

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
 Data File : VN082372.D
 Acq On : 29 May 2024 15:53
 Operator : JC\MD
 Sample : P2609-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 509

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.295	220	228	239	rBV2	8543	22963	1.88%	0.331%
2	3.436	245	252	253	rBV	10041	14576	1.20%	0.210%
3	6.647	787	798	808	rBV3	17687	56300	4.62%	0.810%
4	7.794	982	993	1000	rBV	146292	381263	31.29%	5.488%
5	7.877	1000	1007	1020	rVB2	246802	623616	51.18%	8.976%
6	8.265	1064	1073	1087	rVB	171072	427397	35.07%	6.152%
7	8.865	1166	1175	1186	rBV	402779	861372	70.69%	12.398%
8	10.241	1403	1409	1419	rBV4	4911	13437	1.10%	0.193%
9	10.453	1436	1445	1454	rBV	652120	1218529	100.00%	17.539%
10	11.812	1663	1676	1691	rBV	624222	1098032	90.11%	15.804%
11	12.823	1838	1848	1860	rBV	473436	829220	68.05%	11.935%
12	13.247	1912	1920	1929	rBV	170776	270022	22.16%	3.887%
13	13.494	1954	1962	1970	rBV	64667	105768	8.68%	1.522%
14	13.782	2003	2011	2019	rBV	585516	980442	80.46%	14.112%
15	15.053	2218	2227	2234	rBV6	5680	12199	1.00%	0.176%
16	15.394	2279	2285	2290	rBV3	18310	32473	2.66%	0.467%

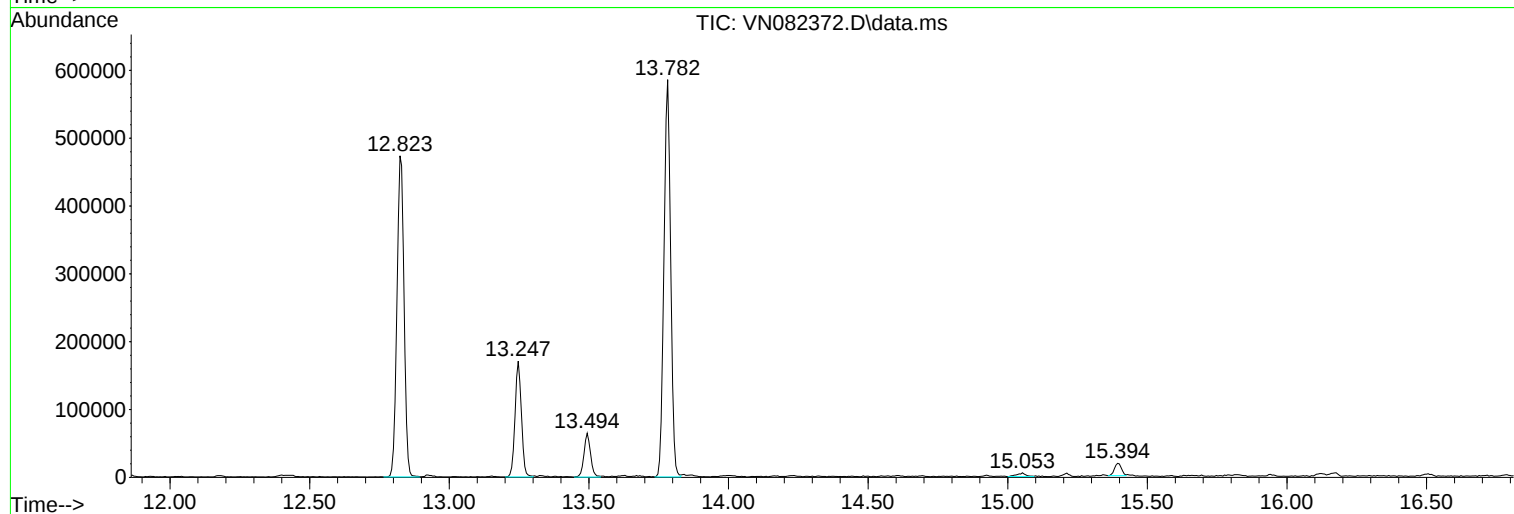
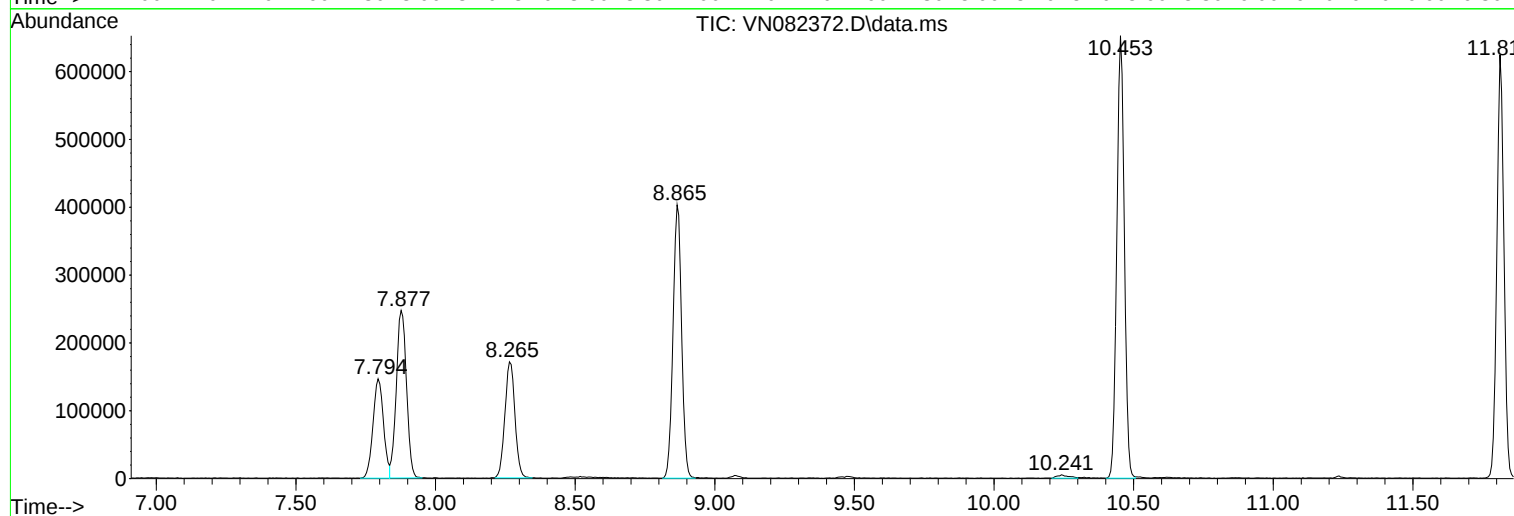
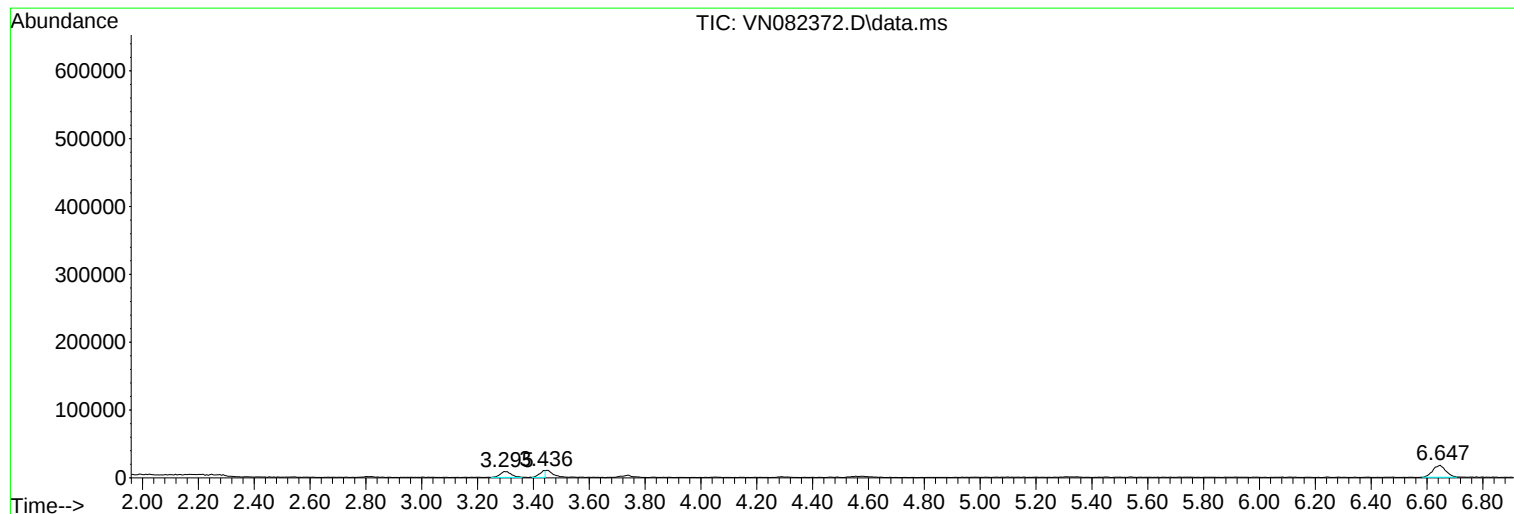
Sum of corrected areas: 6947609

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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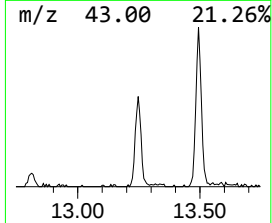
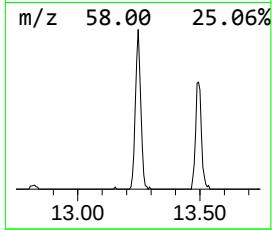
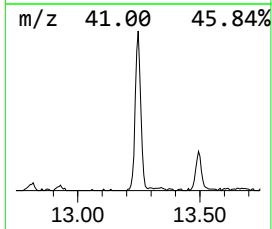
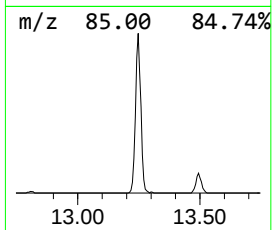
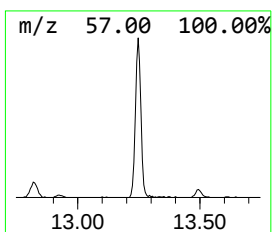
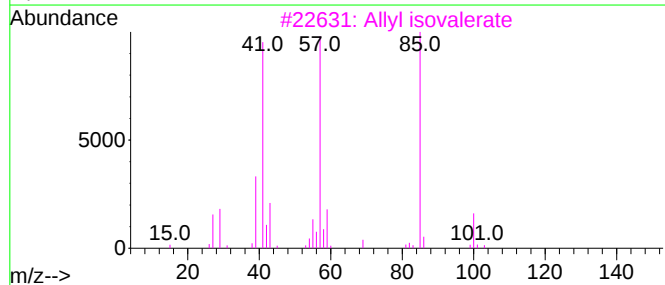
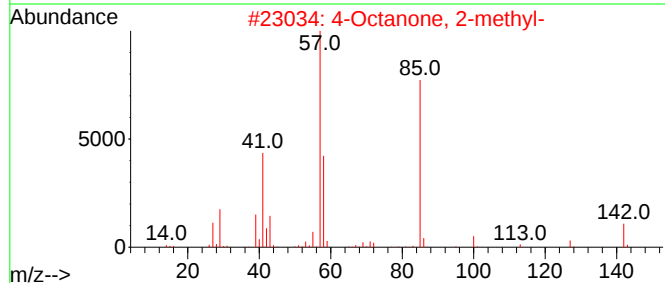
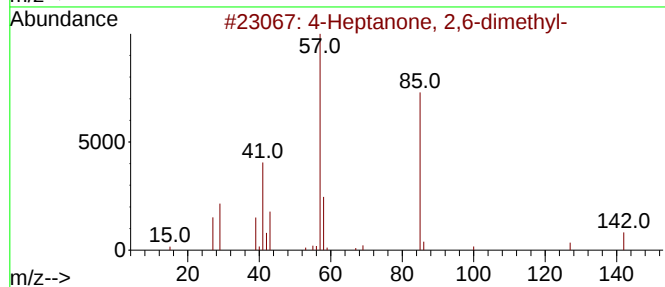
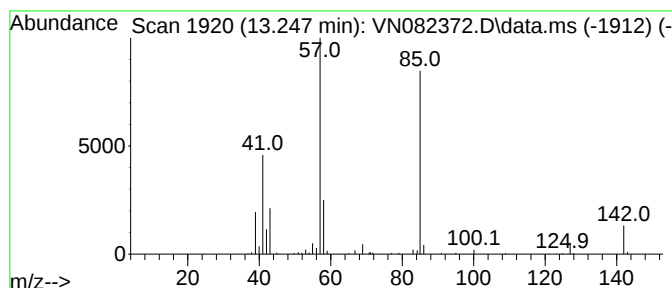
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.247	13.77 ug/l	270022	1,4-Dichlorobenzene-d4	13.782

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	80
3			Allyl isovalerate	142	C8H14O2	002835-39-4	59
4			5-Nonanone	142	C9H18O	000502-56-7	59
5			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50



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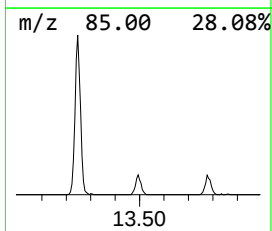
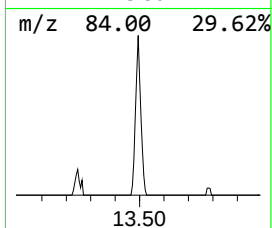
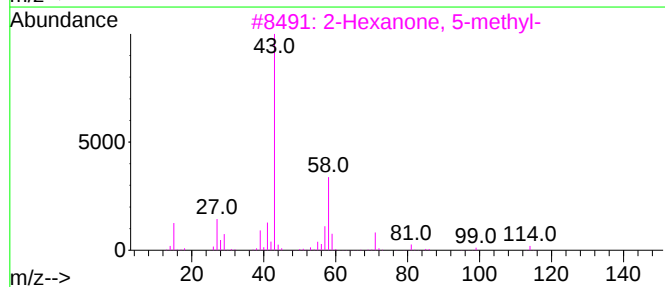
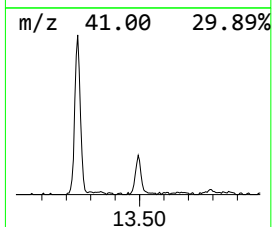
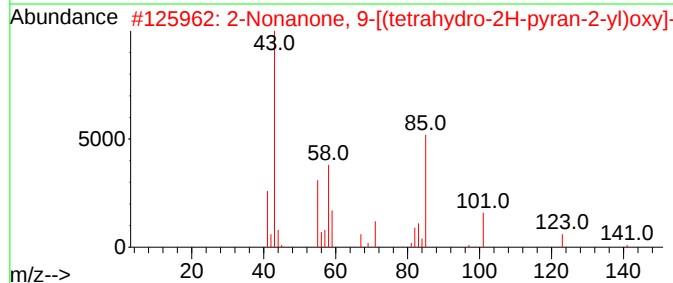
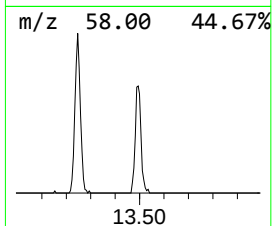
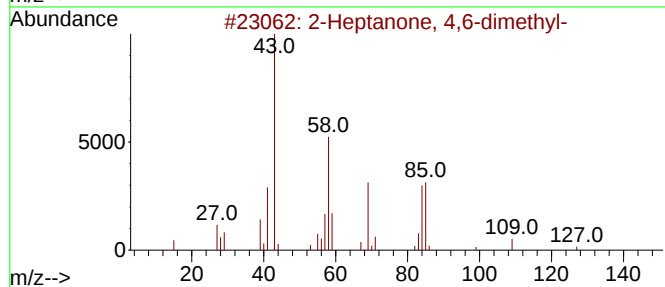
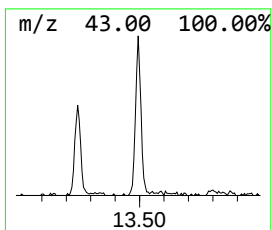
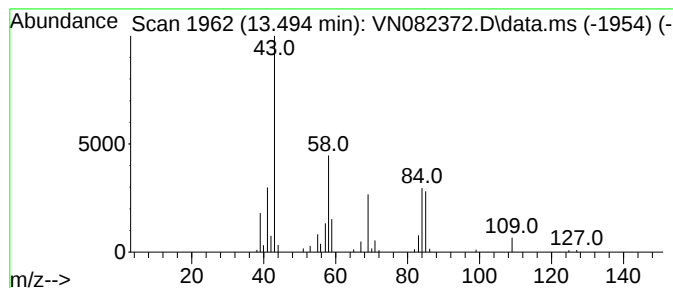
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.494	5.39 ug/l	105768	1,4-Dichlorobenzene-d4	13.782

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	72
2			2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	64
3			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	47
4			3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	47
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	13.247	13.8	ug/l	270022	4	13.782	980442	50.0
2-Heptanone, 4,...	13.494	5.4	ug/l	105768	4	13.782	980442	50.0