

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022724\
 Data File : VX040495.D
 Acq On : 27 Feb 2024 17:22
 Operator : JC/MD
 Sample : P1613-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1848

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\82X022624W.M
 Title : SW846 8260

Signal : TIC: VX040495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	206	212	227	rVB	37726	60326	14.61%	2.076%
2	5.391	694	706	722	rBV3	47475	141213	34.20%	4.859%
3	5.550	722	732	752	rVB	77627	221194	53.57%	7.611%
4	5.958	788	799	812	rBV	56921	150324	36.41%	5.172%
5	6.763	921	931	942	rBV	125709	298426	72.28%	10.268%
6	8.647	1233	1240	1247	rBV	261579	412868	100.00%	14.205%
7	8.720	1247	1252	1266	rVB	67137	106751	25.86%	3.673%
8	10.055	1464	1471	1481	rBV	289943	389758	94.40%	13.410%
9	10.195	1490	1494	1499	rVB2	5418	7603	1.84%	0.262%
10	10.299	1506	1511	1517	rBV	22905	32222	7.80%	1.109%
11	10.640	1563	1567	1574	rBV	8077	10769	2.61%	0.371%
12	11.079	1634	1639	1650	rBV	232477	303587	73.53%	10.445%
13	11.567	1714	1719	1733	rBV	187652	248237	60.13%	8.541%
14	11.683	1733	1738	1747	rVB3	6652	9963	2.41%	0.343%
15	11.829	1757	1762	1768	rBV	37246	51537	12.48%	1.773%
16	11.884	1768	1771	1780	rVV3	11480	15794	3.83%	0.543%
17	11.975	1782	1786	1789	rVV3	2931	4290	1.04%	0.148%
18	12.024	1789	1794	1802	rVV	314417	406528	98.46%	13.987%
19	12.103	1803	1807	1812	rVB2	9502	11788	2.86%	0.406%
20	12.524	1872	1876	1882	rBV5	4489	5953	1.44%	0.205%
21	13.731	2070	2074	2079	rBV3	8732	12935	3.13%	0.445%
22	13.780	2079	2082	2091	rVB2	3196	4349	1.05%	0.150%

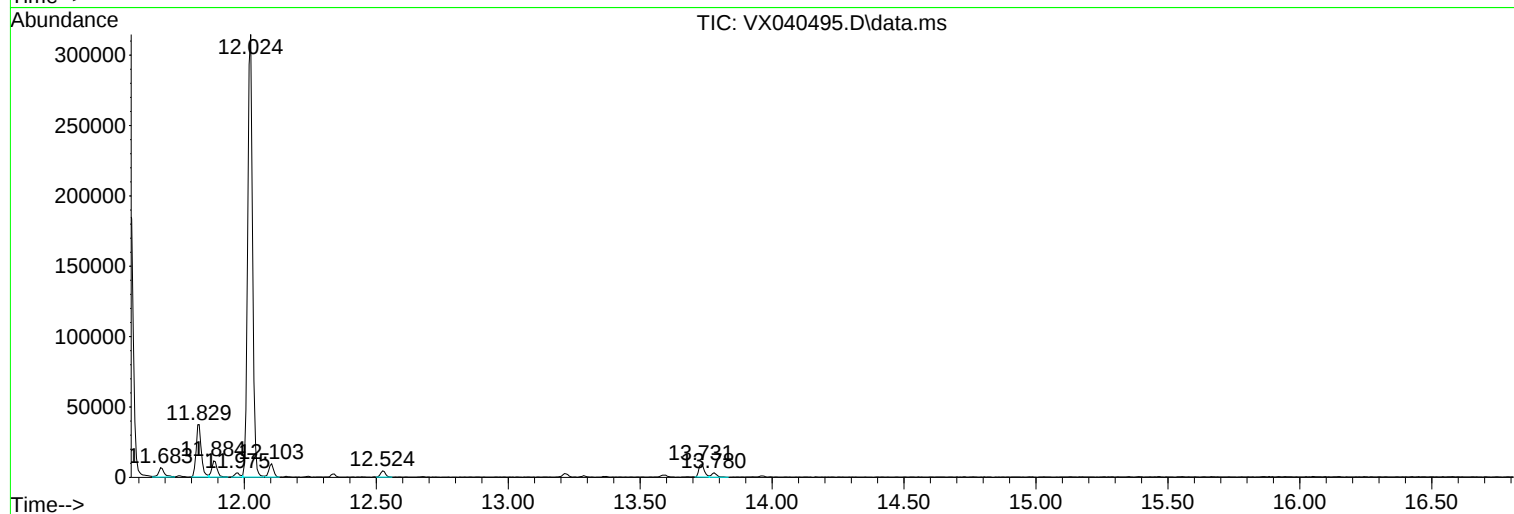
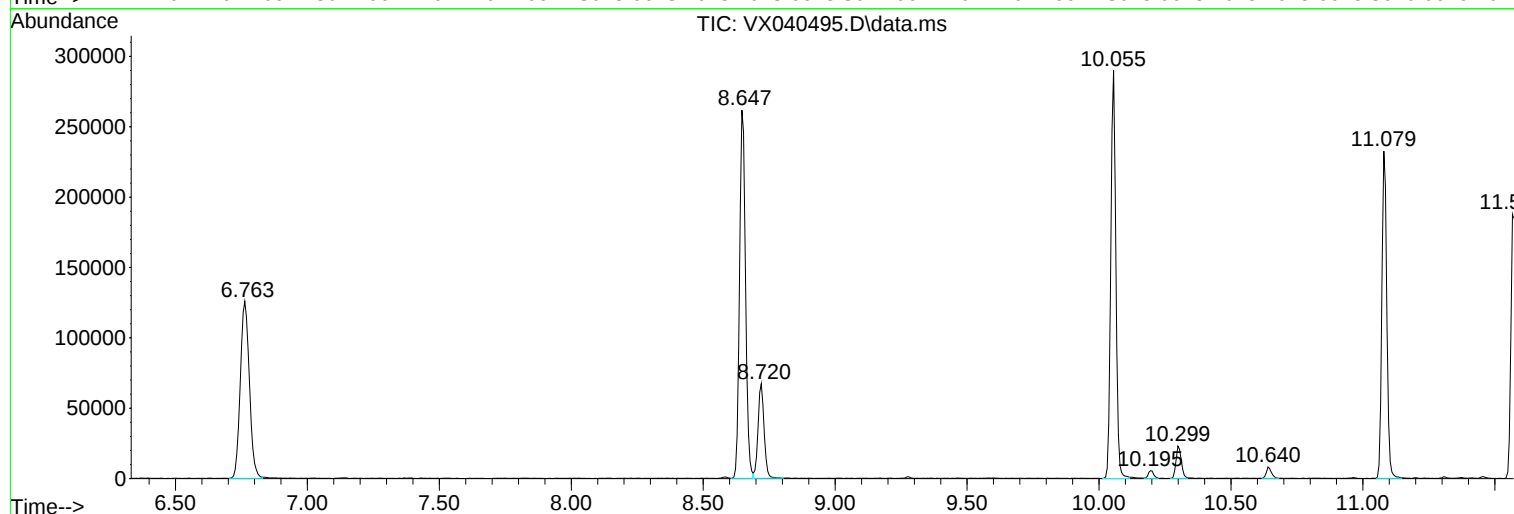
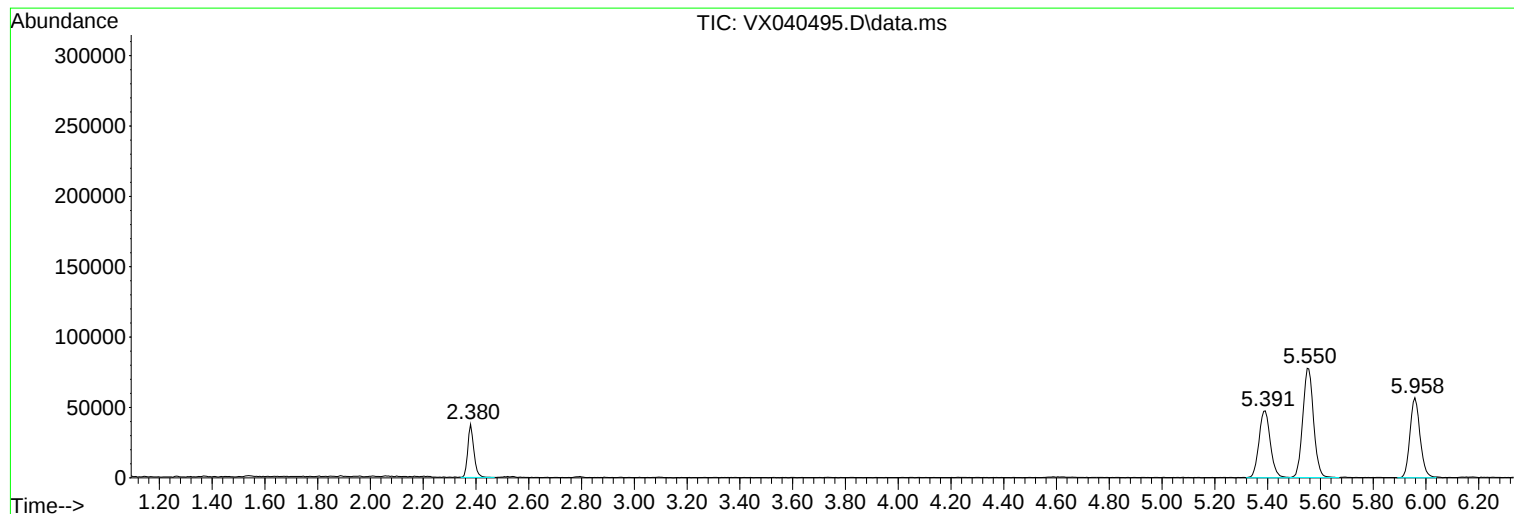
Sum of corrected areas: 2906415

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Instrument :
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ClientSampleId :
1848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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



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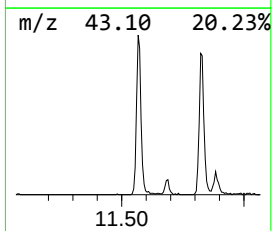
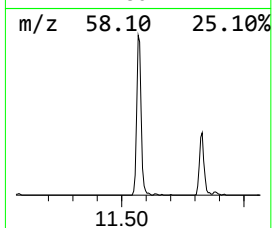
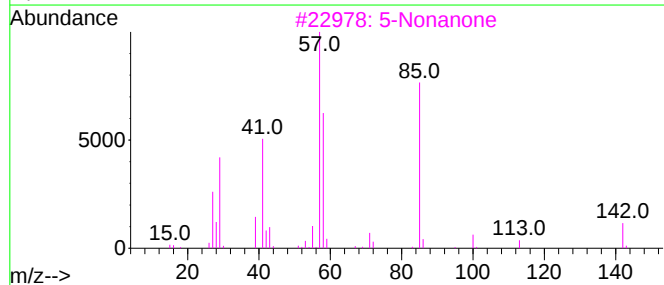
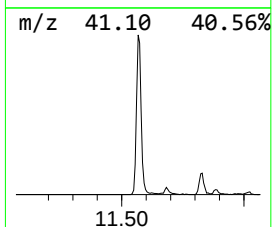
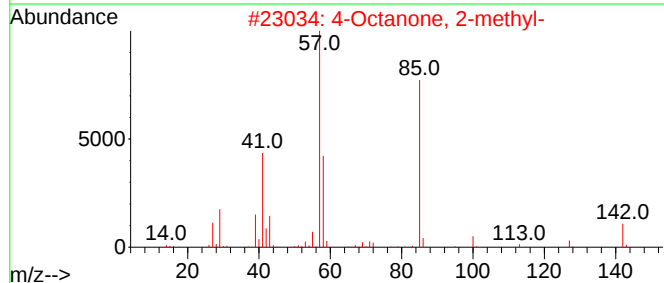
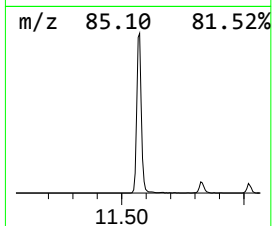
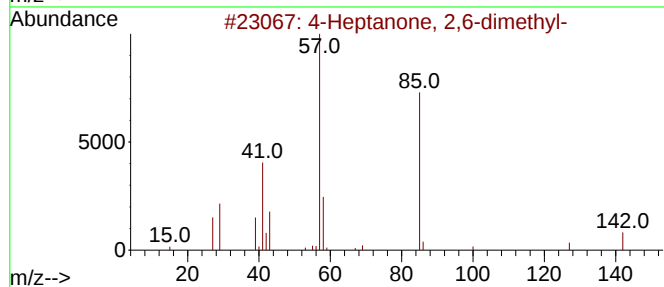
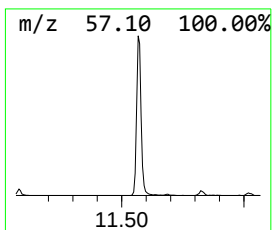
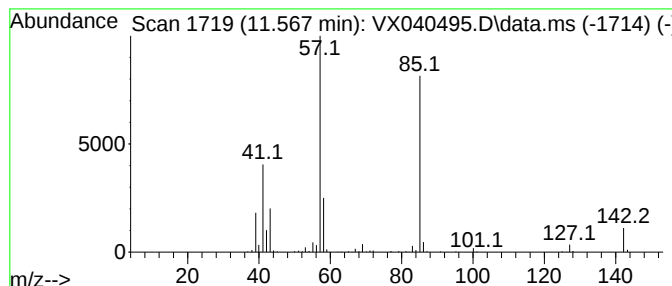
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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.
11.567	30.53 ug/l	248237	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2		4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
3		5-Nonanone	142	C9H18O	000502-56-7	64
4		4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	56
5		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47



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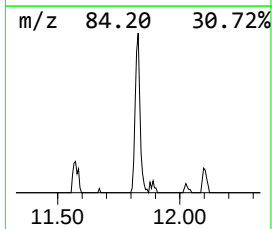
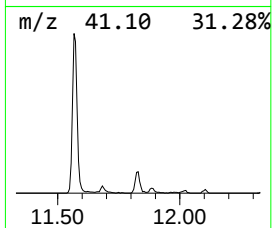
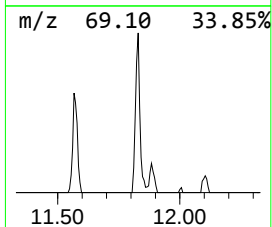
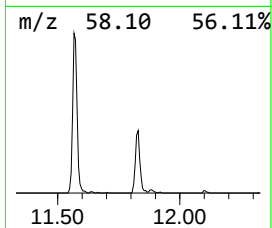
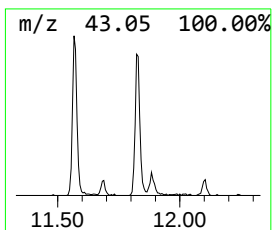
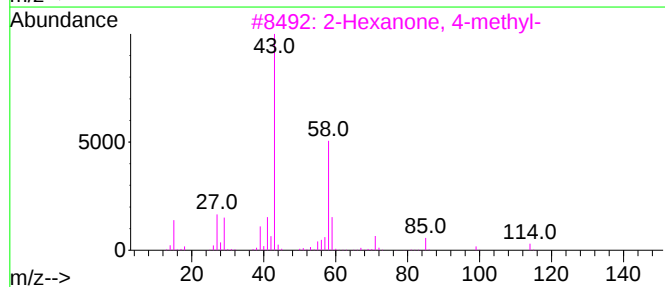
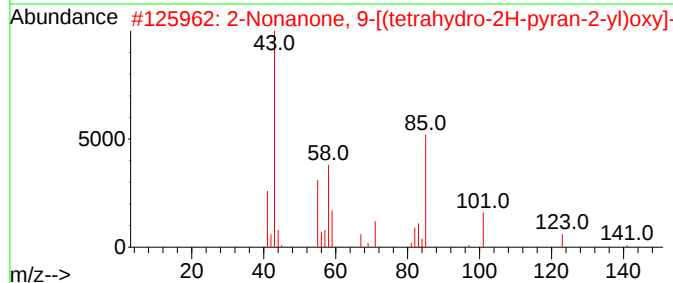
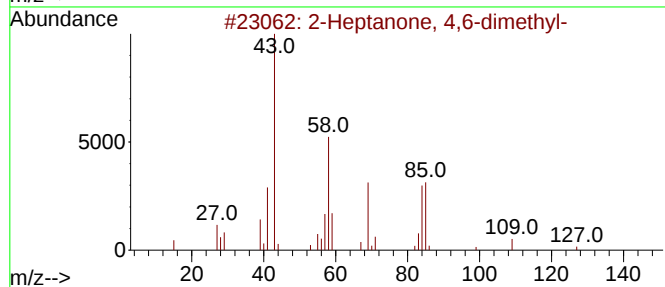
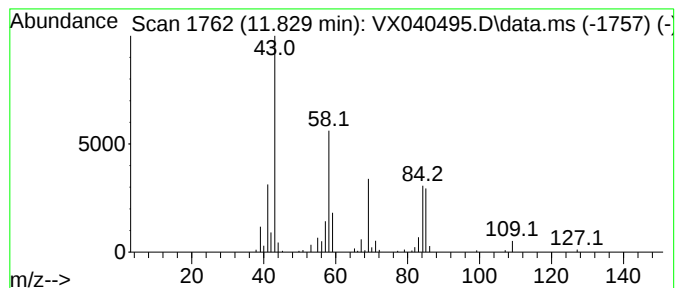
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.829	6.34 ug/l	51537	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	78
2			2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	50
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	50
4			Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	50
5			1,3-Dioxane-2-propanol, 2-methyl-	160	C8H16O3	036651-31-7	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	11.567	30.5	ug/l	248237	4	12.024	406528	50.0
2-Heptanone, 4,...	11.829	6.3	ug/l	51537	4	12.024	406528	50.0