

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090424\
 Data File : VN083644.D
 Acq On : 04 Sep 2024 13:06
 Operator : JC\MD
 Sample : P3744-02
 Misc : 2.07g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 60244

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_N\methods\82N083024W.M
 Title : SW846 8260

Signal : TIC: VN083644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	52	57	74	rVB2	72742	145572	12.82%	2.218%
2	2.801	137	144	145	rBV2	8297	13454	1.18%	0.205%
3	2.883	148	158	159	rBV6	10724	29134	2.57%	0.444%
4	6.283	726	736	749	rBV3	38615	119362	10.51%	1.819%
5	8.159	1046	1055	1060	rBV	135190	337800	29.74%	5.147%
6	8.218	1060	1065	1080	rVB	247515	531251	46.77%	8.095%
7	8.571	1115	1125	1136	rBV	147605	324711	28.59%	4.948%
8	9.094	1205	1214	1225	rBV	392224	816315	71.87%	12.439%
9	10.565	1455	1464	1472	rBV	539575	1000883	88.12%	15.251%
10	11.865	1675	1685	1696	rBV	629392	1135827	100.00%	17.307%
11	12.847	1845	1852	1863	rBV	456668	787250	69.31%	11.996%
12	13.335	1929	1935	1941	rBV	73239	113193	9.97%	1.725%
13	13.688	1989	1995	1999	rBV2	17057	29641	2.61%	0.452%
14	13.788	2006	2012	2021	rBV	636071	1093786	96.30%	16.666%
15	13.876	2021	2027	2035	rVB3	14211	24919	2.19%	0.380%
16	14.553	2136	2142	2147	rBV6	8786	16774	1.48%	0.256%
17	15.388	2280	2284	2288	rBV6	7330	12838	1.13%	0.196%
18	15.829	2355	2359	2365	rVB5	18047	30094	2.65%	0.459%

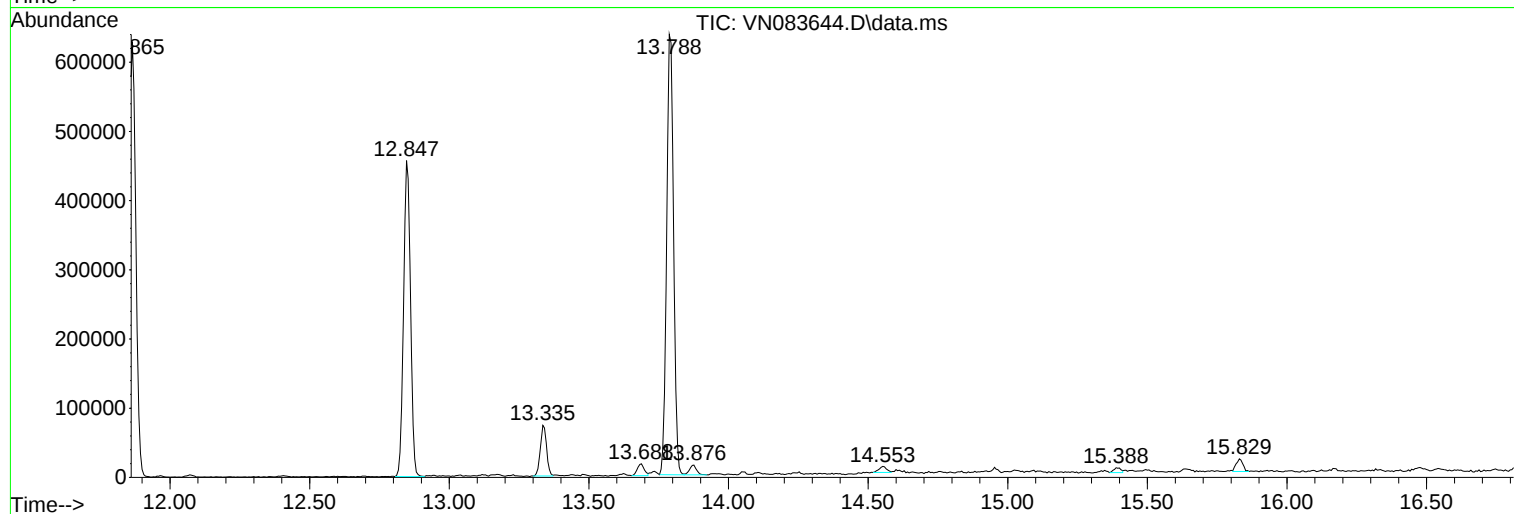
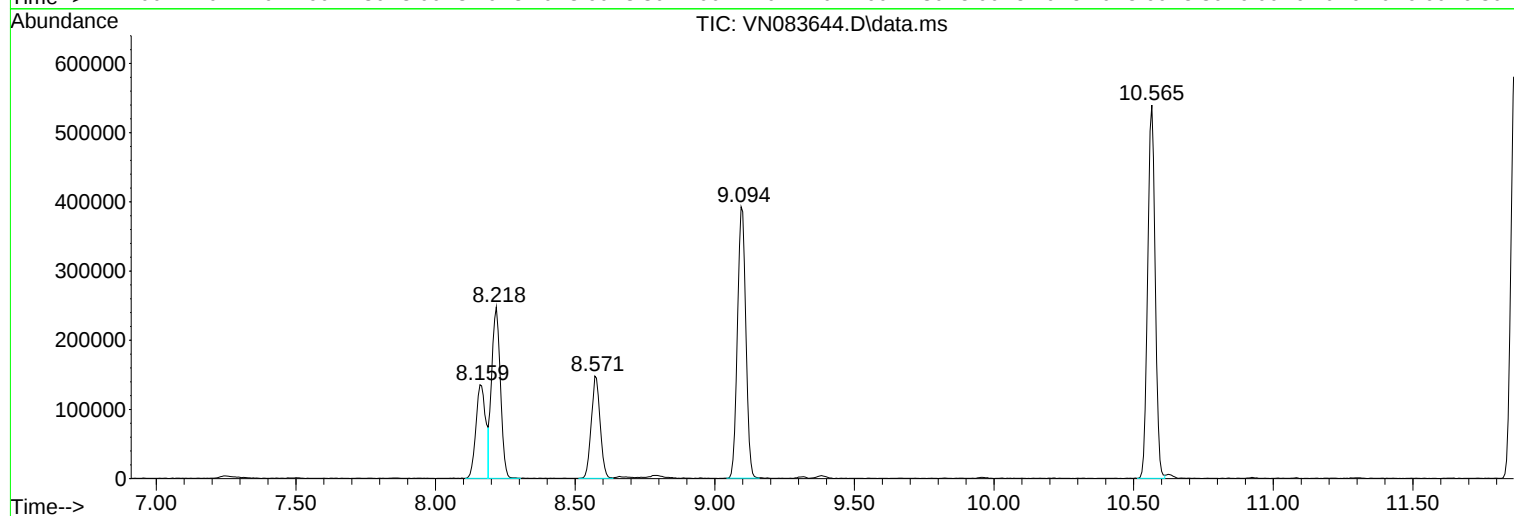
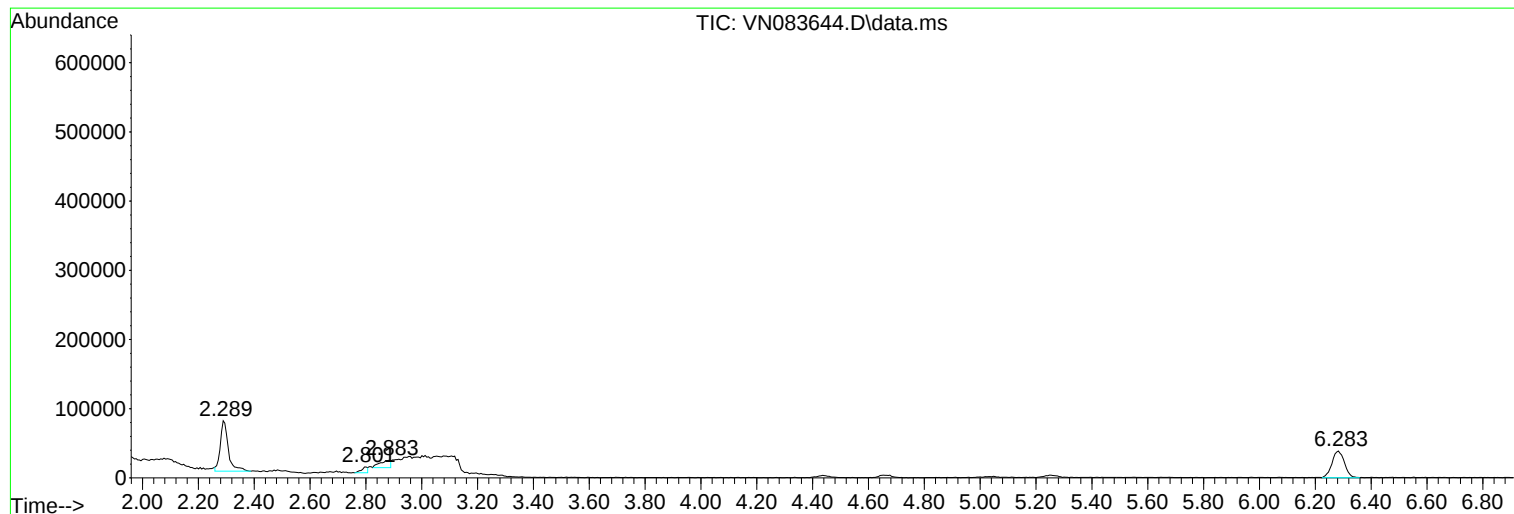
Sum of corrected areas: 6562804

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Quant Title : SW846 8260

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



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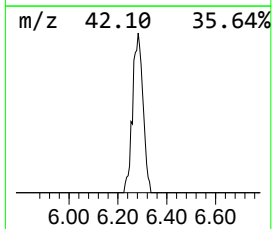
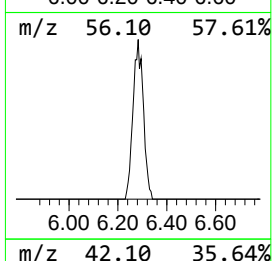
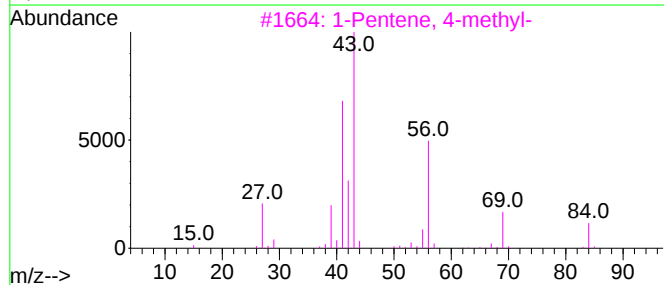
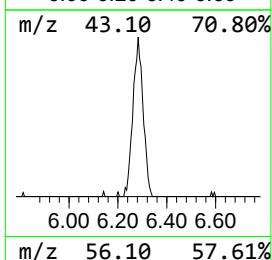
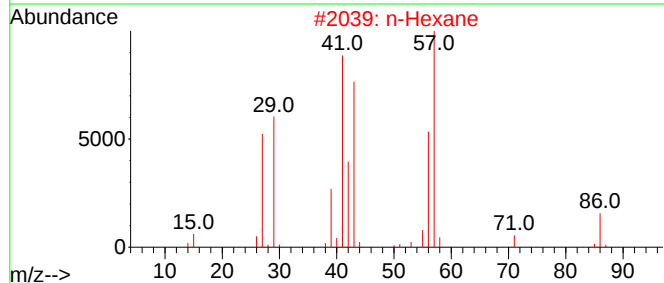
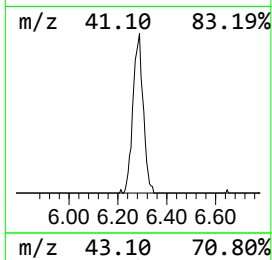
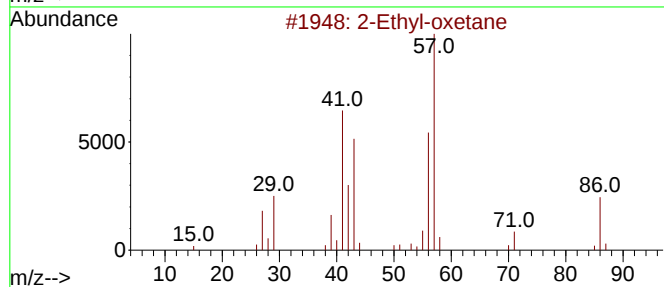
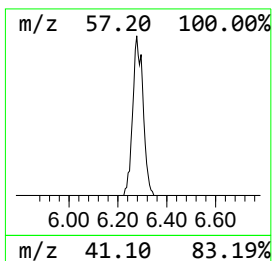
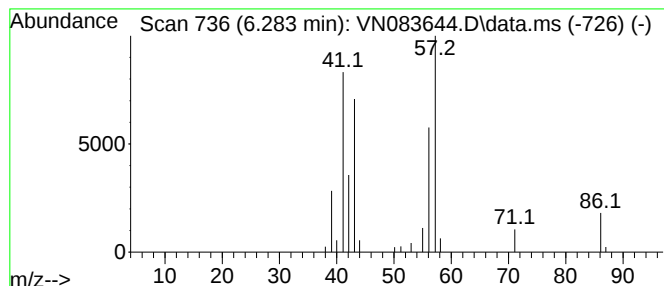
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Ethyl-oxetane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.283	11.23 ug/l	119362	Pentafluorobenzene	8.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	90
2			n-Hexane	86	C6H14	000110-54-3	87
3			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40
4			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
5			1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	38



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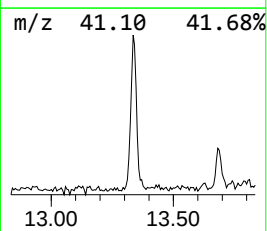
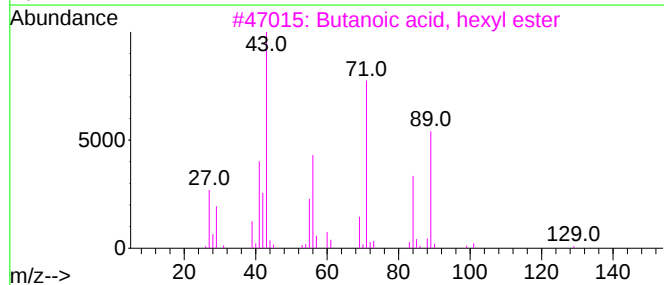
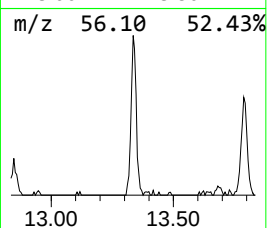
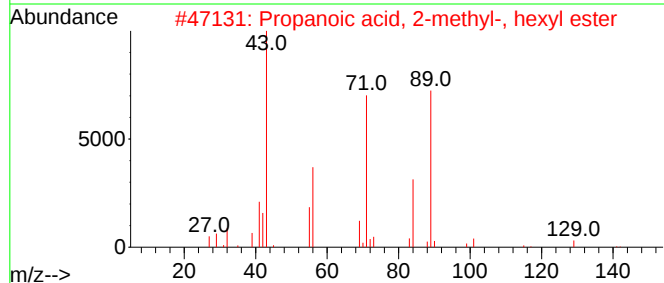
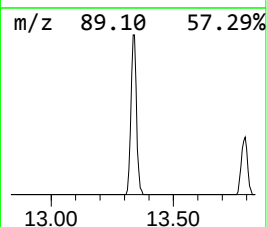
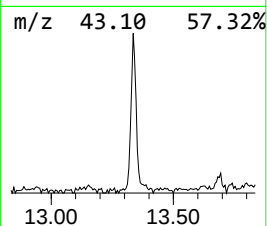
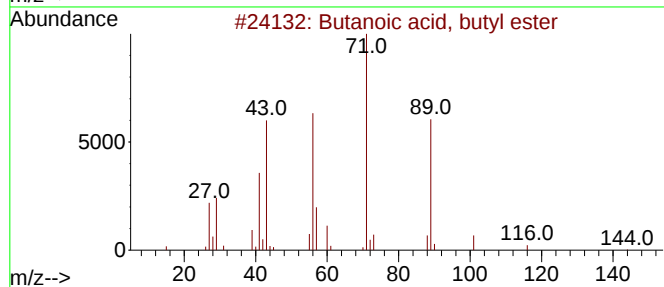
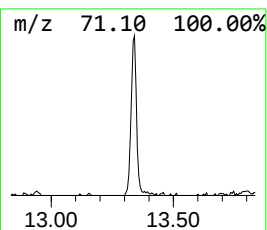
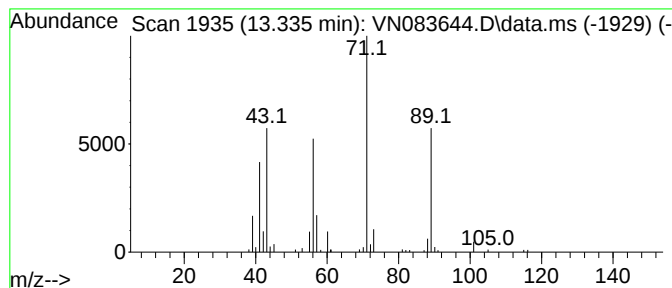
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	5.17 ug/l	113193	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Ethyl-oxetane	6.283	11.2	ug/l	119362	1	8.218	531251	50.0
Butanoic acid, ...	13.335	5.2	ug/l	113193	4	13.788	1093790	50.0