

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020822\
 Data File : VX026829.D
 Acq On : 08 Feb 2022 17:56
 Operator : JC/MD
 Sample : N1429-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-21D

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: VX026829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	44	47	55	rVB	159136	172130	4.52%	2.327%
2	3.099	323	330	341	rVB2	33016	68196	1.79%	0.922%
3	4.495	546	559	579	rBV	1394349	3810313	100.00%	51.510%
4	5.391	695	706	716	rBV	71802	207660	5.45%	2.807%
5	5.556	724	733	756	rVB	128167	383364	10.06%	5.183%
6	5.964	789	800	810	rBV	78325	209526	5.50%	2.832%
7	6.763	921	931	953	rBV	193341	463981	12.18%	6.272%
8	8.653	1234	1241	1251	rVB	391818	622543	16.34%	8.416%
9	10.055	1462	1471	1478	rBV	386732	524251	13.76%	7.087%
10	11.085	1634	1640	1645	rBV	295942	394772	10.36%	5.337%
11	12.024	1789	1794	1807	rBV	400336	481253	12.63%	6.506%
12	13.146	1972	1978	1983	rBV	45056	59258	1.56%	0.801%

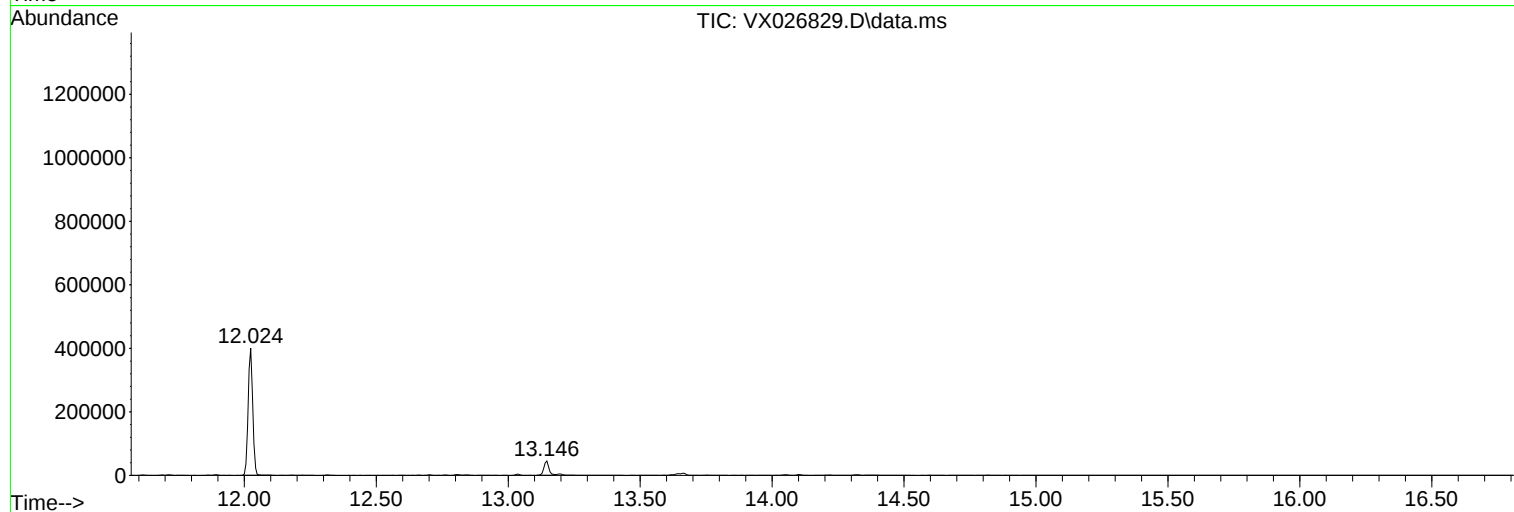
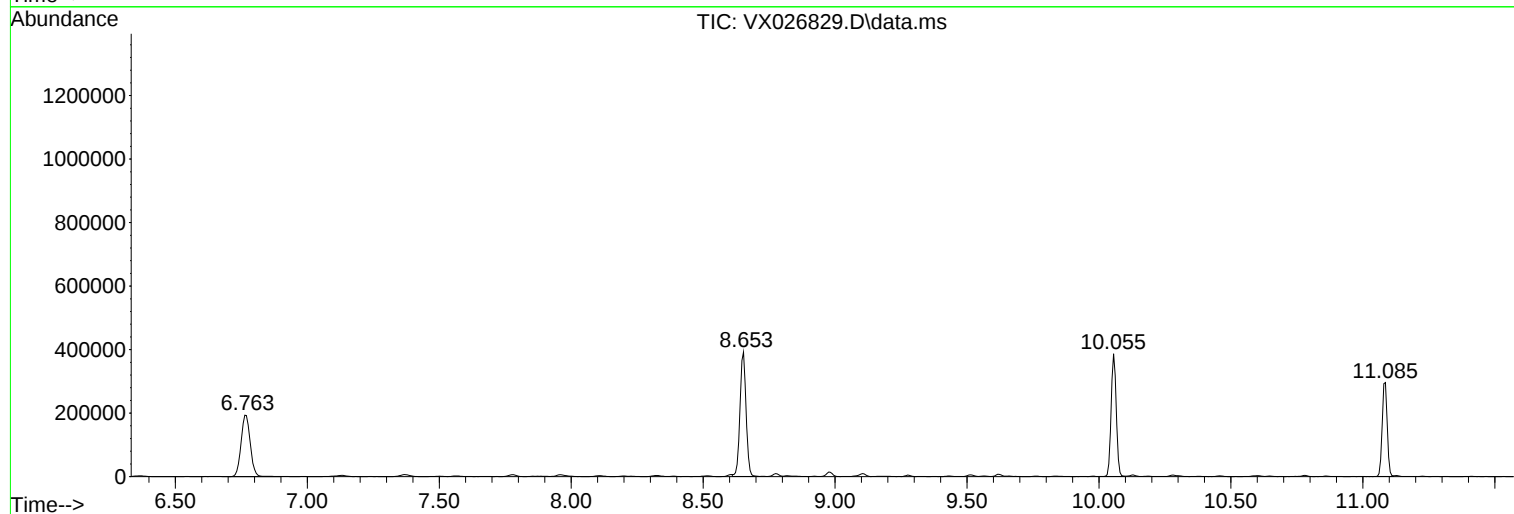
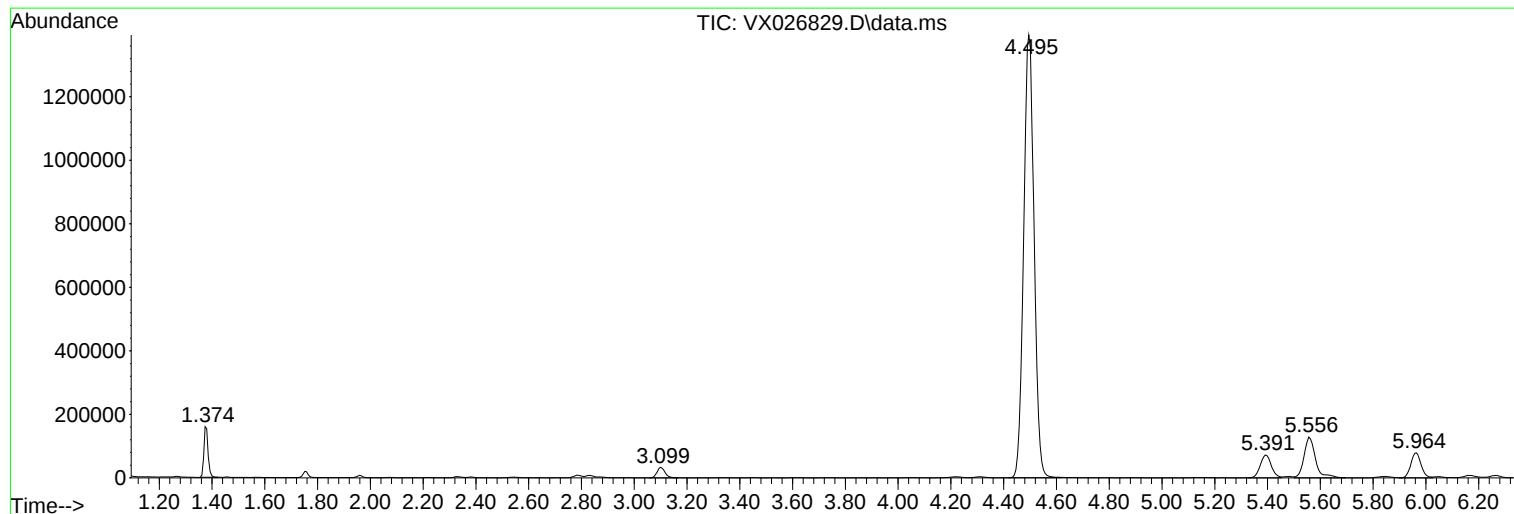
Sum of corrected areas: 7397247

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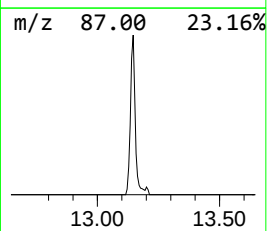
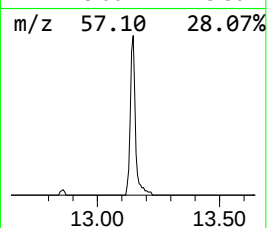
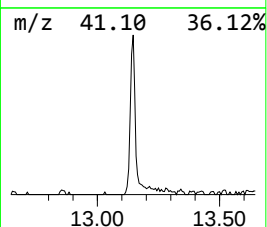
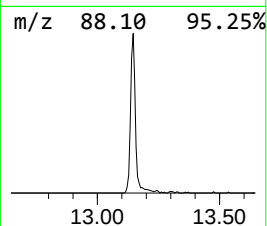
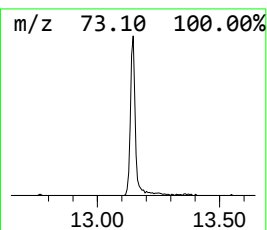
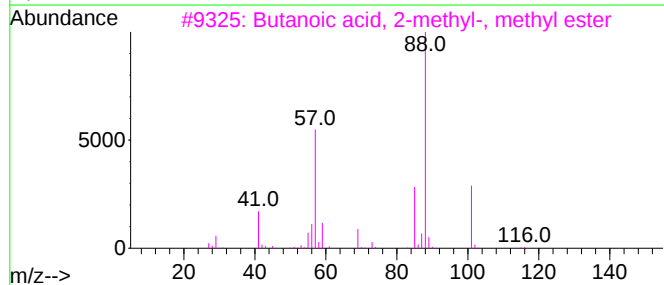
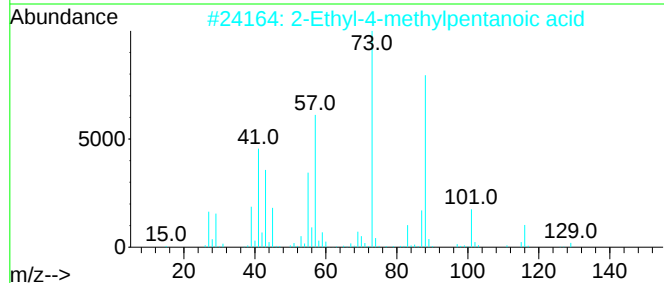
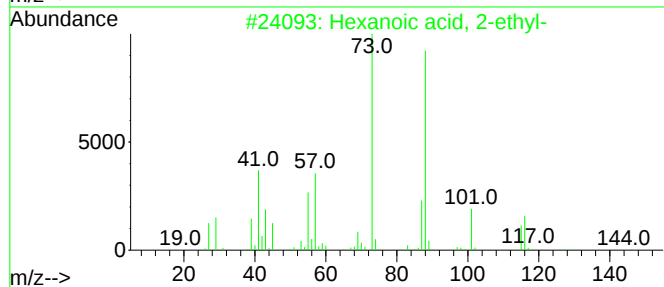
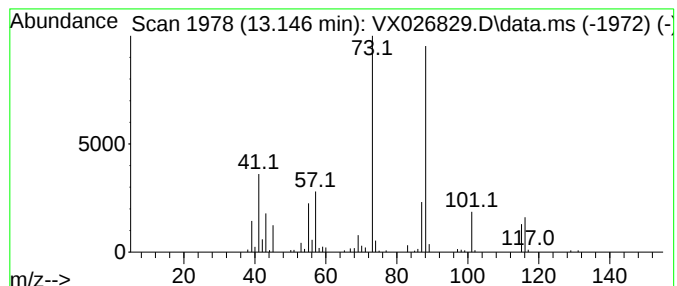
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020822W.M
Quant Title : SW846 8260

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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	6.16 ug/l	59258	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			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
4			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	13.146	6.2	ug/l	59258	4	12.024	481253	50.0