

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020325\
 Data File : VX044817.D
 Acq On : 03 Feb 2025 16:08
 Operator : JC/MD
 Sample : Q1239-10
 Misc : 5.10g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 357

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\82X011525W.M
 Title : SW846 8260

Signal : TIC: VX044817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	31	rBV2	8279	10859	1.70%	0.316%
2	1.569	71	79	80	rBV5	5387	10836	1.70%	0.316%
3	2.940	298	304	314	rBV3	5052	12660	1.98%	0.369%
4	5.379	693	704	721	rBV	68593	209905	32.85%	6.116%
5	5.544	721	731	754	rVV	102143	300693	47.06%	8.762%
6	5.952	788	798	814	rBV	78063	213549	33.42%	6.222%
7	6.367	858	866	877	rBV5	1930	7423	1.16%	0.216%
8	6.757	921	930	952	rBV	185167	463792	72.58%	13.514%
9	7.208	999	1004	1012	rVB3	3183	7034	1.10%	0.205%
10	8.647	1229	1240	1249	rBV	376321	638990	100.00%	18.619%
11	10.055	1465	1471	1486	rBV	363116	546429	85.51%	15.922%
12	11.079	1634	1639	1652	rBV	293686	398115	62.30%	11.600%
13	12.018	1788	1793	1803	rBV	367811	487623	76.31%	14.208%
14	13.140	1972	1977	1986	rBV	45497	65042	10.18%	1.895%
15	13.286	1998	2001	2008	rVB3	4646	7797	1.22%	0.227%
16	13.841	2088	2092	2098	rVB3	4720	7602	1.19%	0.222%
17	14.609	2215	2218	2221	rVV5	5809	9098	1.42%	0.265%
18	14.639	2221	2223	2232	rVB5	5225	8476	1.33%	0.247%
19	15.188	2306	2313	2325	rBV7	11478	26011	4.07%	0.758%

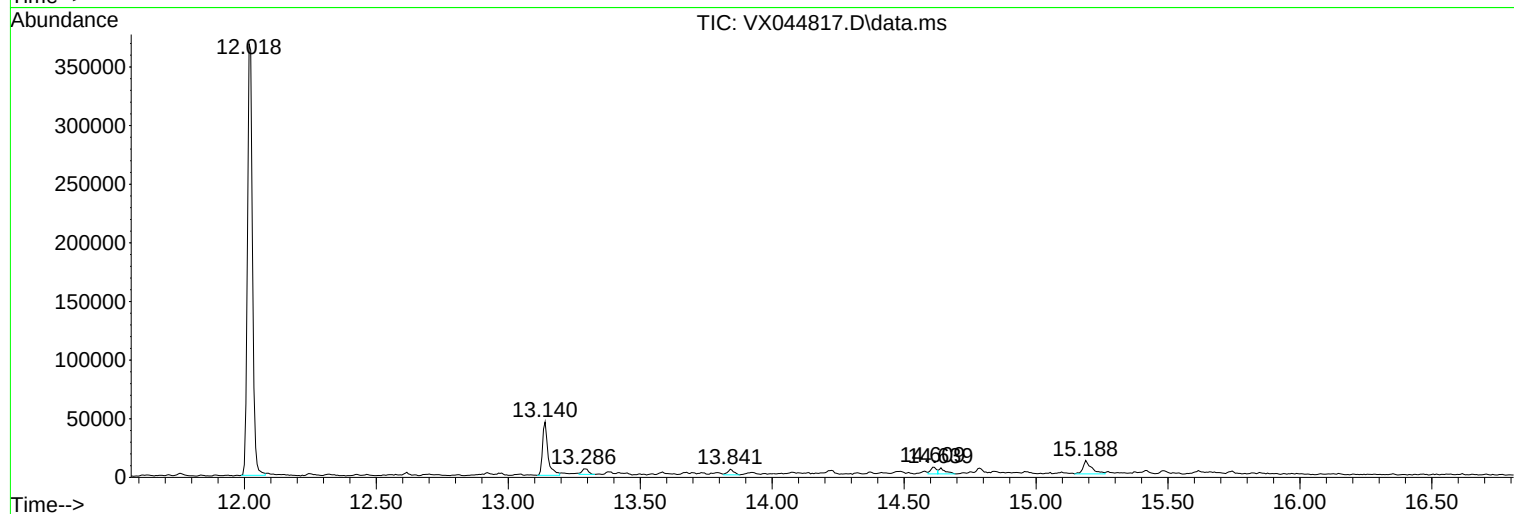
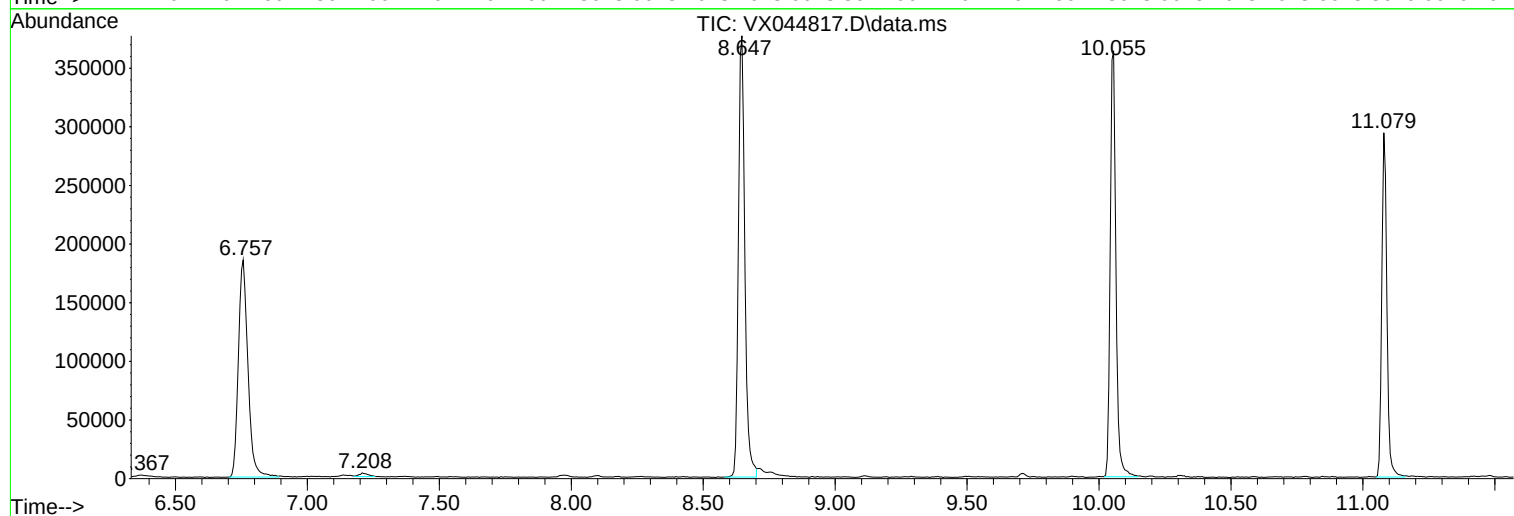
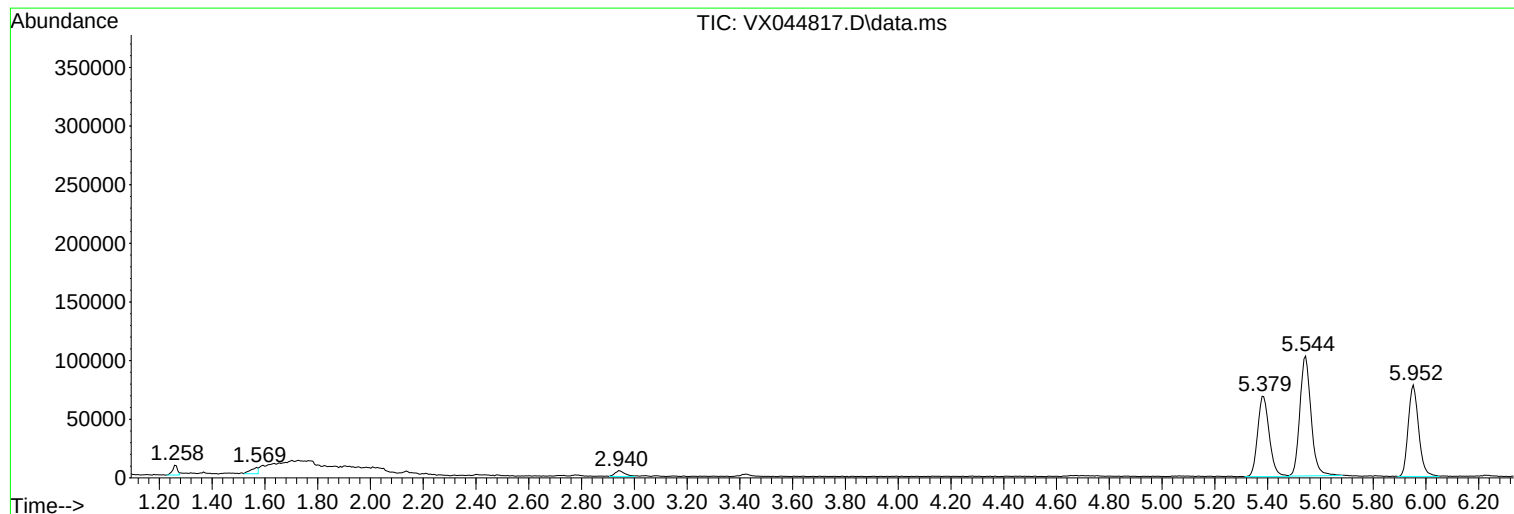
Sum of corrected areas: 3431934

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011525W.M
Quant Title : SW846 8260

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



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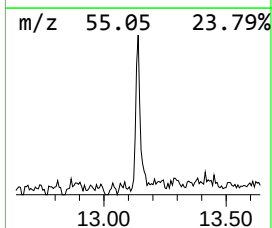
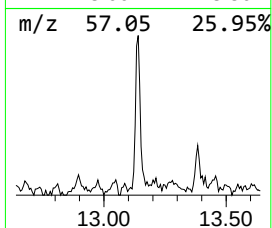
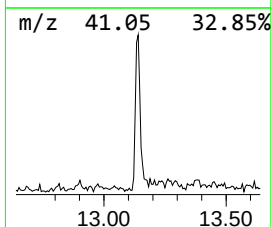
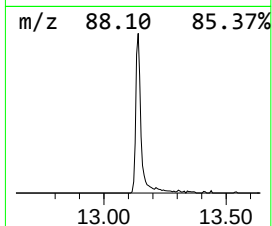
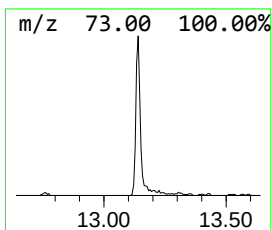
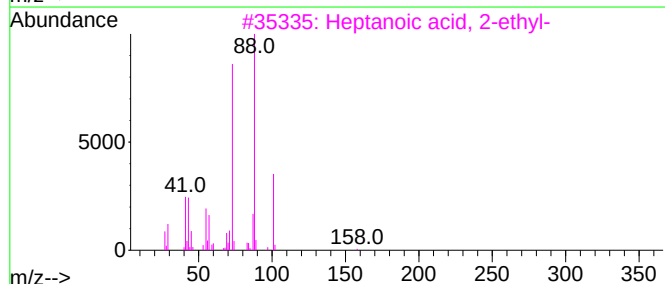
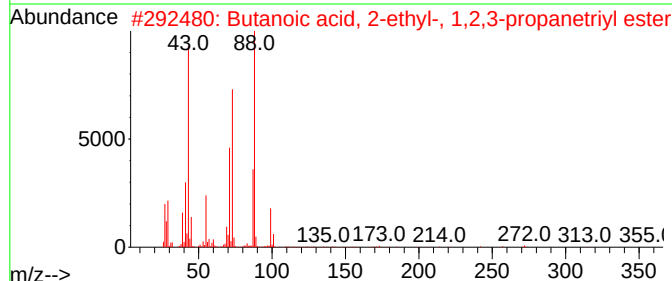
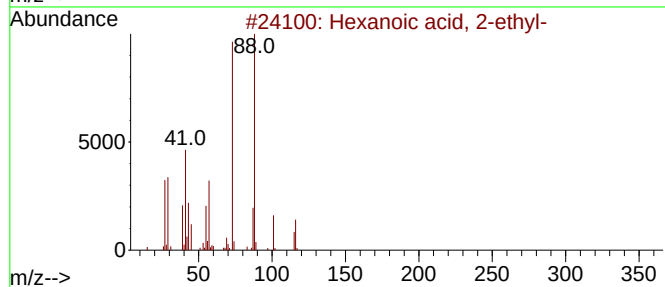
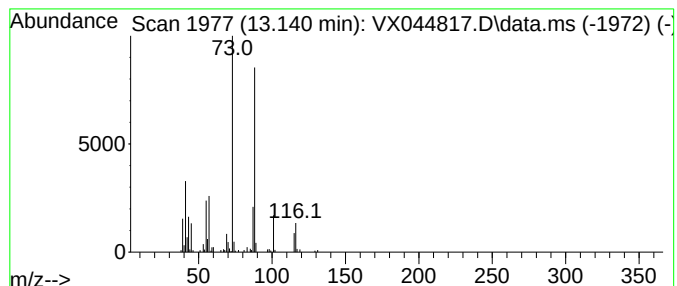
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011525W.M
Quant Title : SW846 8260

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.
13.140	6.67 ug/l	65042	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			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	59
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	13.140	6.7	ug/l	65042	4	12.024	487623	50.0