

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030624\
 Data File : VN081326.D
 Acq On : 06 Mar 2024 15:02
 Operator : JC\MD
 Sample : P1683-04 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3525

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\82N030524W.M

Title : SW846 8260

Signal : TIC: VN081326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.224	890	896	904	rVB6	9392	23555	1.34%	0.232%
2	8.171	1047	1057	1061	rBV	241578	573979	32.76%	5.652%
3	8.224	1061	1066	1081	rVB	426041	983565	56.13%	9.686%
4	8.583	1115	1127	1134	rBV	270102	621704	35.48%	6.122%
5	8.659	1134	1140	1143	rBV4	30537	72638	4.15%	0.715%
6	9.106	1206	1216	1227	rBV	647757	1326861	75.73%	13.067%
7	10.571	1456	1465	1478	rBV	970481	1752206	100.00%	17.255%
8	11.871	1674	1686	1696	rBV	819847	1491919	85.15%	14.692%
9	12.424	1774	1780	1785	rVB4	11937	19852	1.13%	0.195%
10	12.853	1845	1853	1863	rBV	604724	1036280	59.14%	10.205%
11	13.259	1912	1922	1929	rBV	199137	338793	19.34%	3.336%
12	13.341	1930	1936	1942	rVB	344145	506714	28.92%	4.990%
13	13.506	1957	1964	1969	rBV5	19934	33049	1.89%	0.325%
14	13.688	1988	1995	2002	rBV4	26263	50392	2.88%	0.496%
15	13.794	2005	2013	2021	rBV	742457	1258471	71.82%	12.393%
16	13.876	2021	2027	2034	rVB2	38986	64554	3.68%	0.636%

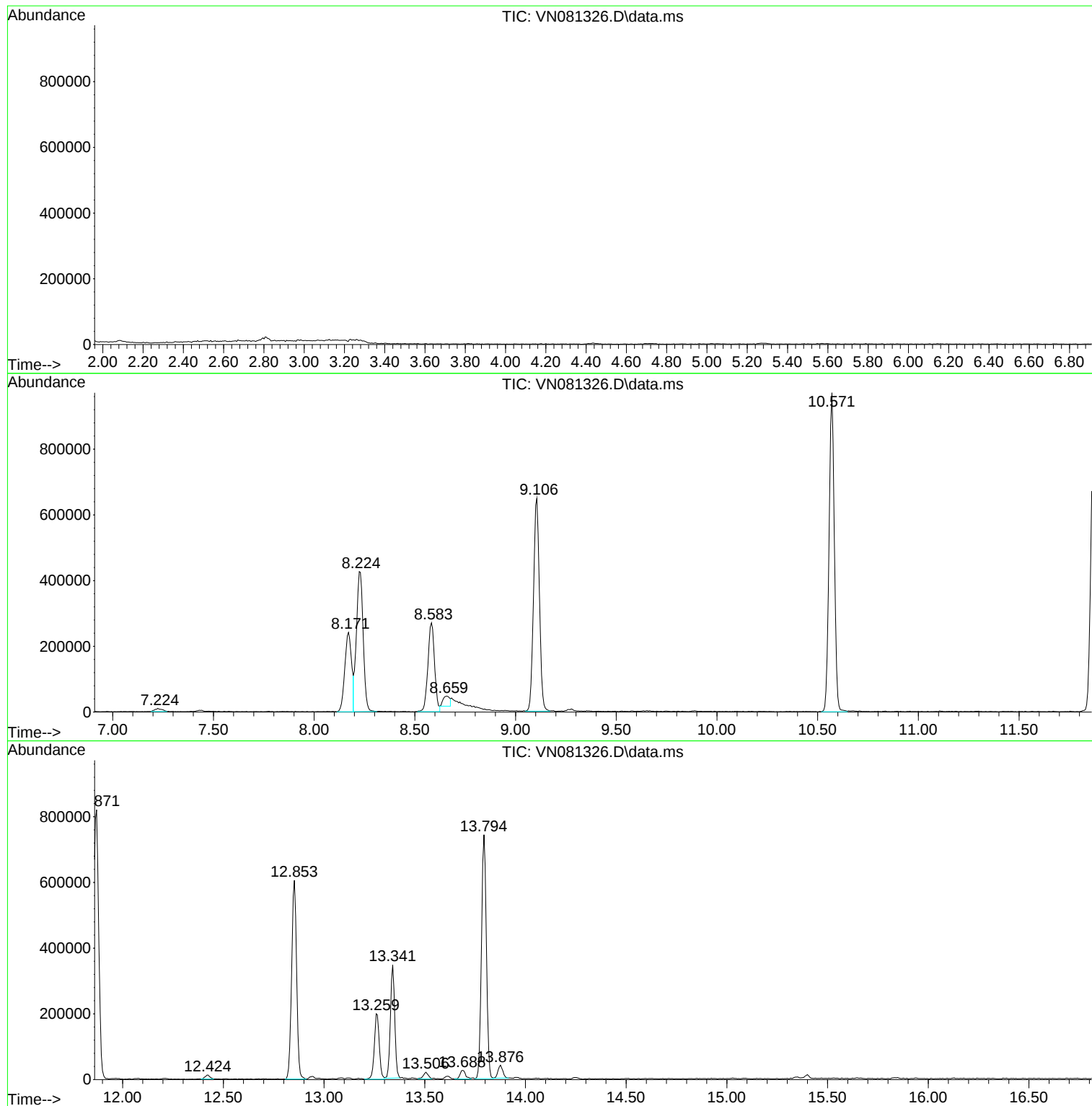
Sum of corrected areas: 10154532

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030524W.M
Quant Title : SW846 8260

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



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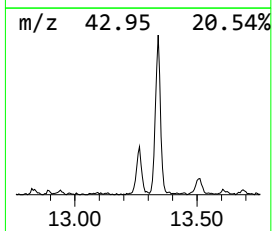
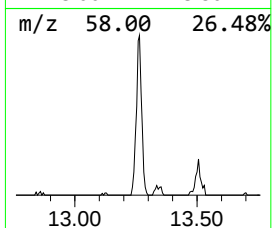
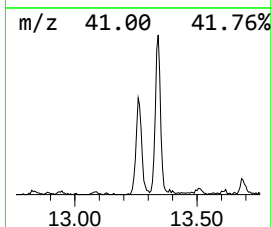
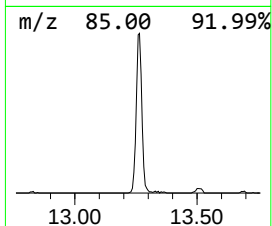
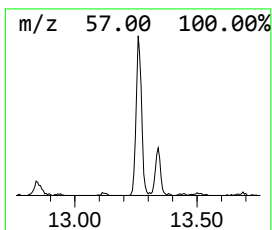
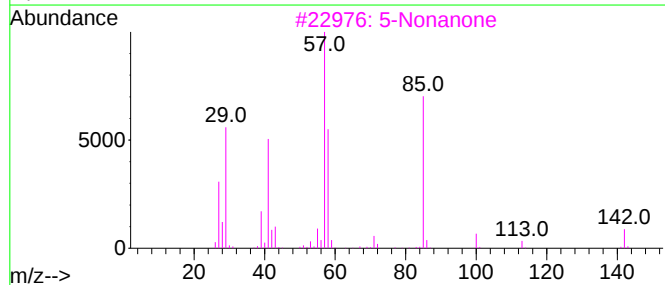
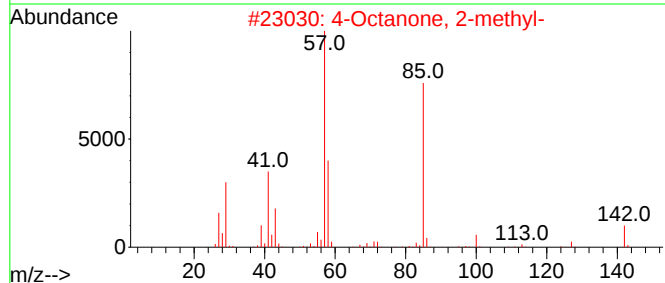
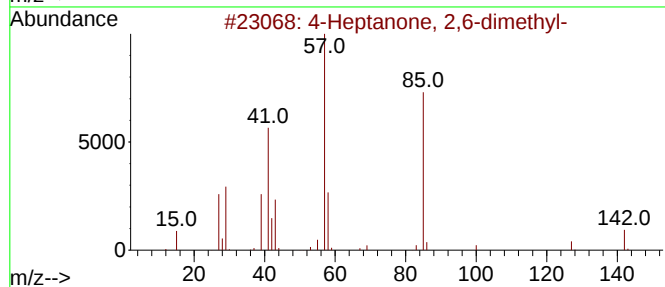
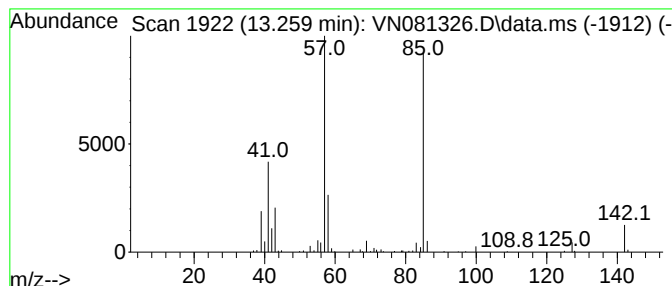
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TIC Integration Parameters: LSCINT.P

Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	13.46 ug/l	338793	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			Allyl isovalerate	142	C8H14O2	002835-39-4	50
5			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47



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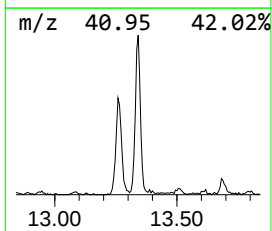
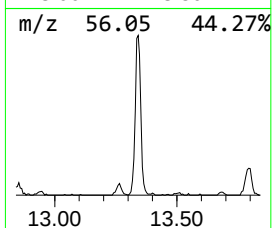
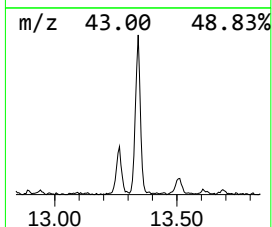
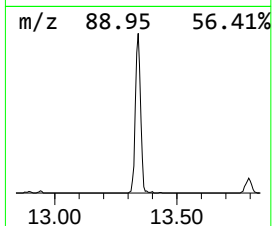
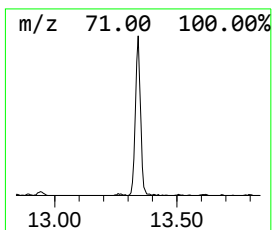
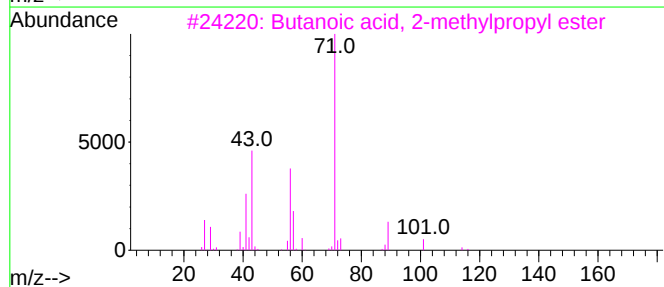
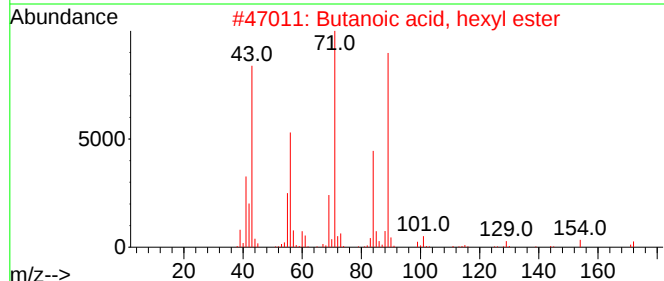
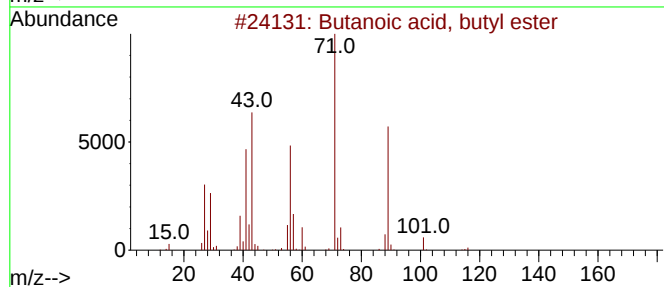
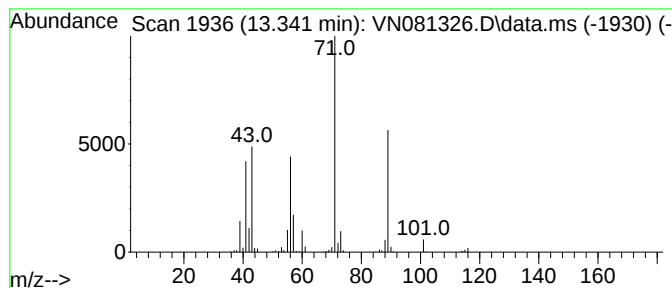
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Peak Number 2 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	20.13 ug/l	506714	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	50
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	13.259	13.5	ug/l	338793	4	13.794	1258470	50.0
Butanoic acid, ...	13.341	20.1	ug/l	506714	4	13.794	1258470	50.0