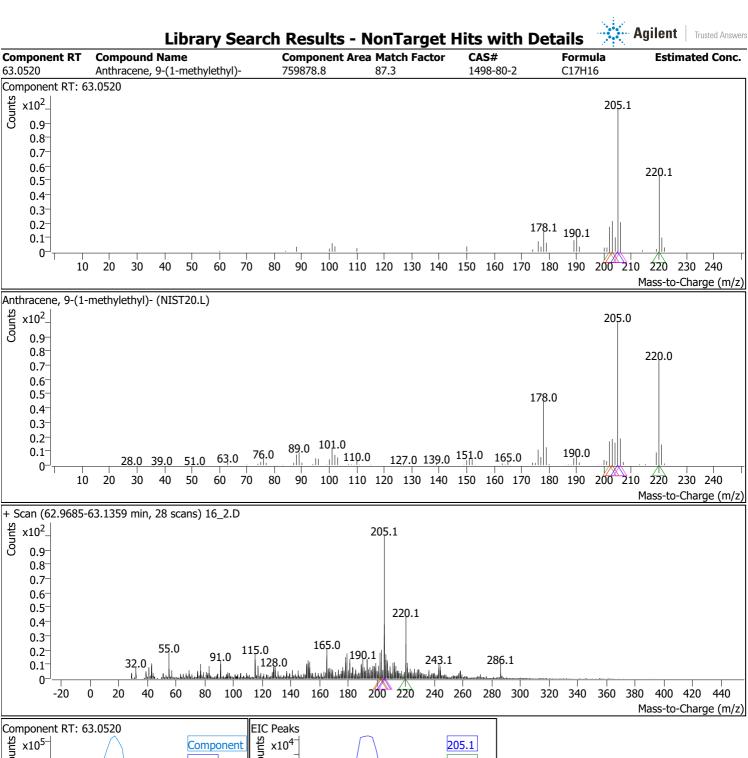
2

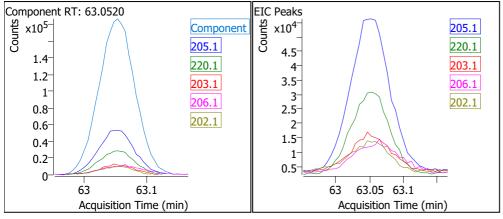
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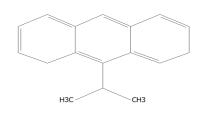
61.5

61.6

Acquisition Time (min)

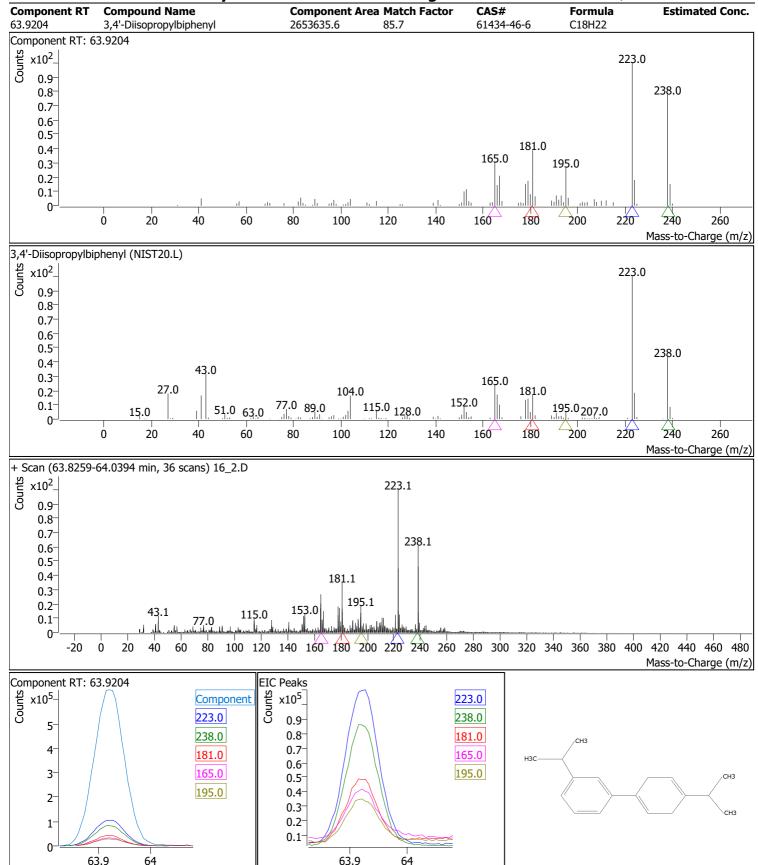












Acquisition Time (min)

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.** 31081-18-2 64.3744 Nonane, 3-methyl-5-propyl-1408141.2 89.8 C13H28 Component RT: 64.3744 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 70 10 20 30 50 80 90 100 110 130 140 150 160 170 180 190 200 120 Mass-to-Charge (m/z) Nonane, 3-methyl-5-propyl- (NIST20.L) Counts x10²_ 0.9 57.0 71.0 0.8 0.7 43.0 0.6 0.5 85.0 0.4 0.3 29.0 0.2 0.1 99.0 112.0 127.0 141.0 184.0 70 10 20 30 50 60 80 90 100 110 120 130 140 150 160 170 180 190 200 Mass-to-Charge (m/z) + Scan (64.3003-64.4503 min, 26 scans) 16_2.D St x10² 0.9 57.1 0.8 0.7 197.1 0.6 71.1 0.5 85.1 43.1 0.4^{-} 0.3 254.2 165.0 0.2 99.1 141.1 239.2 29.1 0.1 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 -20 Mass-to-Charge (m/z) Component RT: 64.3744 **EIC Peaks** Counts Counts x10⁵ x10⁴ 57.0 Component

64.35

64.4

Acquisition Time (min)

64.45

57.0

71.0

43.0

85.0

41.0

5

3

2-

3

2

1 0.5 0

64.35

64.4

Acquisition Time (min)

2.5

1.5

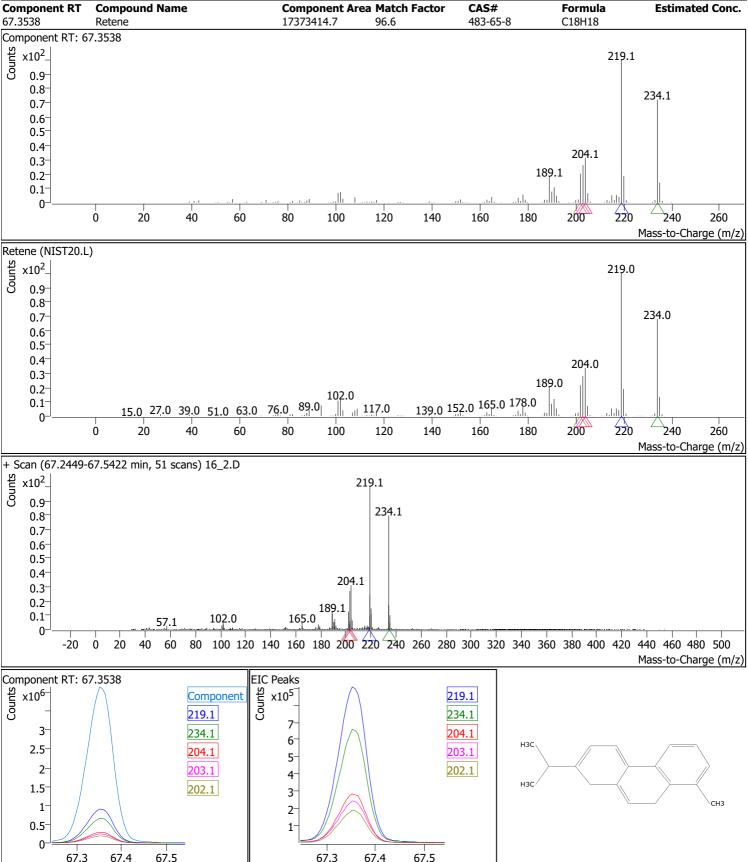
71.0

43.0

85.0

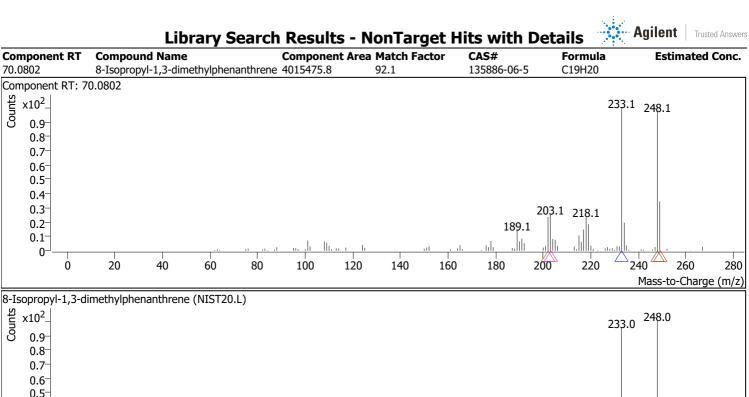
41.0

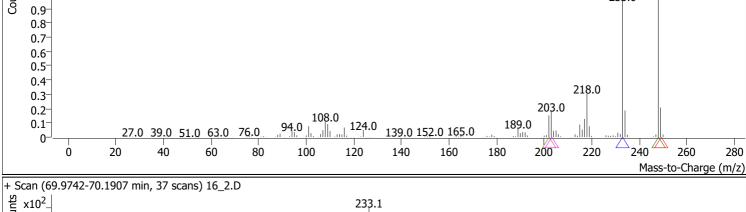


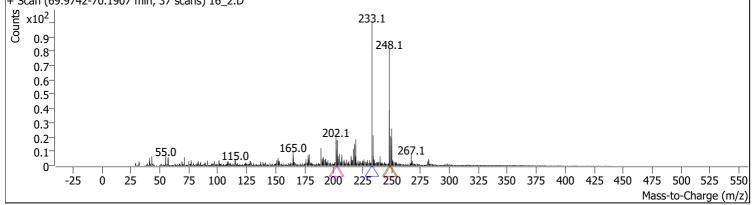


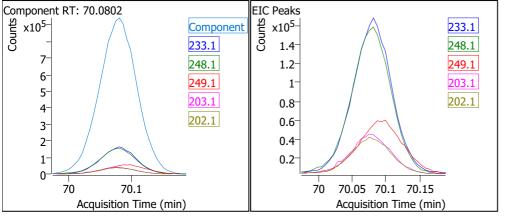
Acquisition Time (min)

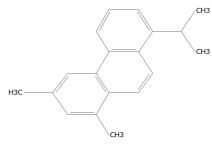
Acquisition Time (min)

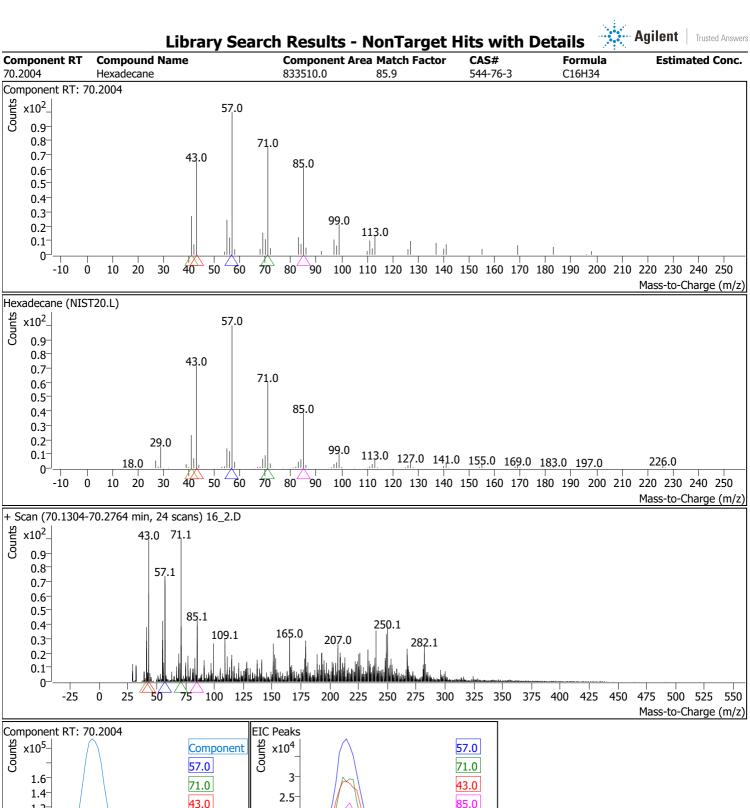


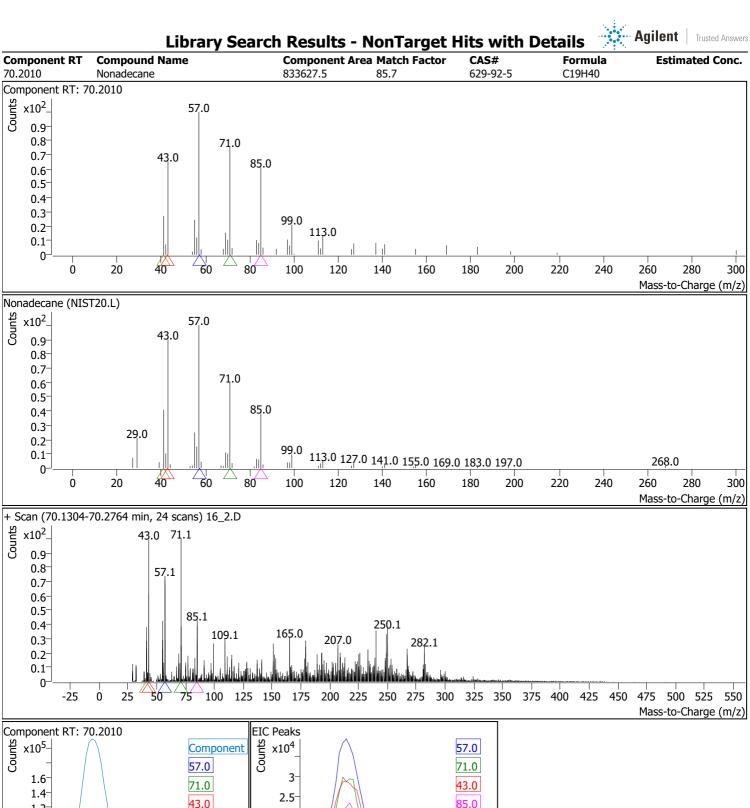


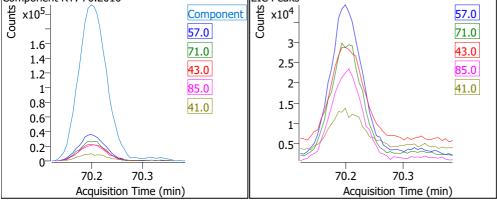






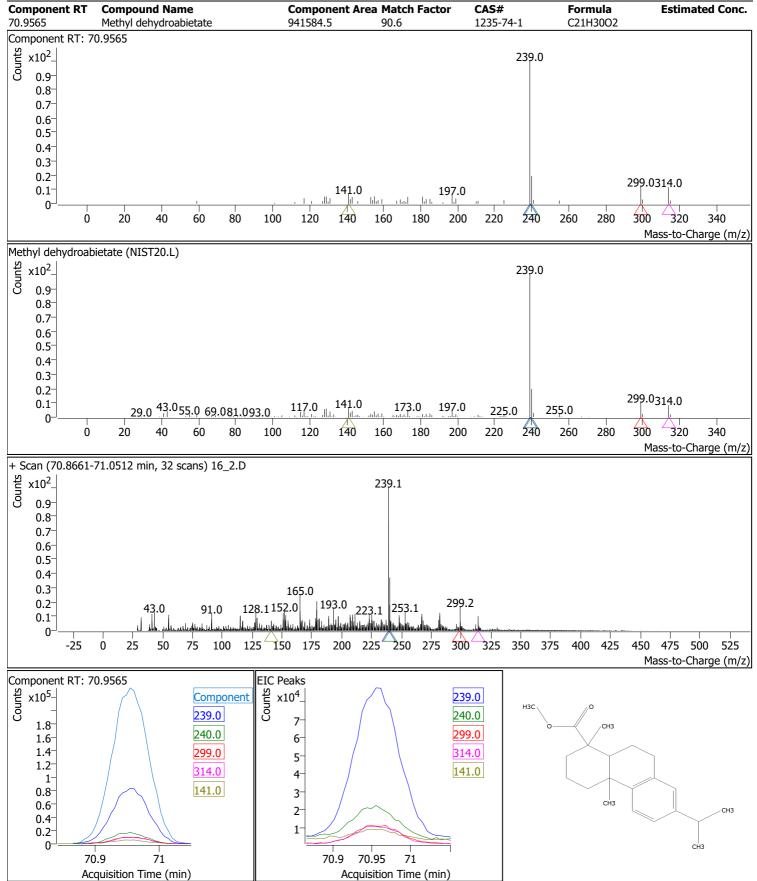












Compound Name Component RT Component Area Match Factor CAS# **Formula Estimated Conc.** 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]-73.6828 8770907.8 5155-70-4 C20H28O2 Component RT: 73.6828 $x10^{2}$ 239.0 285.0 0.9 0.8 0.7 0.6 0.5 0.4^{-} 197.0 300.0 0.3 141.0 0.2 0.1 300 200 240 280 320 0 20 40 60 80 100 120 140 160 180 220 260 Mass-to-Charge (m/z) 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1S-(1.alpha.,4a.alpha.,10a.beta.)]- (NIST20.L) Counts x10²_ 285.0 0.9 0.8 239.0 0.7° 0.6 0.5 0.4 300.0 0.3 197.0 43.0 0.2 141.0 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 (73.5652-73.8629 min, 51 scans) 16_2.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 43.0 91.0 115.0 179.0 0.1 25 200 225 250 275 [^]300 325 350 375 400 425 450 475 500 525 550 575 50 75 100 125 150 175 -25 Mass-to-Charge (m/z) Component RT: 73.6828 EIC Peaks y x10⁶ x10⁵ 285.0 Component 239.0 239.0 1.8 СНЗ 285.0 197.0 1.6 1.2 1.4 197.0 300.0 1 1.2 300.0 141.0 0.8 1 141.0 0.6 0.8

73.7

73.8 Acquisition Time (min)

0.6

0.4

0.2

73.6

0.4

 0.2^{-}

73.6

73.7

73.8

Acquisition Time (min)

73.9

