

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031125\
 Data File : VX045229.D
 Acq On : 11 Mar 2025 17:06
 Operator : JC/MD
 Sample : Q1541-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 205703

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\82X022825W.M

Title : SW846 8260

Signal : TIC: VX045229.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	70	84	85	rBV8	5403	17287	3.58%	0.645%
2	2.379	208	212	219	rBV	3037	5374	1.11%	0.201%
3	5.385	694	705	722	rBV	55000	163835	33.92%	6.115%
4	5.543	722	731	746	rVV	77253	220233	45.60%	8.219%
5	5.952	788	798	813	rBV2	65680	173223	35.86%	6.465%
6	6.757	920	930	943	rBV	140835	342587	70.93%	12.786%
7	8.646	1233	1240	1257	rBV	298665	483020	100.00%	18.027%
8	10.049	1465	1470	1484	rBV	300930	424554	87.90%	15.845%
9	11.079	1634	1639	1650	rBV	224679	292205	60.50%	10.905%
10	11.567	1714	1719	1733	rBV	94319	137874	28.54%	5.146%
11	11.829	1756	1762	1768	rBV	26046	41701	8.63%	1.556%
12	11.884	1768	1771	1776	rVB4	9580	12341	2.55%	0.461%
13	12.018	1788	1793	1801	rVV	280831	356073	73.72%	13.289%
14	12.097	1803	1806	1812	rVB5	6229	9141	1.89%	0.341%

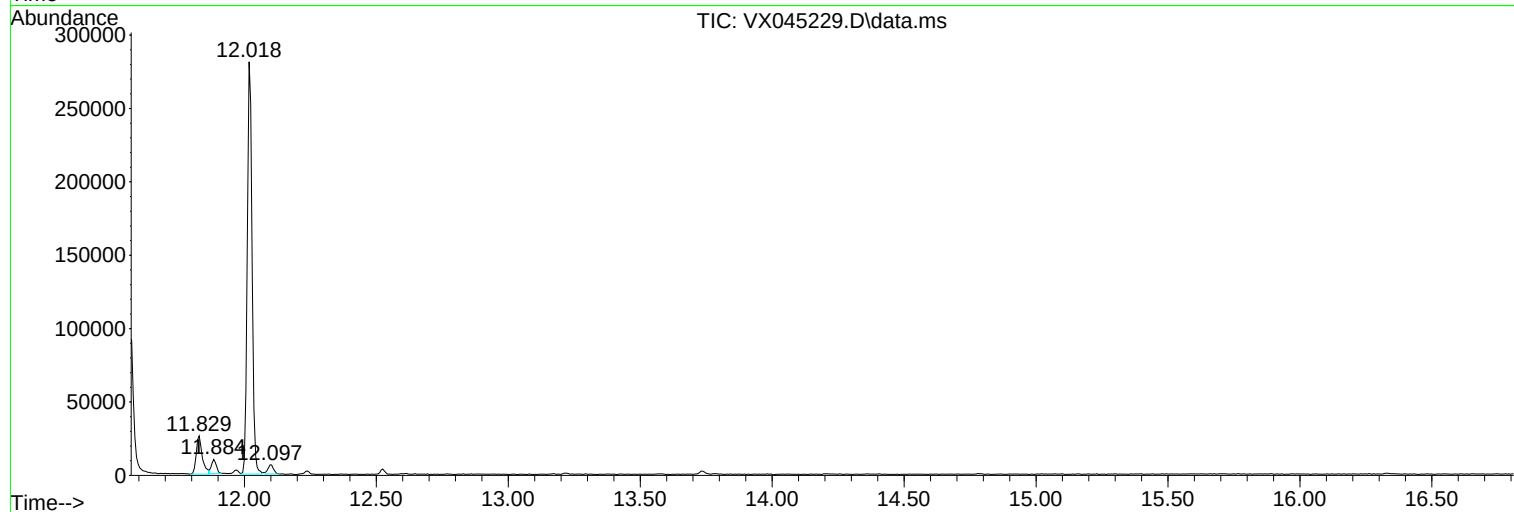
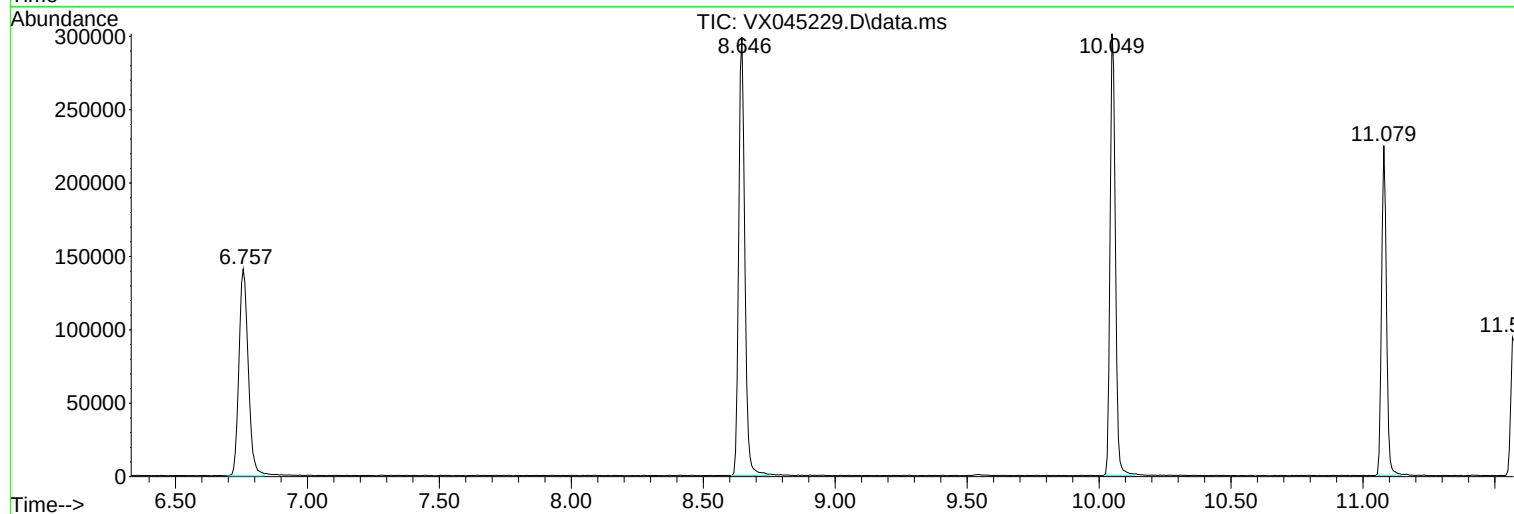
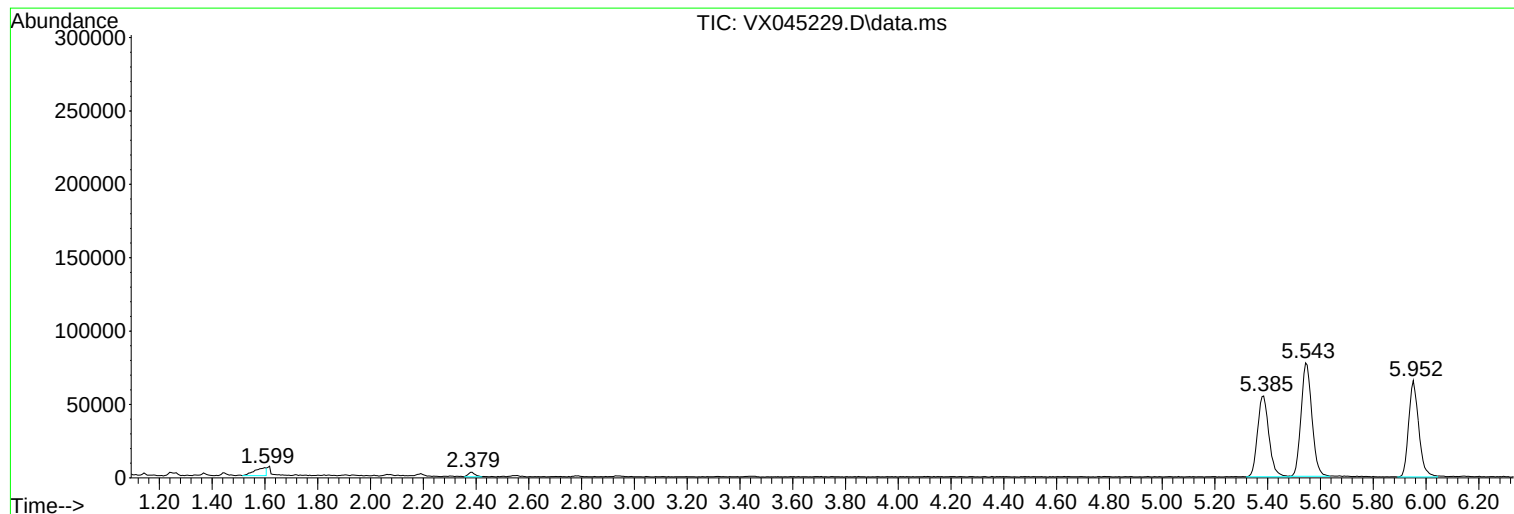
Sum of corrected areas: 2679448

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022825W.M
Quant Title : SW846 8260

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



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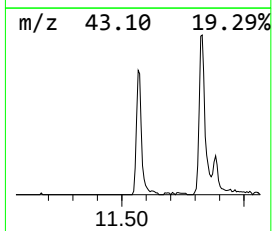
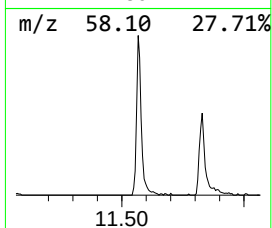
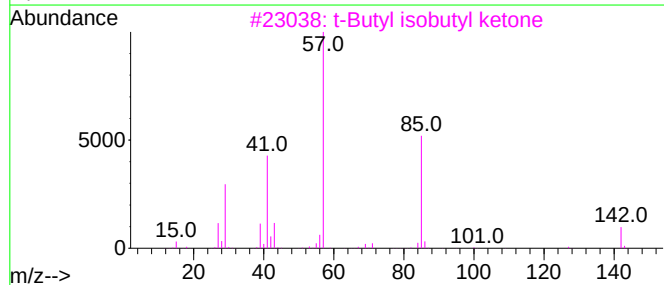
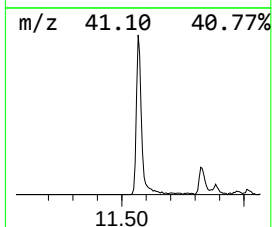
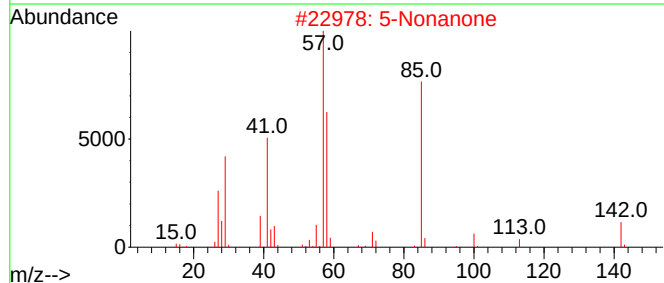
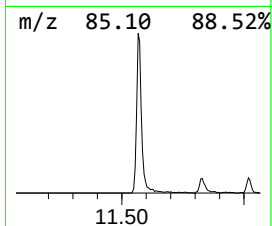
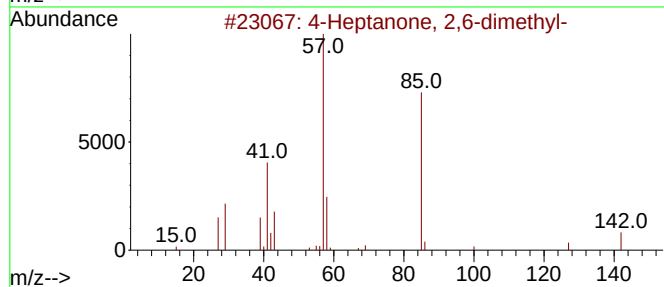
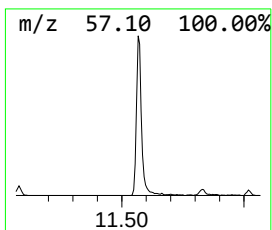
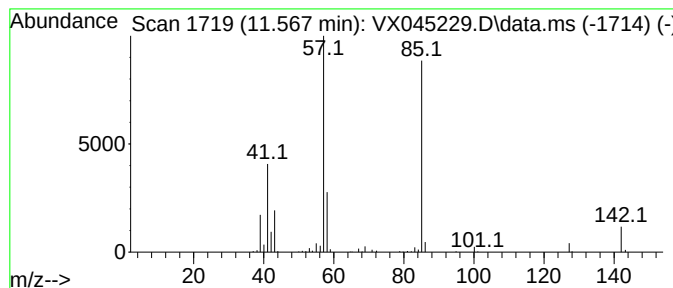
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022825W.M
Quant Title : SW846 8260

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	19.36 ug/l	137874	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			5-Nonanone	142	C9H18O	000502-56-7	64
3			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	64
4			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
5			2,4-Heptanedione, 6-methyl-	142	C8H14O2	003002-23-1	59



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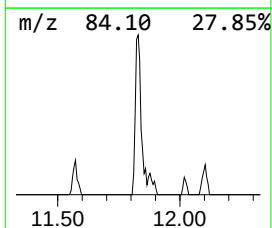
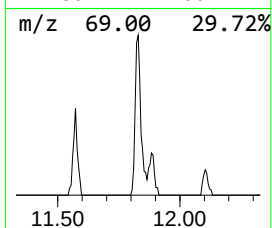
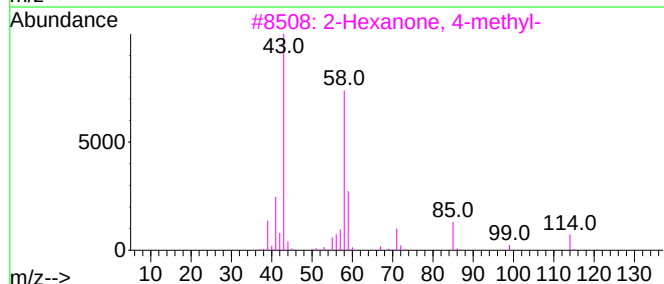
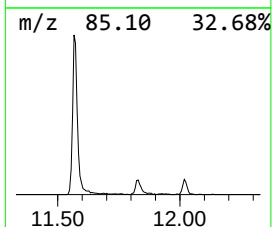
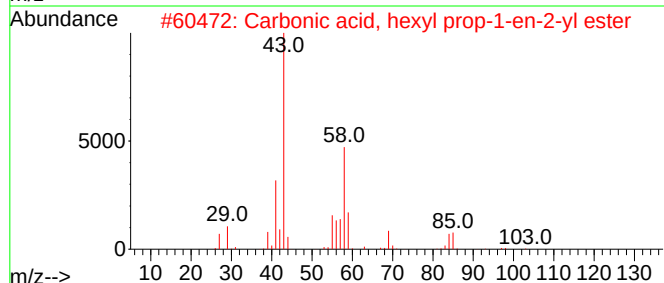
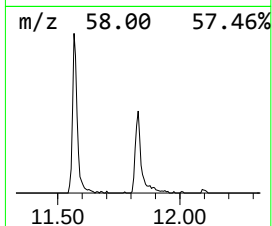
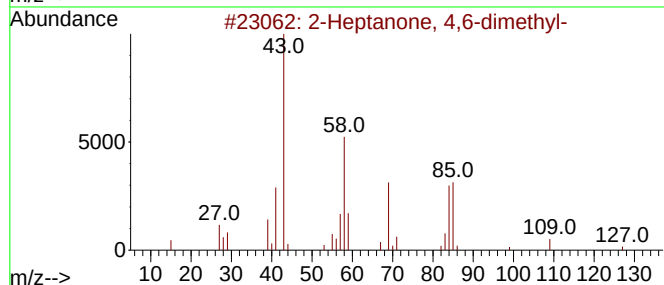
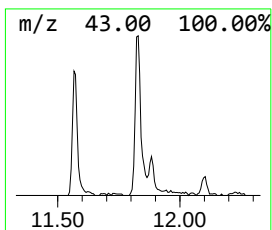
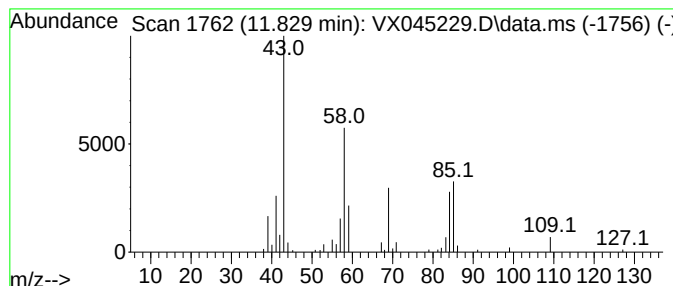
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.829	5.86 ug/l	41701	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	86
2		Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	78
3		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	42
4		Hexane, 3-ethyl-	114	C8H18	000619-99-8	38
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	37



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone, 2,...	11.567	19.4	ug/l	137874	4	12.018	356073	50.0
2-Heptanone, 4,...	11.829	5.9	ug/l	41701	4	12.018	356073	50.0