

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020325\
 Data File : VX044814.D
 Acq On : 03 Feb 2025 14:59
 Operator : JC/MD
 Sample : Q1239-07
 Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RBR22266

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: VX044814.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	21	28	31	rBV2	7594	11478	1.73%	0.310%
2	1.563	71	78	79	rBV5	5403	10277	1.55%	0.278%
3	2.941	297	304	313	rBV	6173	16424	2.48%	0.444%
4	5.379	694	704	719	rBV2	69546	211810	31.93%	5.730%
5	5.544	721	731	748	rBV2	105036	305202	46.01%	8.256%
6	5.952	787	798	816	rBV	79077	221570	33.40%	5.994%
7	6.757	920	930	946	rBV	189155	474979	71.60%	12.849%
8	7.208	999	1004	1012	rVB6	2934	7295	1.10%	0.197%
9	8.647	1232	1240	1248	rBV	402758	663408	100.00%	17.946%
10	8.720	1248	1252	1269	rVB	24074	53469	8.06%	1.446%
11	10.055	1465	1471	1487	rBV	377496	573366	86.43%	15.510%
12	11.079	1634	1639	1653	rBV	309576	409962	61.80%	11.090%
13	12.018	1788	1793	1809	rVB	380504	496532	74.85%	13.432%
14	13.140	1968	1977	1990	rBV	98221	149232	22.49%	4.037%
15	13.780	2076	2082	2089	rBV	6809	9008	1.36%	0.244%
16	14.640	2217	2223	2228	rBV	5714	8128	1.23%	0.220%
17	14.780	2236	2246	2251	rBV5	3836	7993	1.20%	0.216%
18	15.188	2306	2313	2323	rBV2	39685	66630	10.04%	1.802%

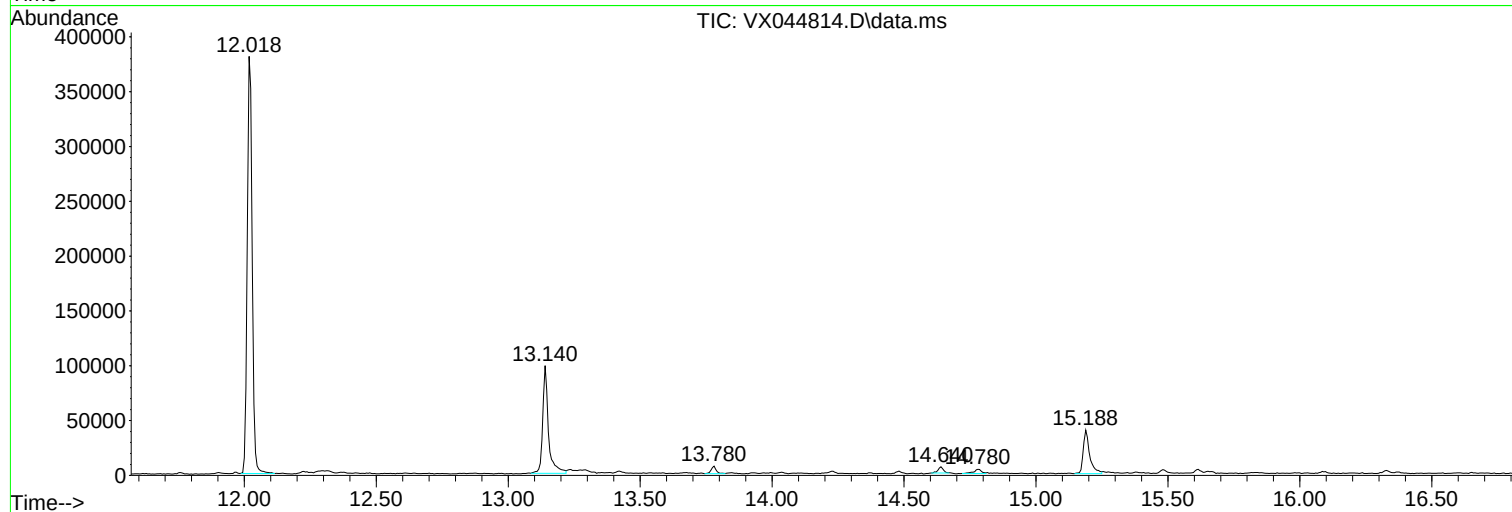
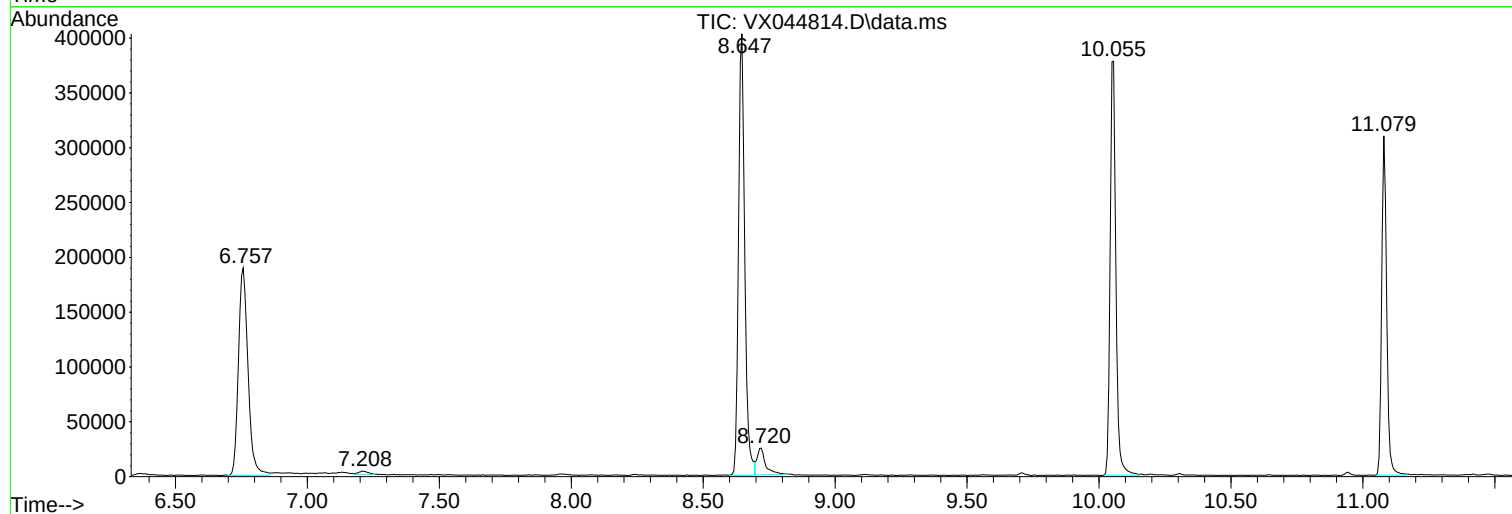
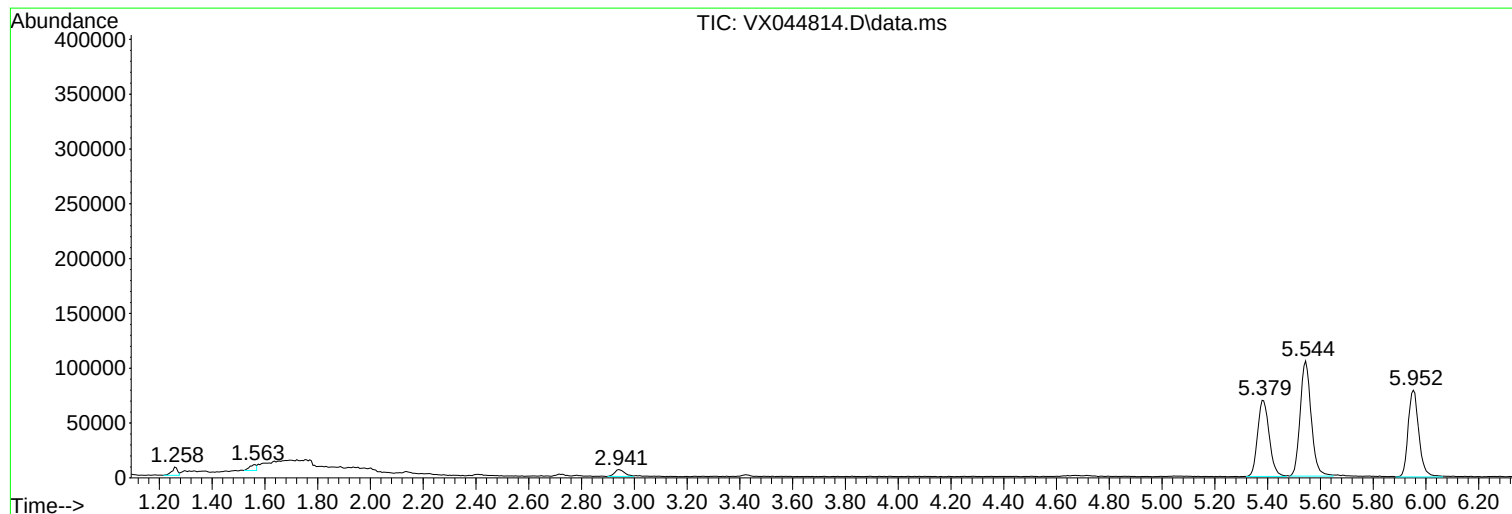
Sum of corrected areas: 3696763

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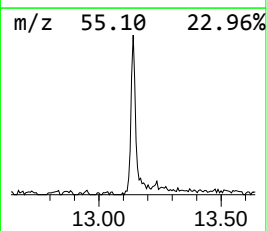
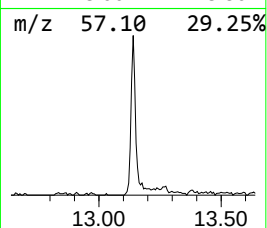
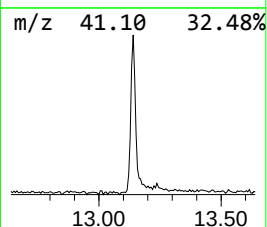
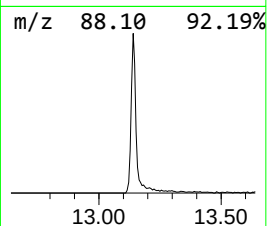
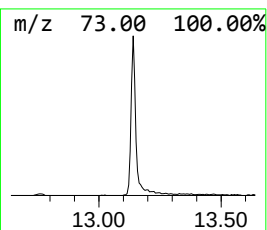
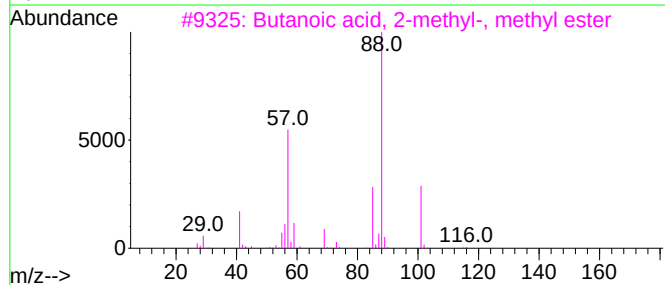
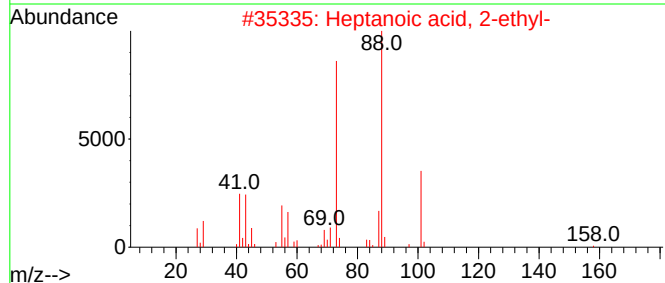
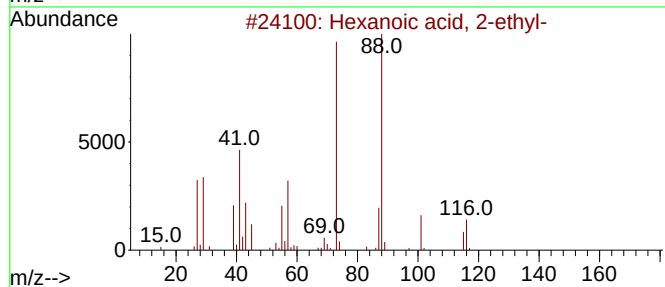
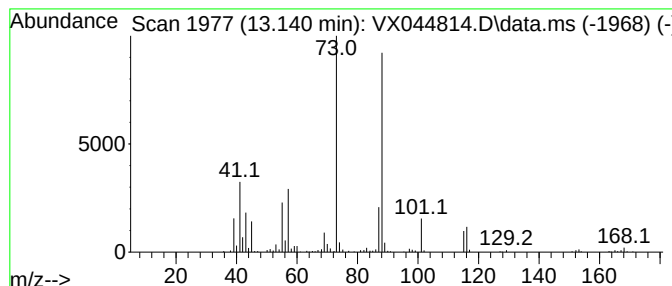
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011525W.M
Quant Title : SW846 8260

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	15.03 ug/l	149232	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	53
3			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
4			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42
5			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40



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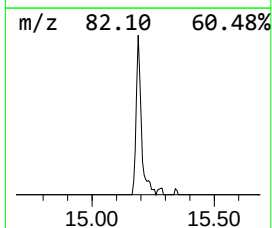
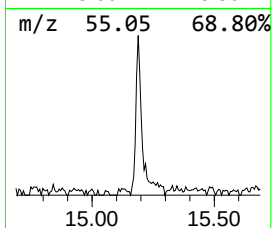
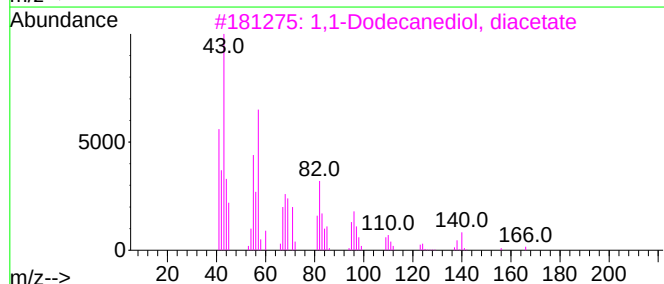
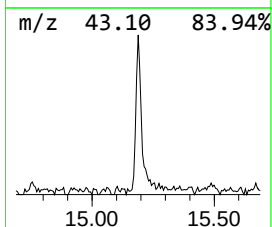
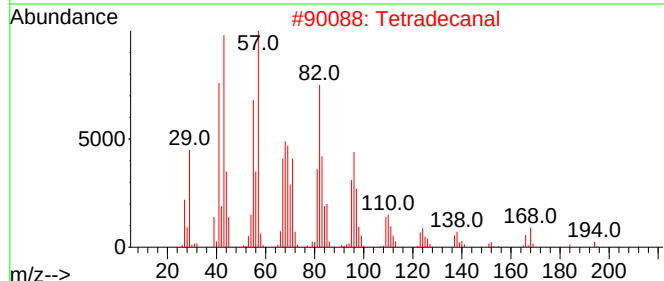
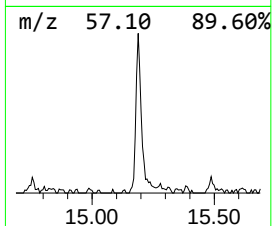
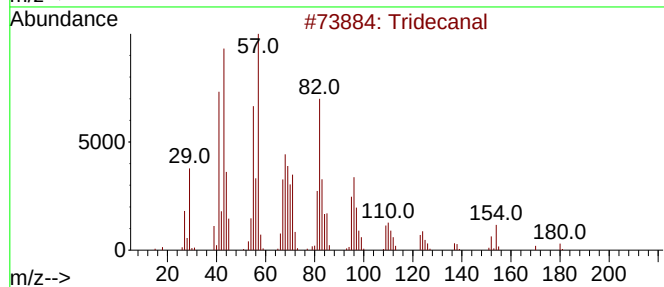
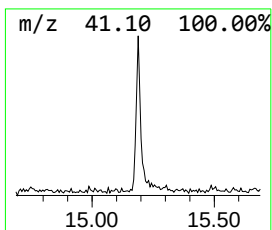
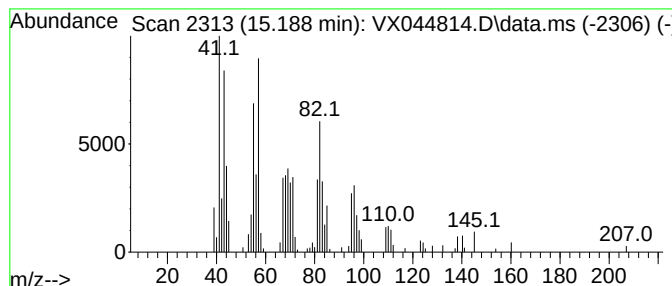
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.188	6.71 ug/l	66630	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanal	198	C13H26O	010486-19-8	76
2			Tetradecanal	212	C14H28O	000124-25-4	64
3			1,1-Dodecanediol, diacetate	286	C16H30O4	056438-07-4	62
4			Dodecanal	184	C12H24O	000112-54-9	60
5			Pentadecanal-	226	C15H30O	002765-11-9	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, ...	13.140	15.0	ug/l	149232	4	12.024	496532	50.0
Tridecanal	15.188	6.7	ug/l	66630	4	12.024	496532	50.0