

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111422\
 Data File : VN075263.D
 Acq On : 14 Nov 2022 14:16
 Operator : JC\MD
 Sample : N5417-02
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1732

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
 Title : SW846 8260

Signal : TIC: VN075263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	34	41	50	rBV3	7157	20934	2.11%	0.313%
2	2.795	121	126	128	rBV	7400	12295	1.24%	0.184%
3	2.954	149	153	156	rBV	16043	22838	2.31%	0.342%
4	3.089	174	176	186	rVB7	20840	42392	4.28%	0.635%
5	5.265	536	546	556	rBV4	5695	17120	1.73%	0.256%
6	5.500	576	586	598	rVB2	4331	13749	1.39%	0.206%
7	6.724	787	794	806	rVB3	6754	20157	2.04%	0.302%
8	8.171	1029	1040	1044	rBV	158102	386637	39.04%	5.787%
9	8.224	1044	1049	1060	rVB	272327	587082	59.27%	8.788%
10	8.577	1100	1109	1119	rBV	162479	365328	36.89%	5.468%
11	9.035	1180	1187	1190	rBV2	6043	10261	1.04%	0.154%
12	9.100	1190	1198	1220	rVB	400550	801068	80.88%	11.991%
13	10.565	1439	1447	1455	rVV	550864	990447	100.00%	14.826%
14	11.300	1566	1572	1579	rVB5	11769	24100	2.43%	0.361%
15	11.865	1660	1668	1678	rBV	520534	897618	90.63%	13.436%
16	12.071	1697	1703	1714	rVB2	22431	46597	4.70%	0.697%
17	12.400	1751	1759	1764	rVB3	9778	20424	2.06%	0.306%
18	12.565	1782	1787	1794	rBV2	15813	26159	2.64%	0.392%
19	12.847	1828	1835	1844	rVB	382449	670607	67.71%	10.038%
20	12.947	1846	1852	1857	rBV2	17509	28851	2.91%	0.432%
21	13.088	1871	1876	1879	rBV2	8614	13112	1.32%	0.196%
22	13.159	1883	1888	1894	rVB2	14708	24639	2.49%	0.369%
23	13.623	1961	1967	1974	rBV3	23304	41402	4.18%	0.620%
24	13.794	1989	1996	2003	rBV	495912	859940	86.82%	12.872%
25	13.870	2003	2009	2017	rVB	101289	173777	17.55%	2.601%
26	14.106	2044	2049	2053	rBV5	14291	24261	2.45%	0.363%
27	14.329	2079	2087	2091	rVB6	6658	17625	1.78%	0.264%
28	14.441	2099	2106	2114	rBV9	5377	14244	1.44%	0.213%
29	14.559	2119	2126	2132	rVV2	31570	60929	6.15%	0.912%
30	14.629	2134	2138	2141	rVV4	12868	21284	2.15%	0.319%
31	14.753	2153	2159	2163	rVB5	10931	20076	2.03%	0.301%
32	14.847	2170	2175	2178	rBV6	5803	10203	1.03%	0.153%
33	14.959	2186	2194	2200	rBV4	13106	27697	2.80%	0.415%
34	15.035	2202	2207	2211	rVV4	14526	27509	2.78%	0.412%
35	15.088	2211	2216	2224	rVB9	14369	41301	4.17%	0.618%
36	15.276	2242	2248	2251	rVV4	5727	10334	1.04%	0.155%

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37	15.312	2251	2254	2261	rVB6	7395	15504	1.57%	0.232%
38	15.435	2271	2275	2277	rVV5	8610	13497	1.36%	0.202%
39	15.594	2297	2302	2306	rBV5	11894	25968	2.62%	0.389%
40	15.741	2322	2327	2332	rBV3	17960	31463	3.18%	0.471%
41	15.829	2338	2342	2353	rVB5	16662	38434	3.88%	0.575%
42	15.929	2353	2359	2360	rBV5	7984	13628	1.38%	0.204%
43	16.011	2368	2373	2378	rVB6	9222	17173	1.73%	0.257%
44	16.106	2385	2389	2395	rBV7	8633	20886	2.11%	0.313%
45	16.400	2434	2439	2447	rBV9	8856	23220	2.34%	0.348%
46	16.553	2460	2465	2471	rVB7	11389	23289	2.35%	0.349%
47	16.629	2471	2478	2485	rBV8	10829	29451	2.97%	0.441%
48	16.711	2485	2492	2496	rBV6	14928	35176	3.55%	0.527%

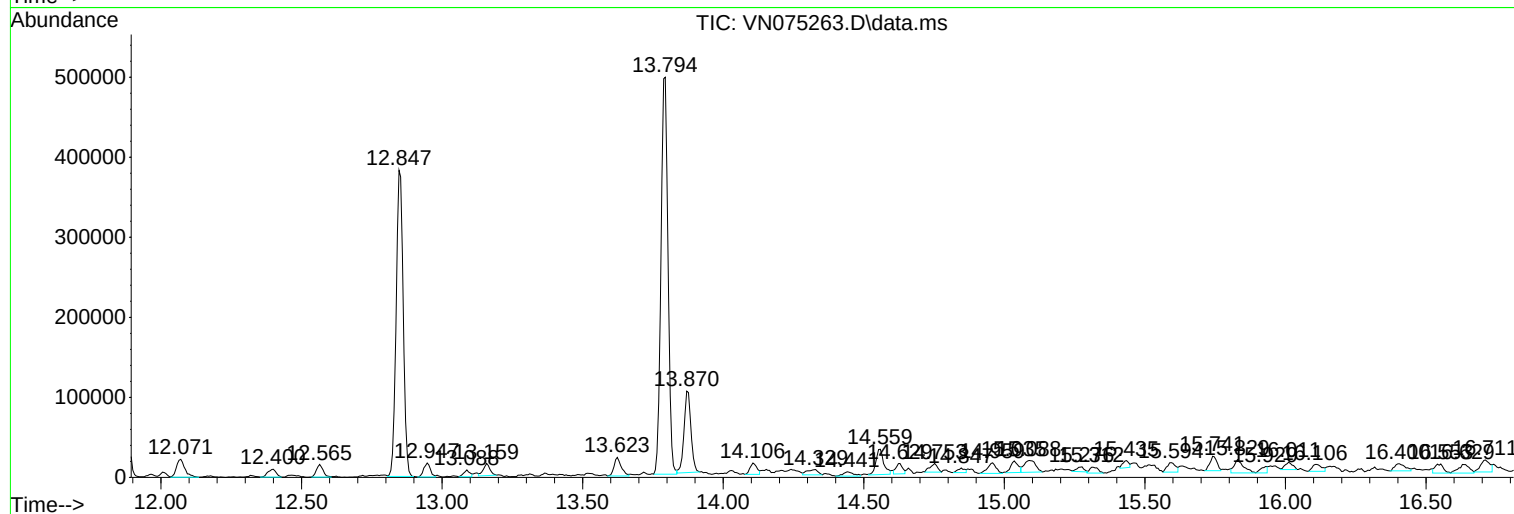
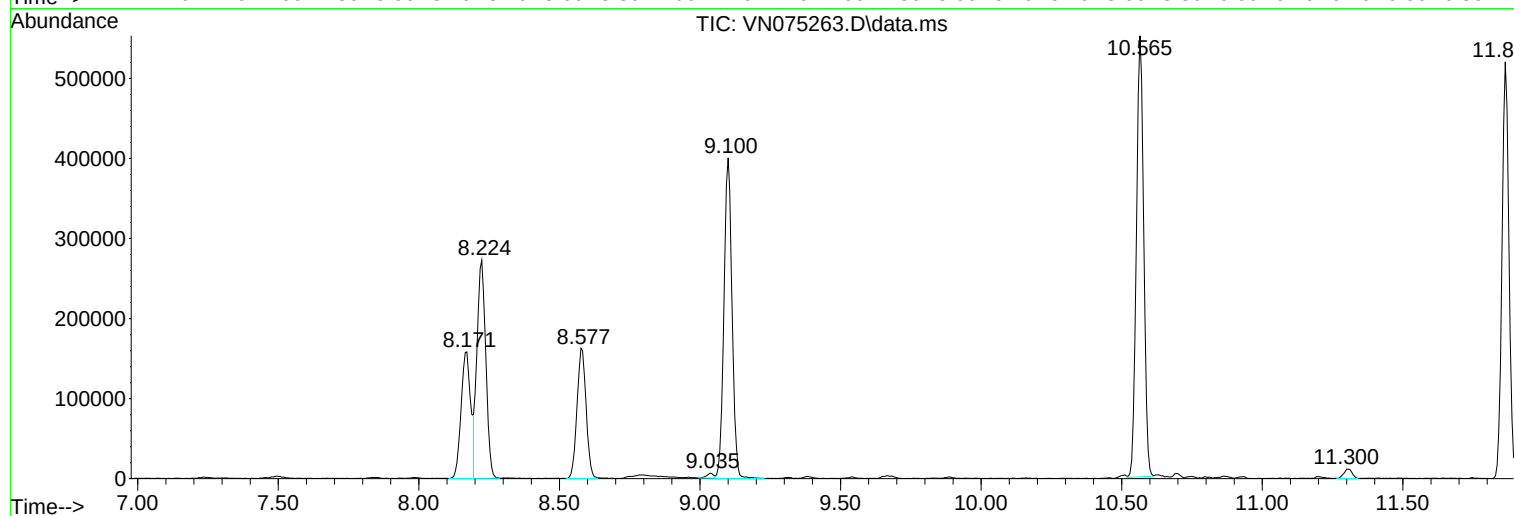
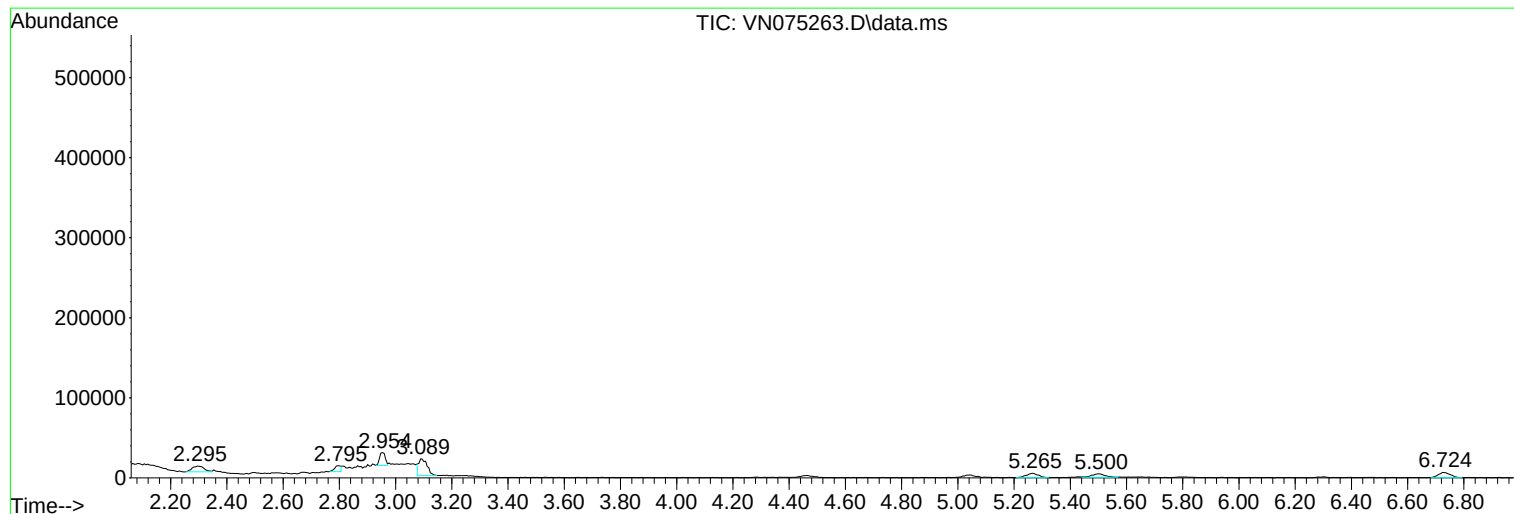
Sum of corrected areas: 6680686

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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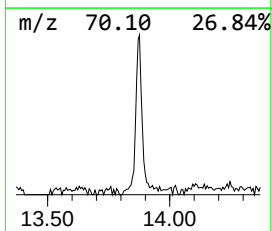
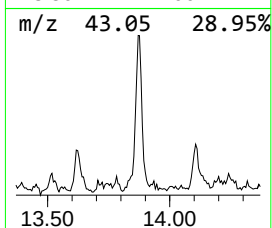
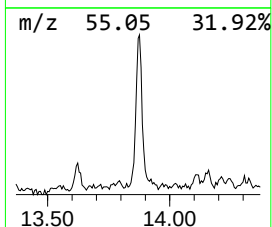
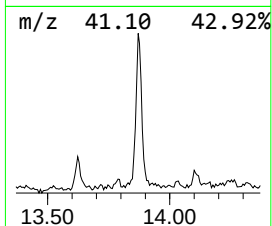
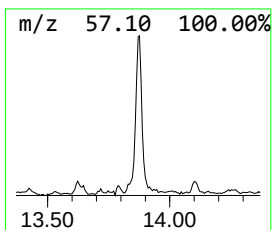
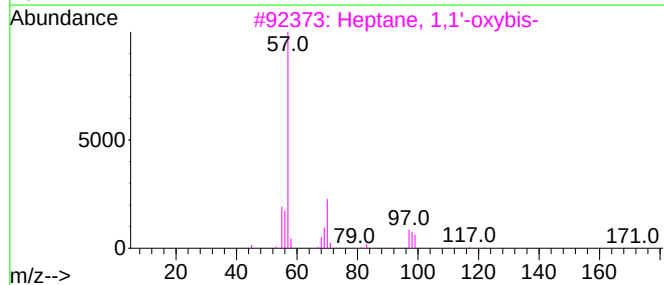
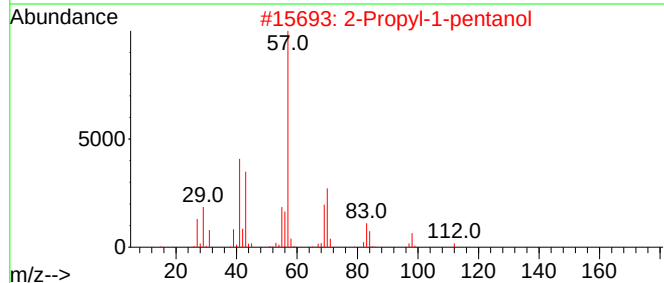
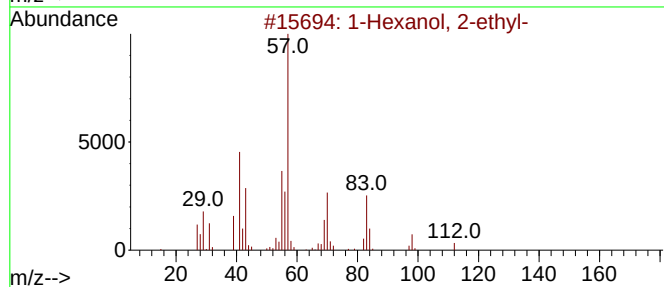
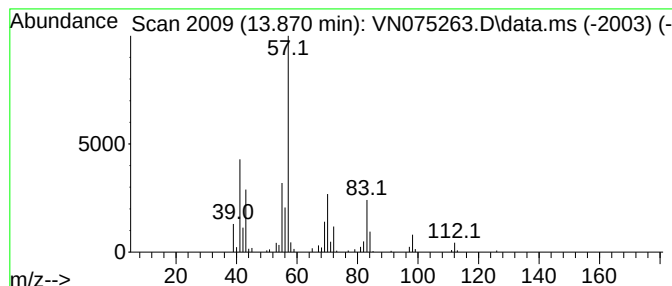
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	10.10 ug/l	173777	1,4-Dichlorobenzene-d4	13.788

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	13.870	10.1	ug/l	173777	4	13.788	859940	50.0