

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060123\
 Data File : VX035959.D
 Acq On : 01 Jun 2023 15:01
 Operator : JC/MD
 Sample : 02997-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DMA-1103

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\82X053123W.M
 Title : SW846 8260

Signal : TIC: VX035959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	37	45	50	rBV4	12643	40585	3.79%	0.623%
2	2.148	171	174	180	rVB4	7460	12597	1.18%	0.193%
3	2.392	206	214	228	rVB2	23055	68584	6.41%	1.053%
4	2.611	238	250	255	rBV3	4184	16979	1.59%	0.261%
5	4.574	562	572	581	rBV2	5223	15130	1.41%	0.232%
6	5.099	648	658	666	rBV2	8025	23045	2.15%	0.354%
7	5.385	693	705	718	rBV	117440	342830	32.03%	5.261%
8	5.550	720	732	749	rVB2	236922	663048	61.94%	10.176%
9	5.958	788	799	815	rBV	146473	384720	35.94%	5.904%
10	6.757	920	930	944	rBV	339249	817985	76.42%	12.553%
11	8.574	1221	1228	1234	rBV	29982	48508	4.53%	0.744%
12	8.647	1234	1240	1248	rVV	692923	1070388	100.00%	16.427%
13	8.720	1248	1252	1258	rVB	13360	21429	2.00%	0.329%
14	9.525	1375	1384	1390	rBV3	7595	13851	1.29%	0.213%
15	10.055	1464	1471	1485	rBV	682157	930048	86.89%	14.273%
16	10.769	1582	1588	1599	rBV	217522	278551	26.02%	4.275%
17	10.878	1599	1606	1619	rVV	51919	84496	7.89%	1.297%
18	11.079	1634	1639	1652	rVB	563835	707148	66.06%	10.852%
19	12.018	1788	1793	1803	rBV	708864	902781	84.34%	13.855%
20	12.219	1821	1826	1836	rBV	28709	47659	4.45%	0.731%
21	12.853	1926	1930	1935	rVB2	9153	11333	1.06%	0.174%
22	13.591	2047	2051	2059	rBV4	8410	14403	1.35%	0.221%

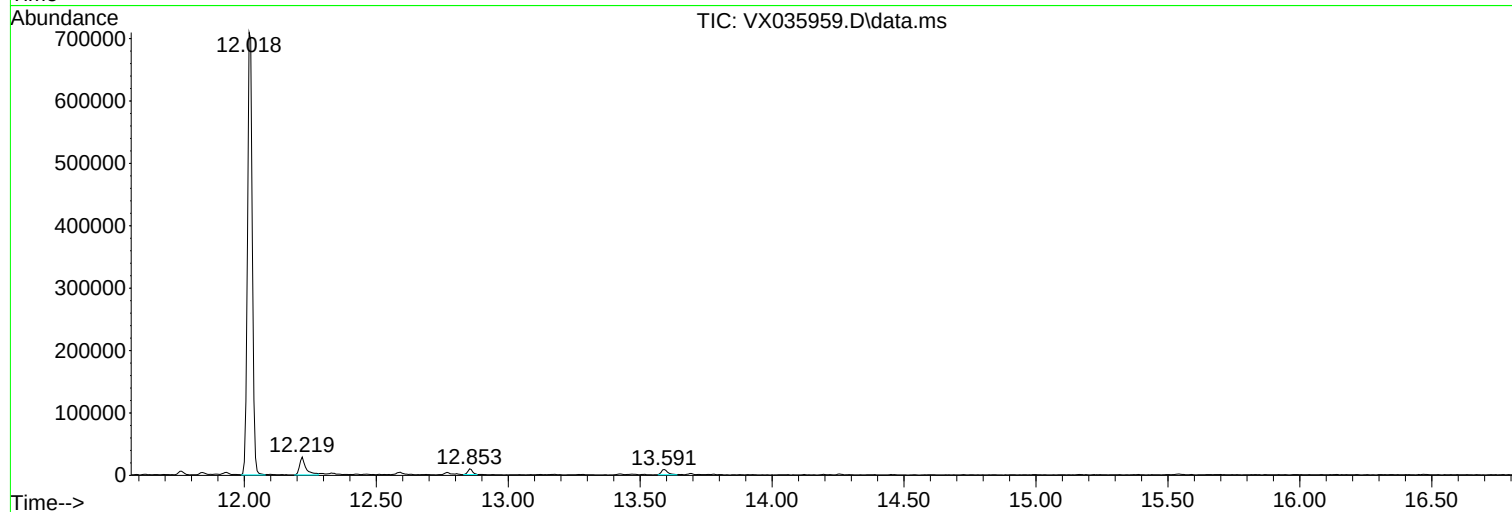
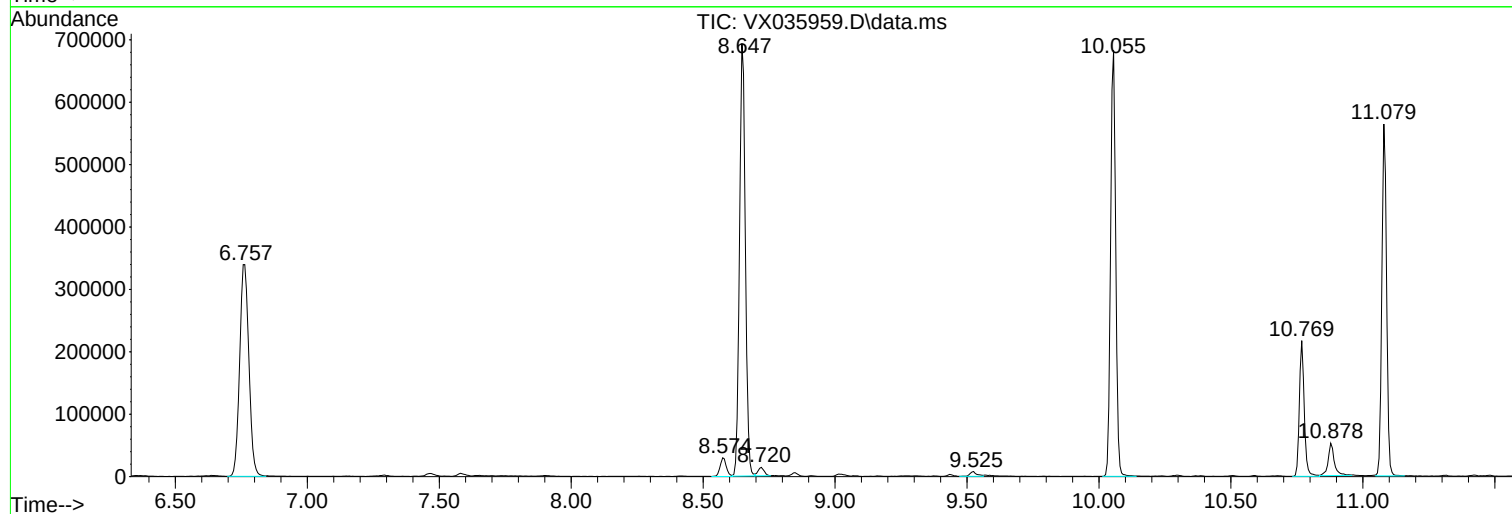
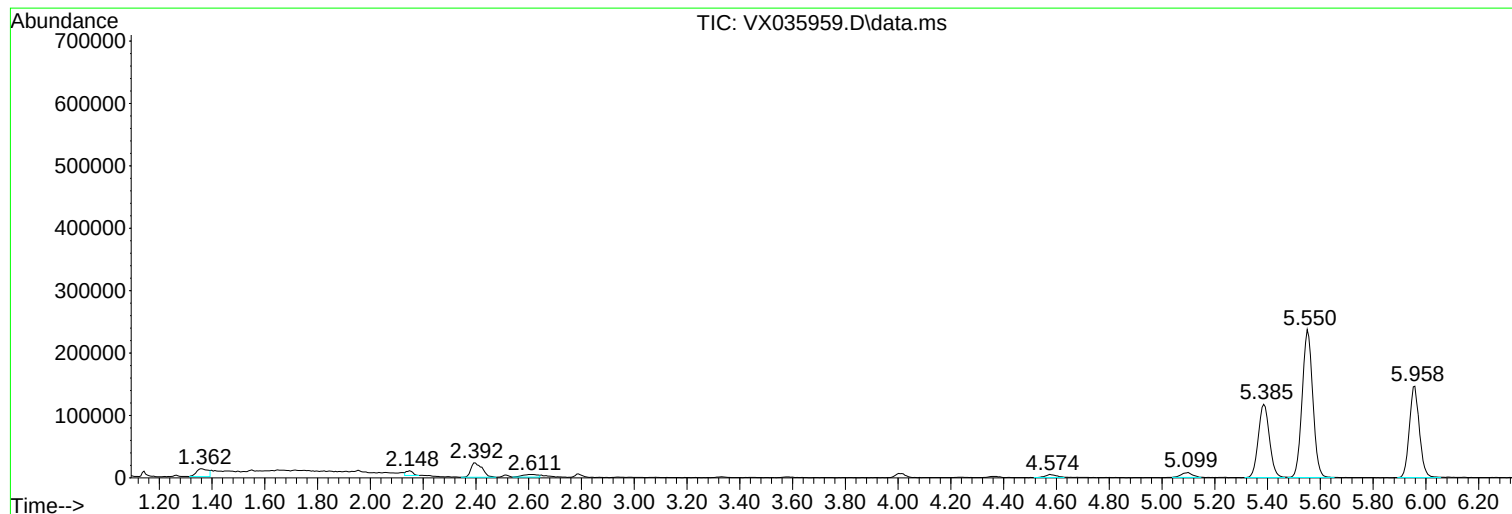
Sum of corrected areas: 6516098

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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



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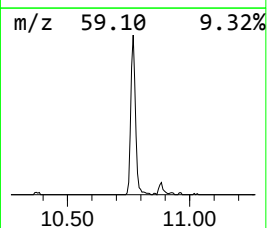
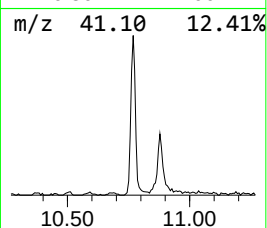
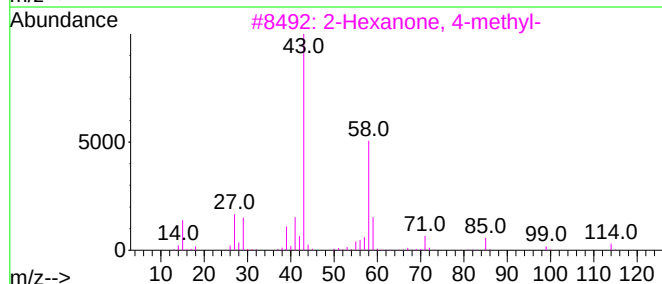
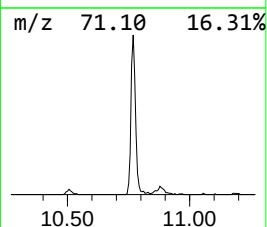
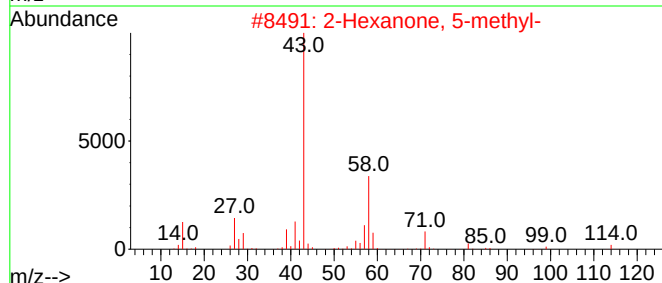
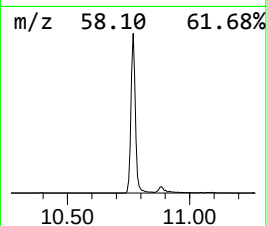
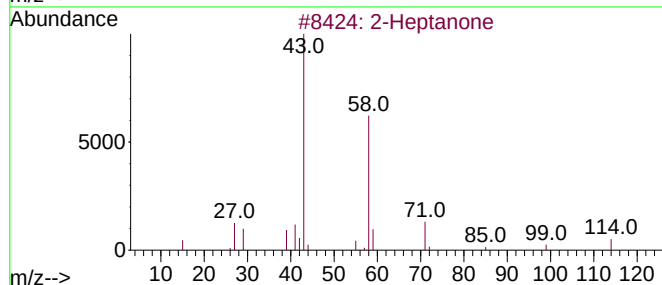
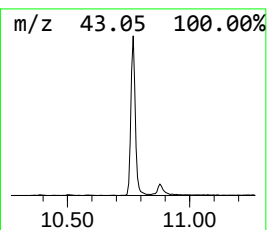
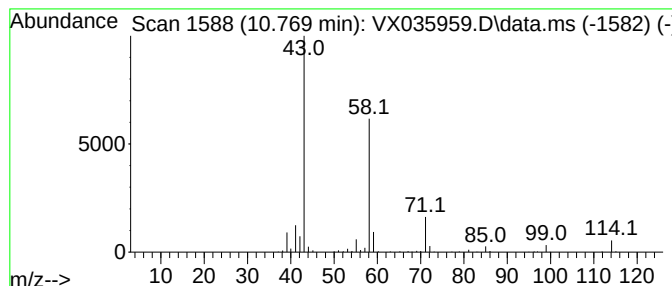
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Heptanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	14.98 ug/l	278551	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4			2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52
5			Butane, 2-(ethenyl-)-2-methyl-	114	C7H14O	029281-39-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Heptanone	10.769	15.0	ug/l	278551	3	10.055	930048	50.0