

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
 Data File : VX029696.D
 Acq On : 22 Jun 2022 14:04
 Operator : JC/MD
 Sample : N3384-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WC-4

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_X\Method\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	25	29	43	rBV	18081	42319	3.47%	0.574%
2	2.965	298	308	318	rBV2	9448	24307	1.99%	0.330%
3	5.098	646	658	672	rBV	20353	59665	4.89%	0.810%
4	5.391	694	706	720	rBV	140204	403129	33.01%	5.471%
5	5.556	720	733	750	rVB	256536	734398	60.14%	9.966%
6	5.958	789	799	812	rBV	147189	391261	32.04%	5.309%
7	6.763	920	931	943	rBV	389495	931936	76.32%	12.647%
8	7.830	1099	1106	1113	rBV	11664	22151	1.81%	0.301%
9	8.653	1234	1241	1249	rBV	778312	1221074	100.00%	16.570%
10	9.524	1378	1384	1394	rBV	59319	83572	6.84%	1.134%
11	10.055	1465	1471	1489	rVB	800625	1054170	86.33%	14.305%
12	10.305	1505	1512	1519	rBV	40882	60035	4.92%	0.815%
13	10.646	1563	1568	1574	rBV	20464	27459	2.25%	0.373%
14	10.860	1598	1603	1614	rBV	93088	120786	9.89%	1.639%
15	11.085	1634	1640	1654	rBV	594329	781448	64.00%	10.604%
16	11.384	1684	1689	1696	rBV	35640	65708	5.38%	0.892%
17	11.451	1696	1700	1709	rVB	14623	20918	1.71%	0.284%
18	11.616	1723	1727	1732	rVB	15989	20597	1.69%	0.280%
19	11.756	1745	1750	1758	rVB	57708	72502	5.94%	0.984%
20	11.841	1760	1764	1770	rBV	17504	23720	1.94%	0.322%
21	12.024	1788	1794	1801	rVV	784150	973558	79.73%	13.211%
22	12.091	1801	1805	1815	rVB	18950	25465	2.09%	0.346%
23	12.244	1821	1830	1833	rBV3	16078	24817	2.03%	0.337%
24	12.317	1838	1842	1852	rVB3	18226	27332	2.24%	0.371%
25	12.536	1872	1878	1880	rBV2	10370	15092	1.24%	0.205%
26	12.615	1885	1891	1895	rBV	15938	19456	1.59%	0.264%
27	12.701	1901	1905	1912	rBV3	7990	12450	1.02%	0.169%
28	12.853	1926	1930	1935	rVB4	19368	25630	2.10%	0.348%
29	12.963	1945	1948	1954	rVB	11336	13294	1.09%	0.180%
30	13.170	1975	1982	1986	rBV2	10534	13992	1.15%	0.190%
31	13.292	1998	2002	2007	rVB2	18371	24676	2.02%	0.335%
32	13.780	2077	2082	2087	rVB	12491	16502	1.35%	0.224%
33	14.639	2219	2223	2227	rBV	13560	15673	1.28%	0.213%

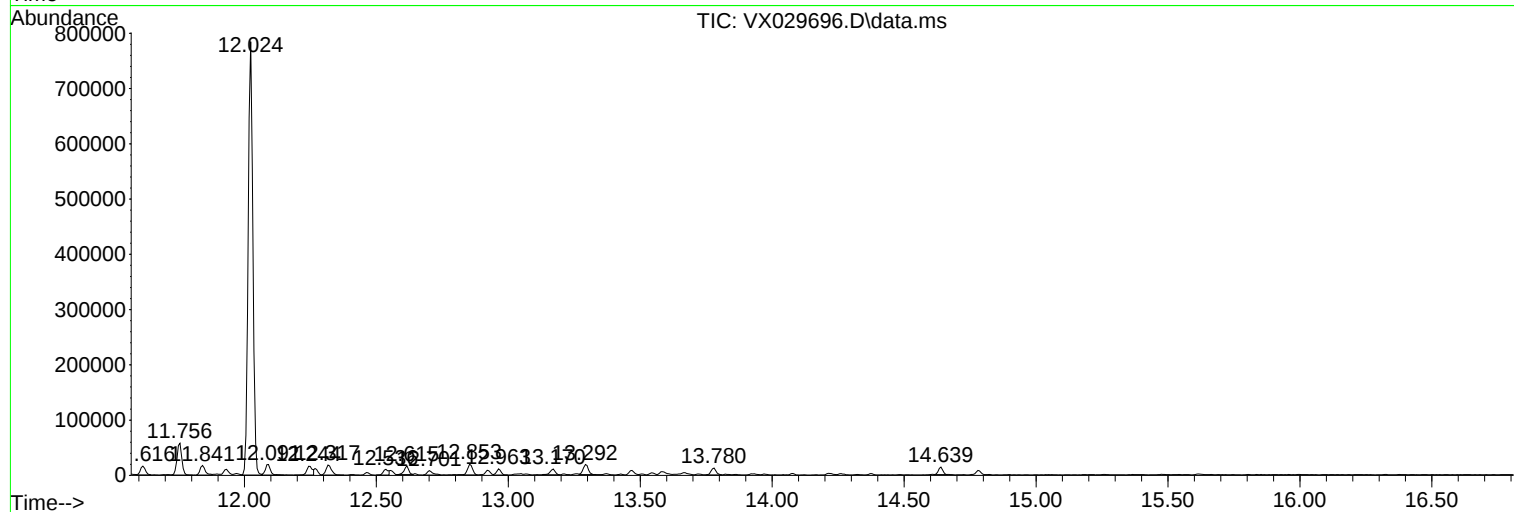
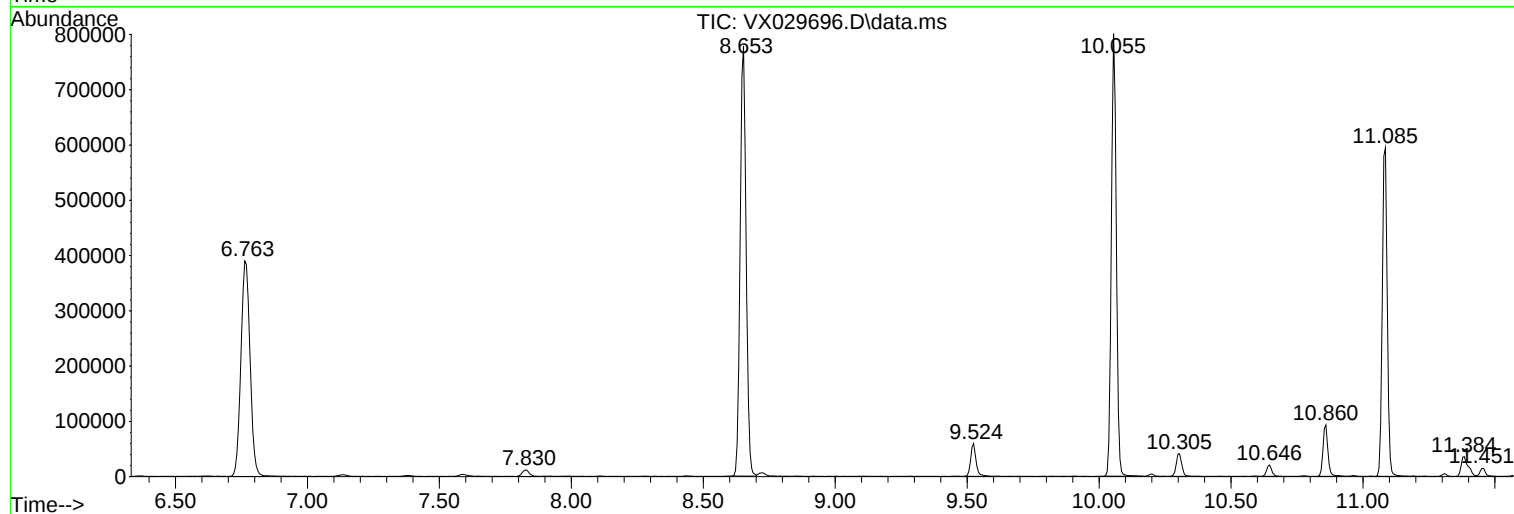
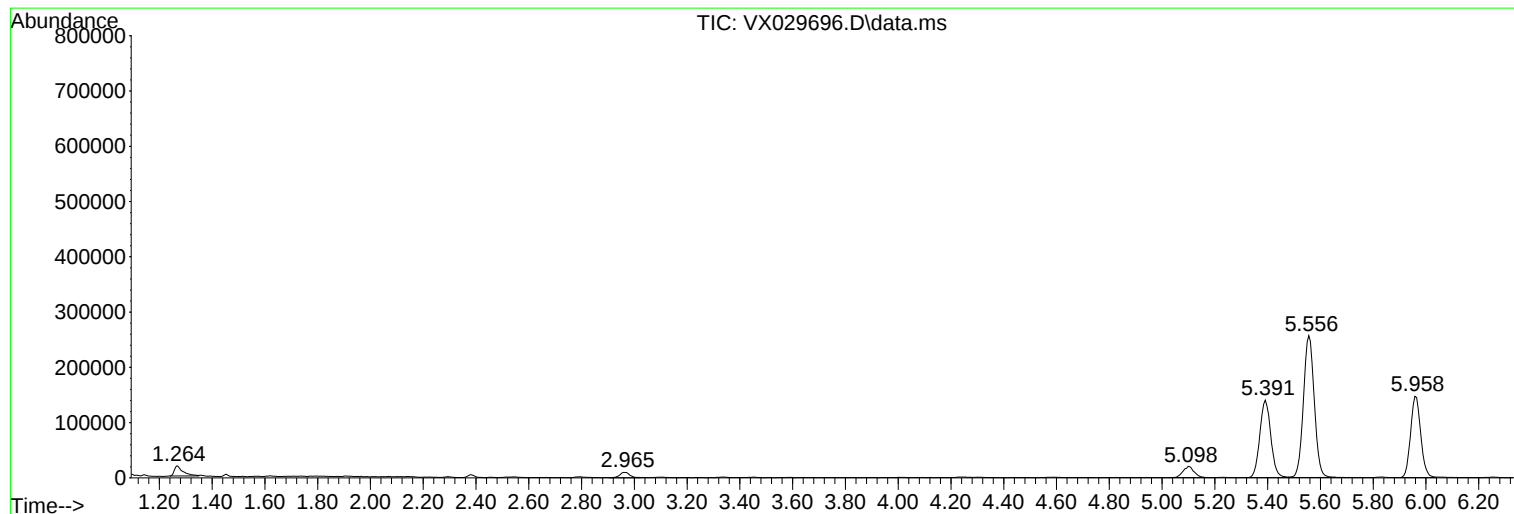
Sum of corrected areas: 7369092

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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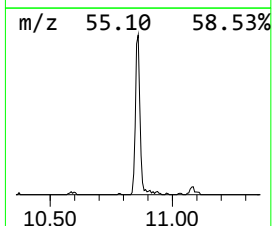
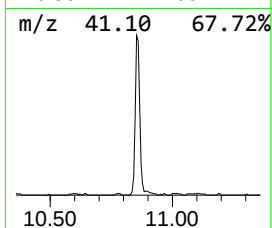
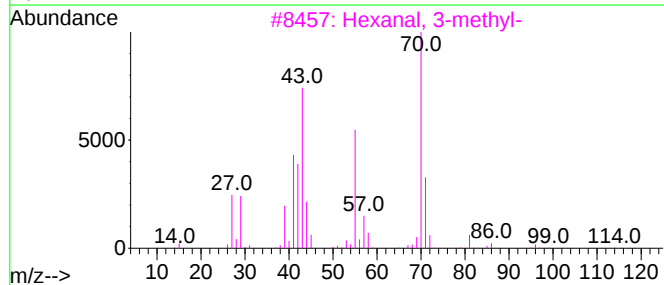
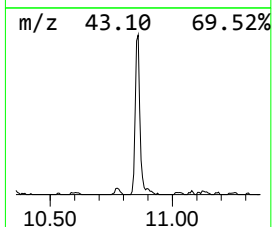
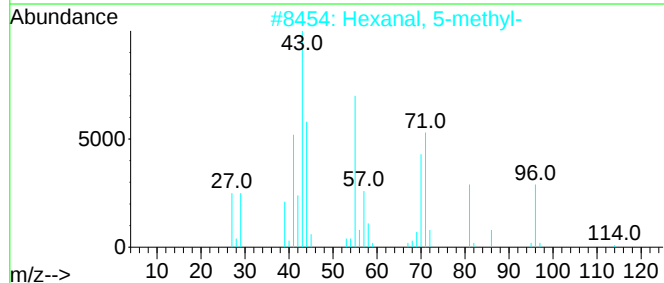
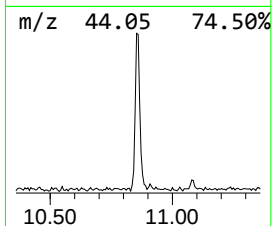
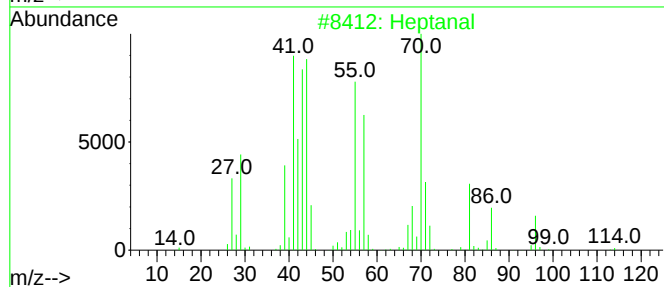
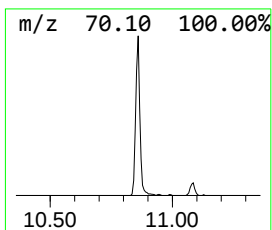
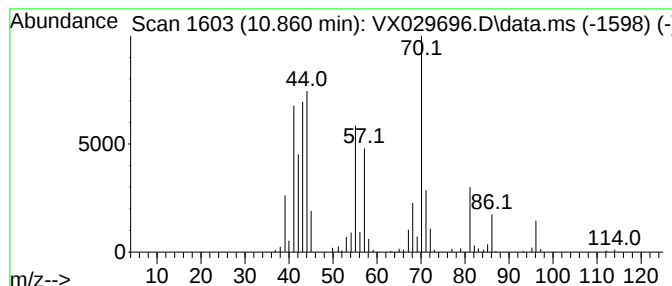
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Heptanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	5.73 ug/l	120786	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Hexanal, 5-methyl-	114	C7H14O	001860-39-5	43
3			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	43
4			Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	38
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptanal	10.860	5.7	ug/l	120786	3	10.055	1054170	50.0