

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030721\
 Data File : VX021040.D
 Acq On : 05 Mar 2021 17:10
 Operator : JC/MD
 Sample : M1575-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 IDW-GW803-AQ-030321

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\82X022421W.M

Title : SW846 8260

Signal : TIC: VX021040.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	62	66	71	rBV	39318	43066	3.39%	0.594%
2	2.417	220	226	235	rVB	16370	27675	2.18%	0.382%
3	2.576	244	253	259	rBV	8927	17857	1.41%	0.246%
4	3.393	384	392	404	rVB3	12930	28620	2.26%	0.395%
5	5.182	683	696	713	rBV	109963	331182	26.10%	4.567%
6	5.464	732	744	758	rBV	140937	402126	31.69%	5.546%
7	5.635	760	773	787	rBV	221236	612287	48.25%	8.444%
8	6.035	830	841	855	rBV	151940	399453	31.48%	5.509%
9	6.829	966	976	992	rBV	366646	888785	70.04%	12.257%
10	7.876	1146	1154	1164	rBV	30863	57332	4.52%	0.791%
11	8.694	1286	1293	1302	rBV	804558	1268995	100.00%	17.500%
12	8.765	1302	1305	1318	rVB	12835	23877	1.88%	0.329%
13	9.565	1434	1441	1449	rBV	25780	39428	3.11%	0.544%
14	10.094	1525	1531	1547	rVB	826084	1130356	89.07%	15.588%
15	10.341	1568	1573	1578	rBV	12111	16705	1.32%	0.230%
16	10.894	1659	1667	1677	rBV	88622	114844	9.05%	1.584%
17	11.118	1700	1705	1719	rVB	646907	853570	67.26%	11.771%
18	11.789	1813	1819	1825	rBV	10046	12816	1.01%	0.177%
19	12.059	1860	1865	1873	rBV	791724	982244	77.40%	13.546%

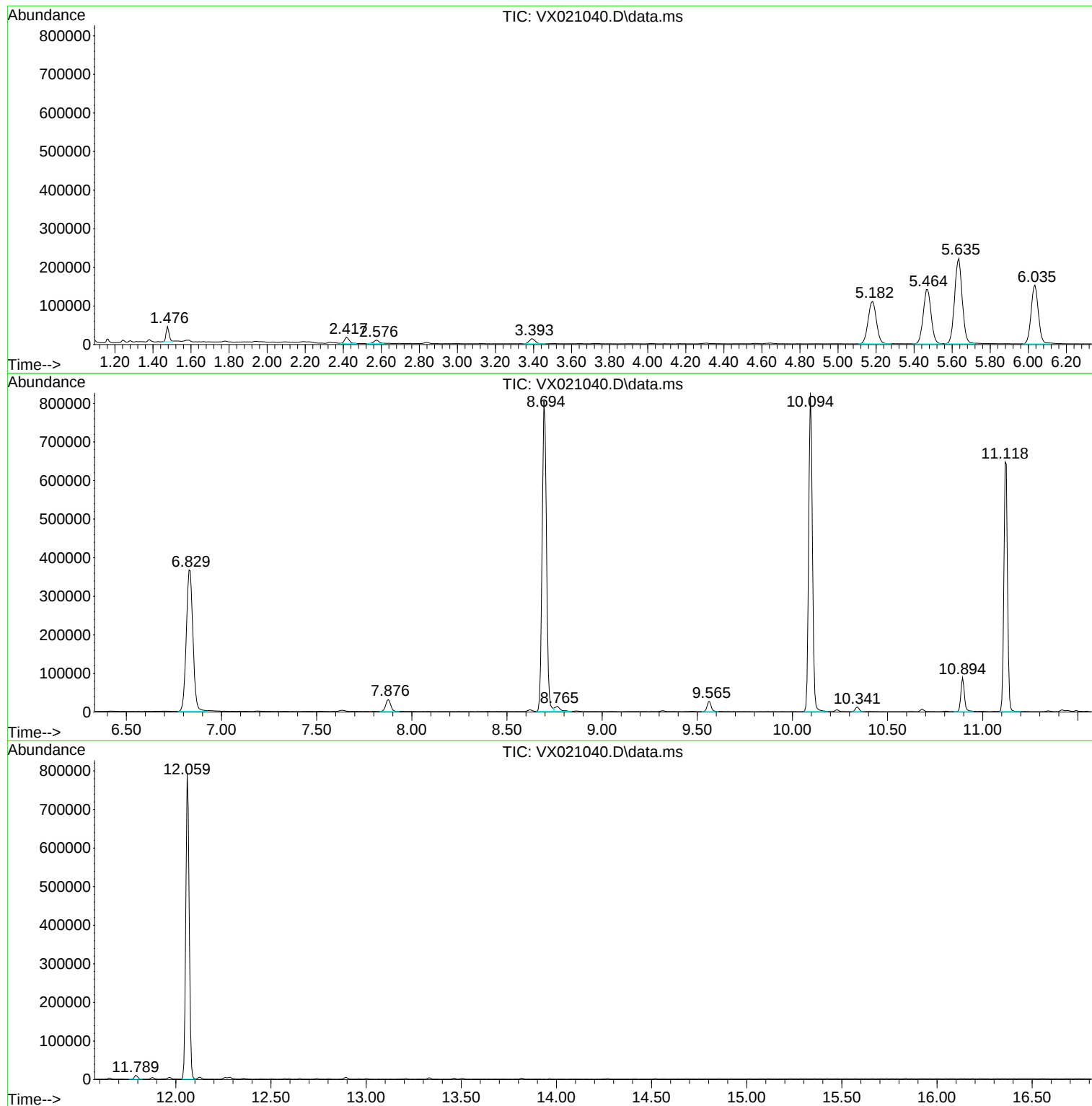
Sum of corrected areas: 7251218

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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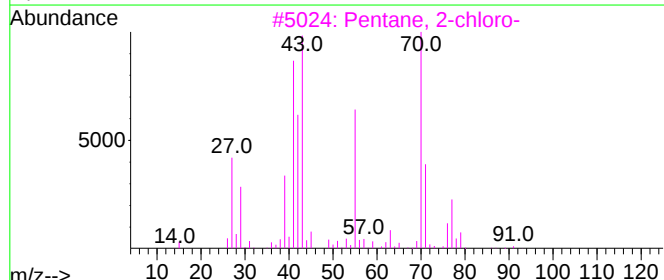
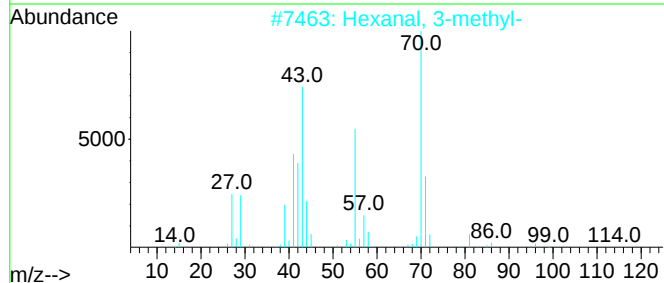
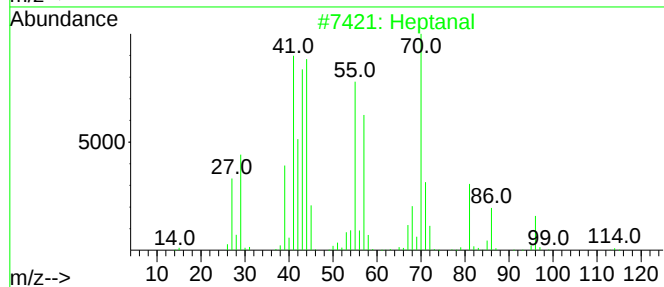
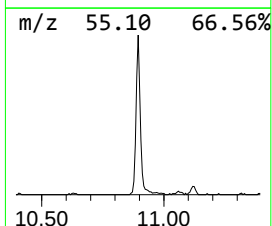
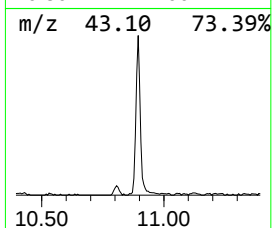
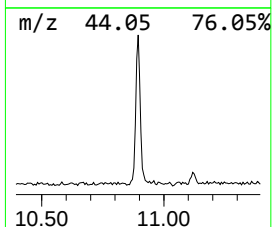
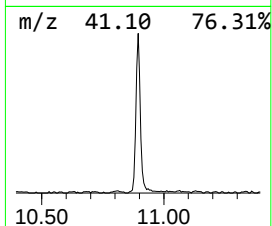
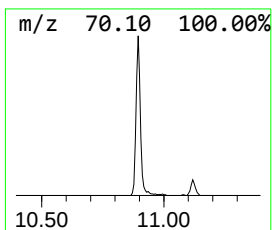
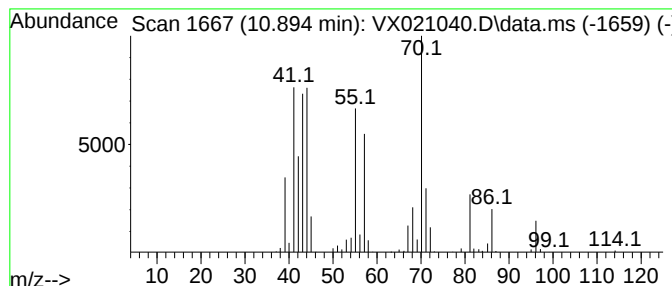
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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Peak Number 1 Heptanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.894	5.08 ug/l	114844	Chlorobenzene-d5	10.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanal	114	C7H14O	000111-71-7	98
2		Hexanal, 3-methyl-	114	C7H14O	019269-28-4	37
3		Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	35
4		Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	35
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptanal	10.894	5.1	ug/l	114844	3	10.094	1130360	50.0