

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
 Data File : VX026832.D
 Acq On : 08 Feb 2022 19:06
 Operator : JC/MD
 Sample : N1431-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SHB-2022

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\82X020822W.M
 Title : SW846 8260

Signal : TIC: VX026832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.544	232	239	251	rVB2	3561	9339	1.48%	0.273%
2	4.495	551	559	569	rVB2	2990	7420	1.18%	0.217%
3	5.391	695	706	722	rBV	73592	213060	33.81%	6.238%
4	5.556	722	733	749	rVB	129294	365277	57.97%	10.694%
5	5.964	789	800	818	rVB	82076	216120	34.30%	6.327%
6	6.769	921	932	944	rBV	198890	475707	75.49%	13.927%
7	8.653	1234	1241	1255	rBV	405149	630162	100.00%	18.449%
8	10.055	1465	1471	1485	rBV	403809	541235	85.89%	15.846%
9	11.085	1634	1640	1652	rBV	317803	407845	64.72%	11.941%
10	12.024	1789	1794	1808	rVB	419249	498670	79.13%	14.600%
11	13.146	1972	1978	1990	rBV	37474	50777	8.06%	1.487%

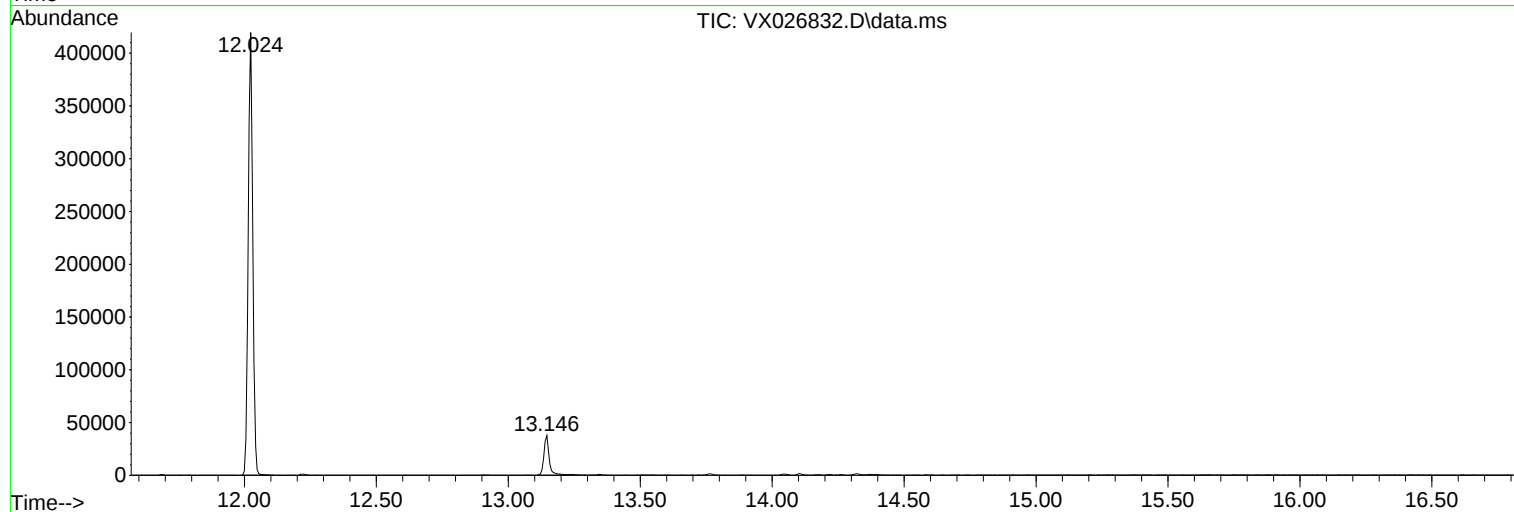
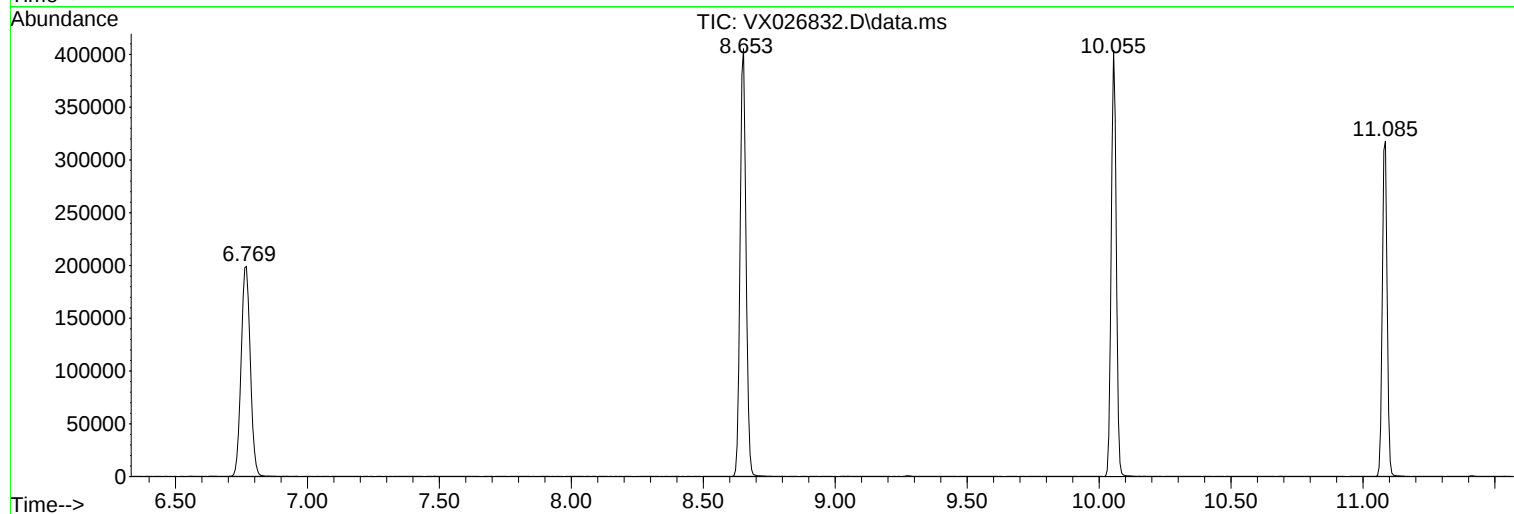
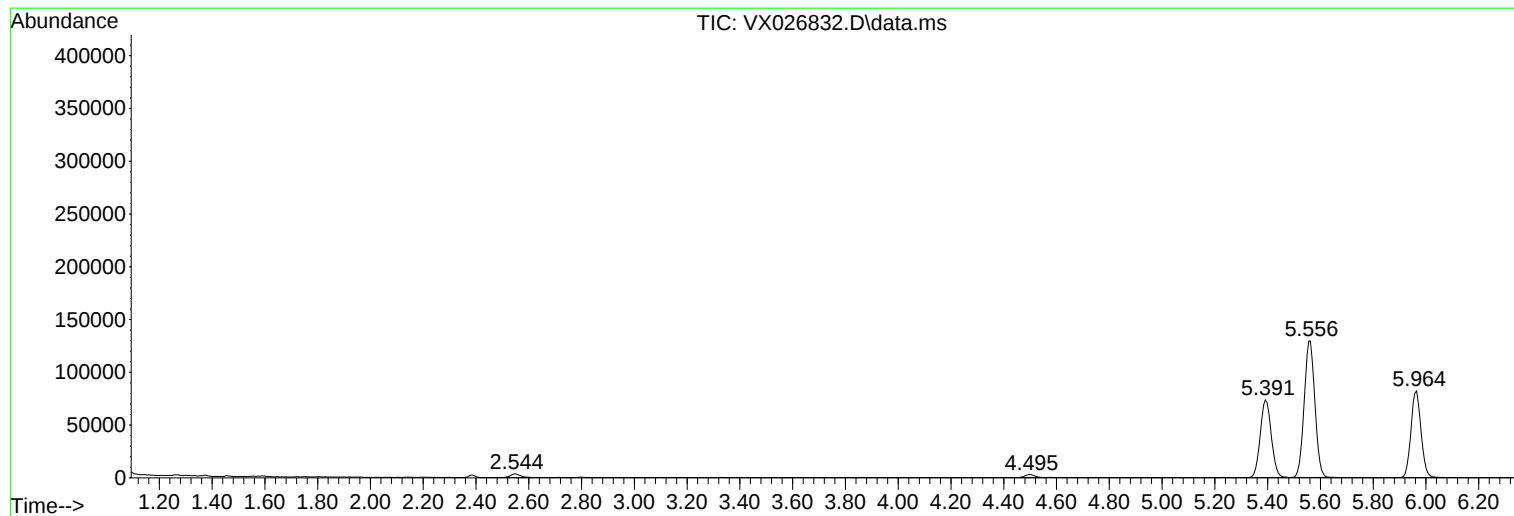
Sum of corrected areas: 3415612

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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



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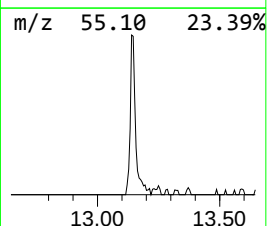
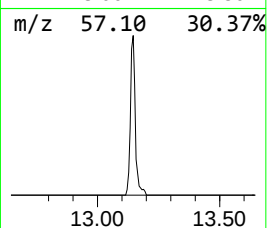
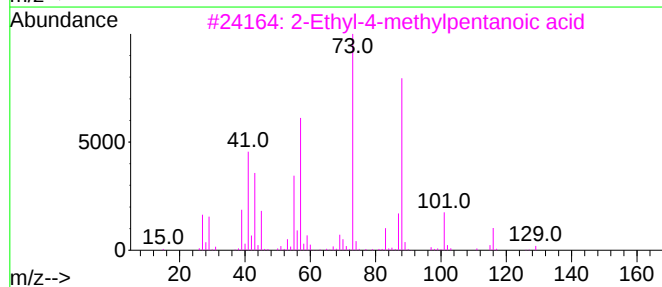
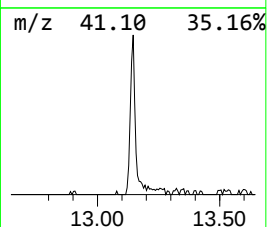
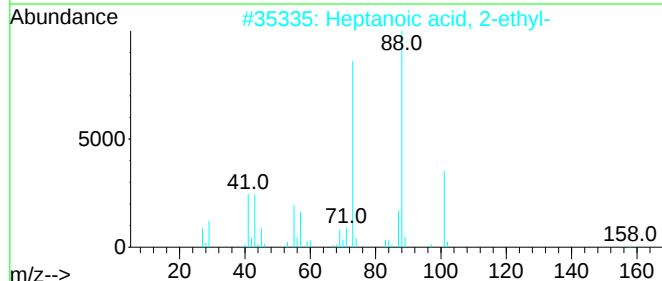
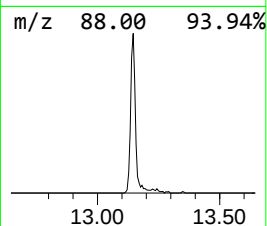
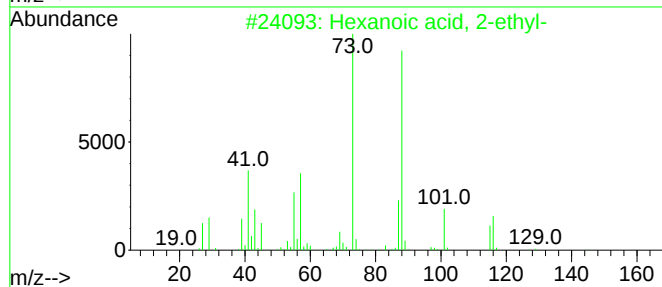
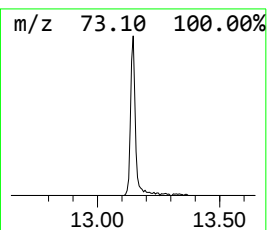
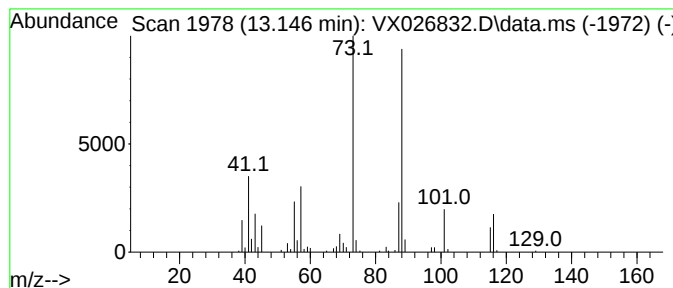
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.146	5.09 ug/l	50777	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
4			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
5			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	13.146	5.1	ug/l	50777	4	12.024	498670	50.0