

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
 Data File : VX035060.D
 Acq On : 13 Apr 2023 13:40
 Operator : JC/MD
 Sample : 02325-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 230412098-02-VOA

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\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.386	206	213	223	rBV2	102875	197293	3.97%	0.773%
2	2.983	297	311	328	rBV	1455811	4898510	98.52%	19.200%
3	3.111	328	332	346	rVB2	36508	90403	1.82%	0.354%
4	4.574	552	572	587	rBV	1509246	4971995	100.00%	19.488%
5	5.007	632	643	665	rVB	558949	1739476	34.99%	6.818%
6	5.385	694	705	717	rBV2	150785	440431	8.86%	1.726%
7	5.550	722	732	745	rVB	276403	780521	15.70%	3.059%
8	5.952	789	798	807	rBV	175113	470898	9.47%	1.846%
9	6.044	807	813	820	rVB	40645	103615	2.08%	0.406%
10	6.245	836	846	857	rBV2	40829	136857	2.75%	0.536%
11	6.763	920	931	948	rBV	429785	1037680	20.87%	4.067%
12	8.574	1222	1228	1233	rBV3	27974	51468	1.04%	0.202%
13	8.647	1233	1240	1247	rBV	890798	1405928	28.28%	5.511%
14	8.720	1247	1252	1260	rVB2	77940	133210	2.68%	0.522%
15	8.805	1260	1266	1271	rBV	46456	77544	1.56%	0.304%
16	9.244	1331	1338	1346	rBV	33251	63168	1.27%	0.248%
17	9.378	1352	1360	1366	rBV	159055	243211	4.89%	0.953%
18	10.055	1460	1471	1483	rBV	901633	1374911	27.65%	5.389%
19	10.195	1489	1494	1504	rBV2	162565	255130	5.13%	1.000%
20	10.299	1504	1511	1518	rVB	187797	279461	5.62%	1.095%
21	10.384	1519	1525	1534	rVB3	26069	55001	1.11%	0.216%
22	10.640	1563	1567	1579	rVB	135645	197106	3.96%	0.773%
23	10.964	1614	1620	1626	rVB2	42734	70009	1.41%	0.274%
24	11.079	1634	1639	1645	rBV	731547	942615	18.96%	3.695%
25	11.378	1682	1688	1695	rBV3	34284	58870	1.18%	0.231%
26	11.506	1705	1709	1715	rVB	43163	62606	1.26%	0.245%
27	11.610	1723	1726	1735	rVB	36732	60427	1.22%	0.237%
28	11.750	1745	1749	1754	rVB	76073	100168	2.01%	0.393%
29	11.884	1763	1771	1778	rBV3	103212	168891	3.40%	0.662%
30	12.024	1788	1794	1801	rBV	874636	1250614	25.15%	4.902%
31	12.097	1801	1806	1810	rVV2	62158	110541	2.22%	0.433%
32	12.146	1810	1814	1823	rVB8	22817	60298	1.21%	0.236%
33	12.244	1824	1830	1840	rBV	83954	134394	2.70%	0.527%
34	12.335	1840	1845	1853	rVB5	26007	50143	1.01%	0.197%
35	12.414	1853	1858	1865	rBV4	26977	53635	1.08%	0.210%
36	12.524	1872	1876	1882	rBV3	62109	111637	2.25%	0.438%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	12.579	1882	1885	1889	rVB2	57750	70416	1.42%	0.276%
38	12.762	1910	1915	1920	rVB2	89076	132520	2.67%	0.519%
39	12.908	1927	1939	1944	rBV	975230	1364228	27.44%	5.347%
40	12.963	1944	1948	1953	rVB4	79413	117628	2.37%	0.461%
41	13.231	1985	1992	1996	rVB3	30690	63212	1.27%	0.248%
42	13.286	1996	2001	2005	rBV3	58686	80223	1.61%	0.314%
43	13.475	2027	2032	2036	rBV2	192528	280930	5.65%	1.101%
44	13.512	2036	2038	2046	rVB3	34879	52418	1.05%	0.205%
45	13.591	2046	2051	2061	rBV2	210285	390639	7.86%	1.531%
46	13.731	2070	2074	2077	rBV3	48124	65286	1.31%	0.256%
47	13.774	2077	2081	2089	rVB	289235	371049	7.46%	1.454%
48	13.926	2101	2106	2115	rBV5	42906	115495	2.32%	0.453%
49	14.097	2128	2134	2141	rBV3	51765	96815	1.95%	0.379%
50	14.780	2241	2246	2252	rVB	53300	73397	1.48%	0.288%

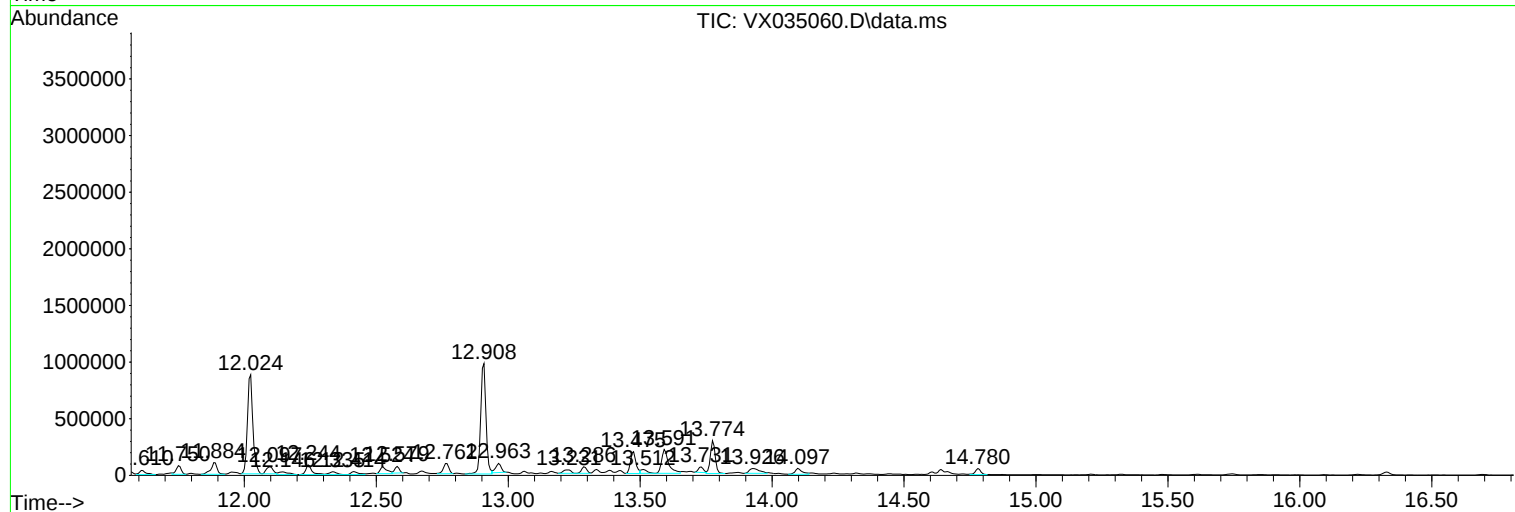
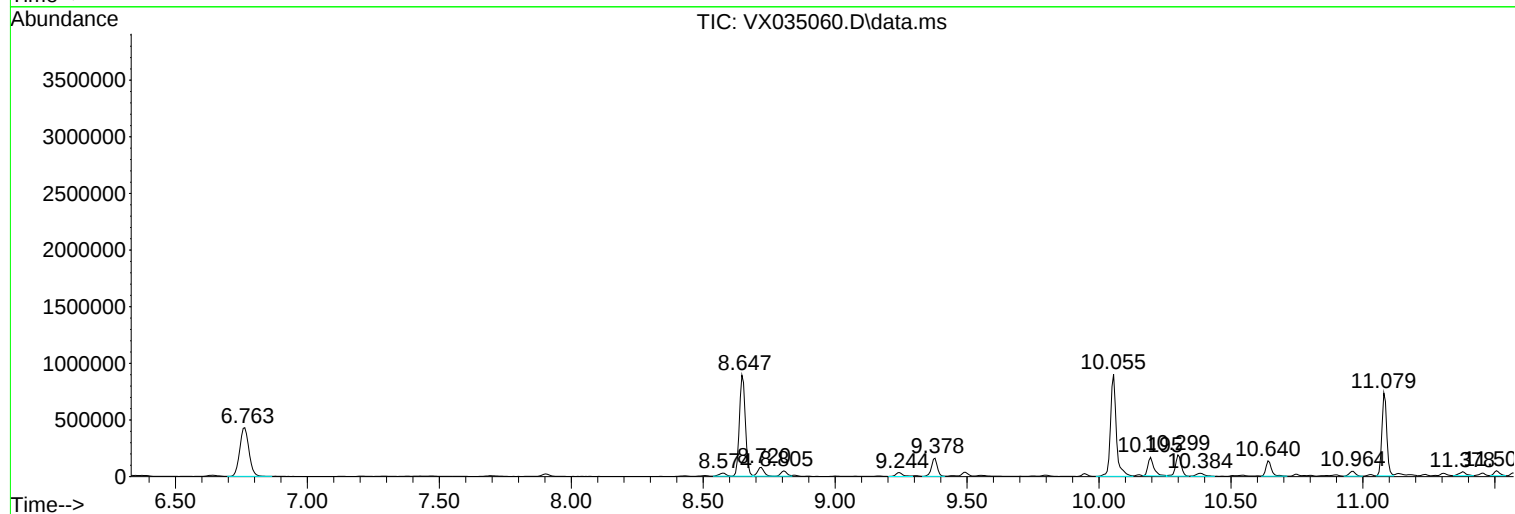
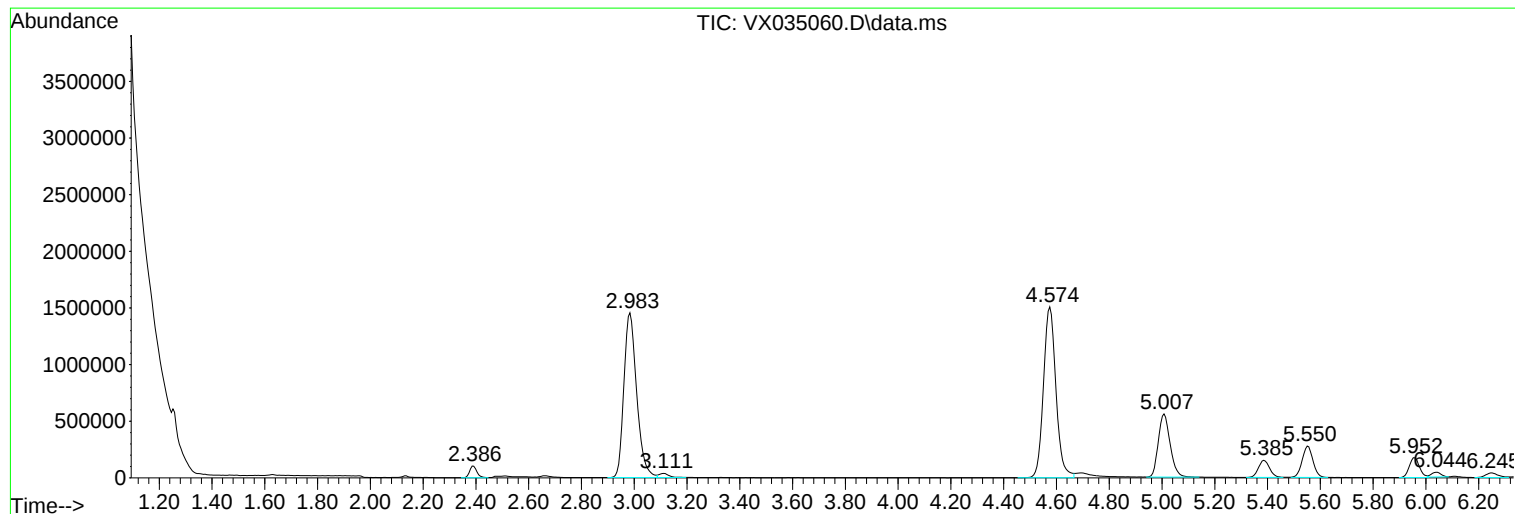
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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230412098-02-VOA

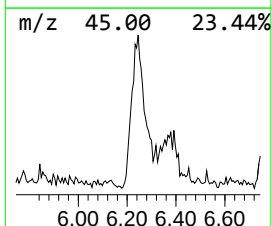
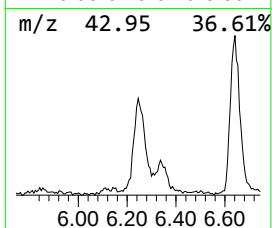
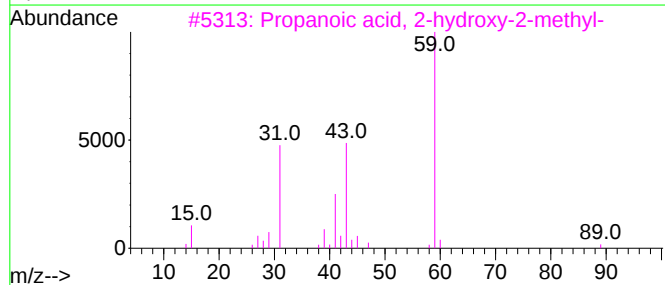
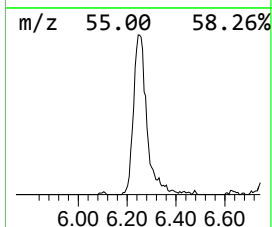
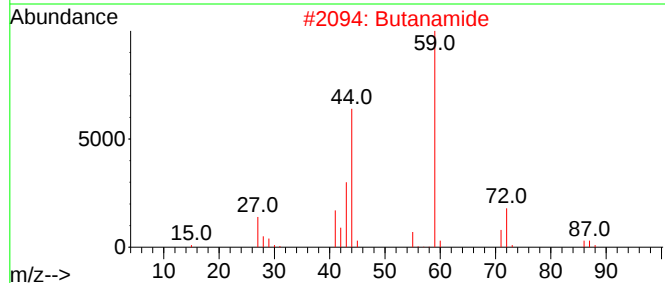
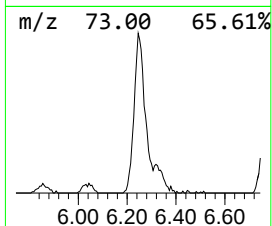
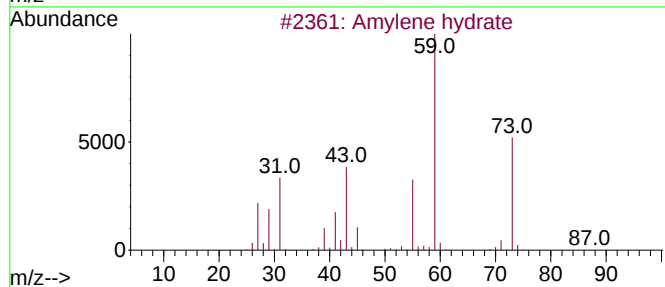
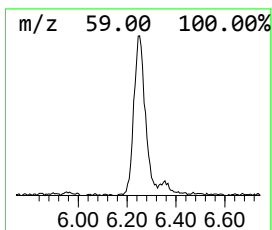
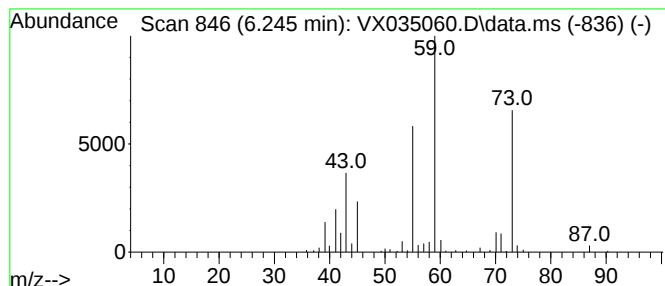
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	6.59 ug/l	136857	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	64
2			Butanamide	87	C4H9NO	000541-35-5	50
3			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	47
4			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	47
5			2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	39



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ClientSampleId :
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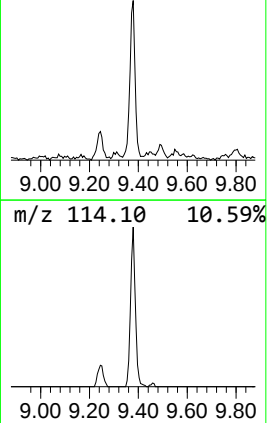
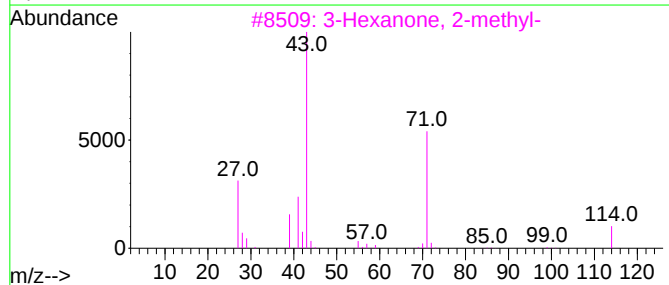
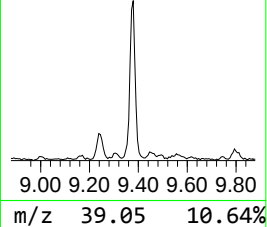
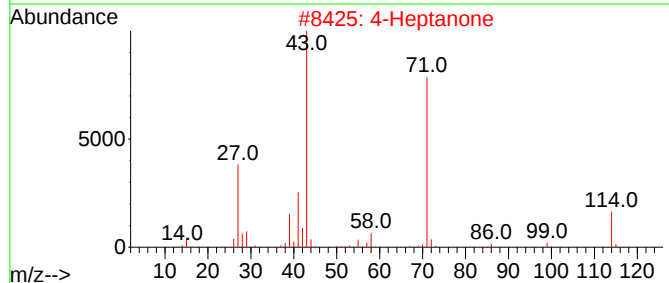
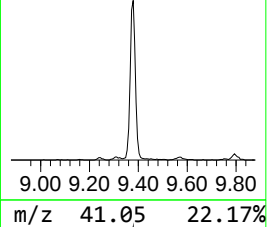
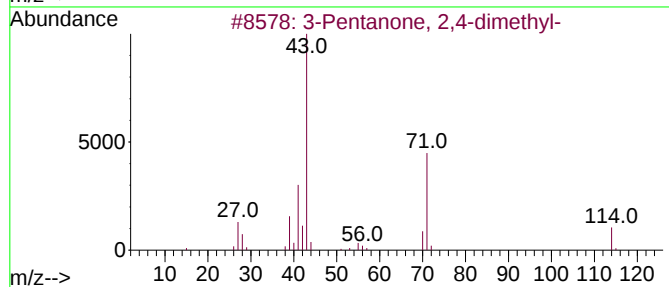
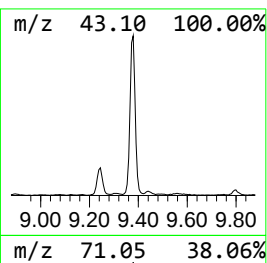
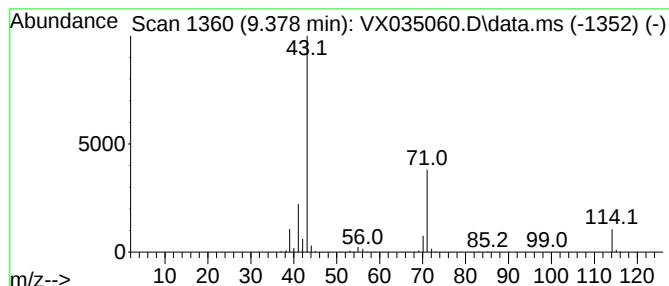
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 2 3-Pentanone, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	8.84 ug/l	243211	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2			4-Heptanone	114	C7H14O	000123-19-3	59
3			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	59
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	38
5			2,5-Hexanedione	114	C6H10O2	000110-13-4	37



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ALS Vial : 8 Sample Multiplier: 1

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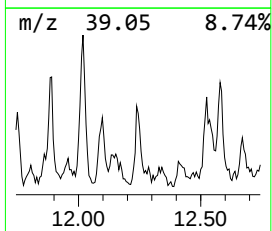
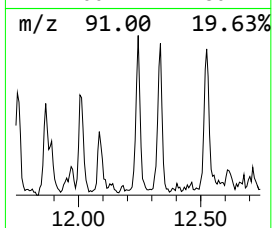
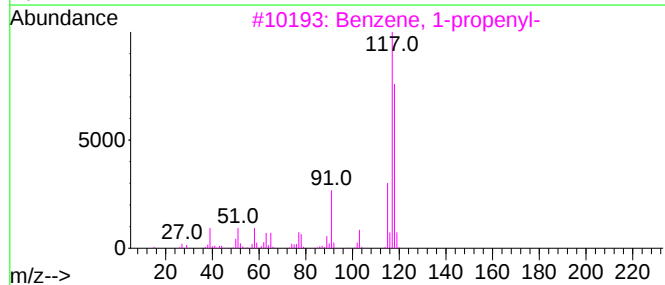
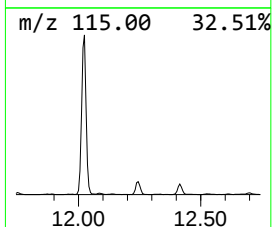
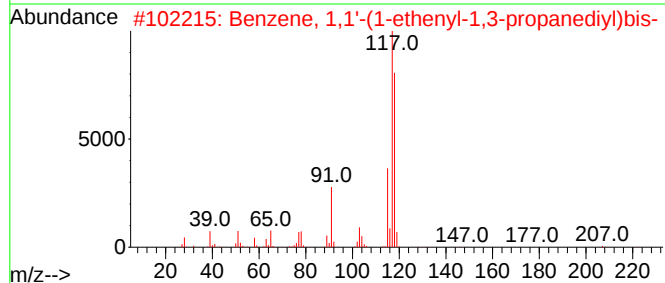
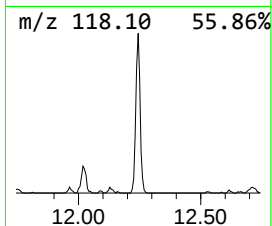
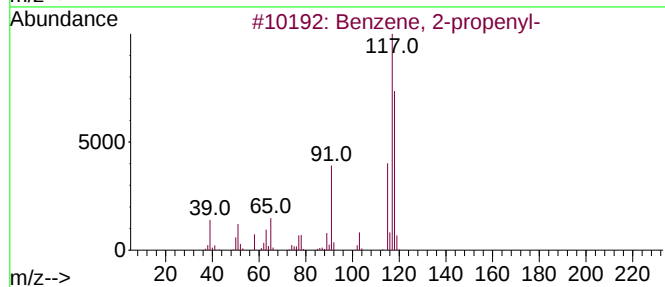
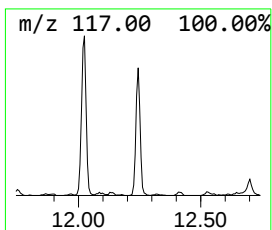
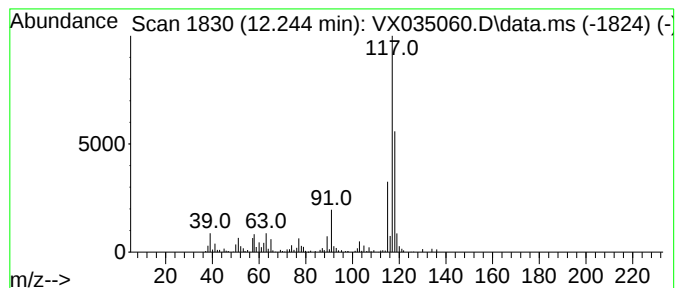
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 2-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	5.37 ug/l	134394	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
2			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	78
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	76
4			Indane	118	C9H10	000496-11-7	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	74



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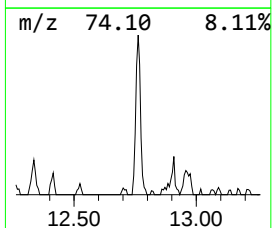
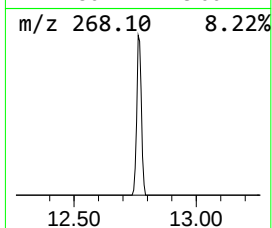
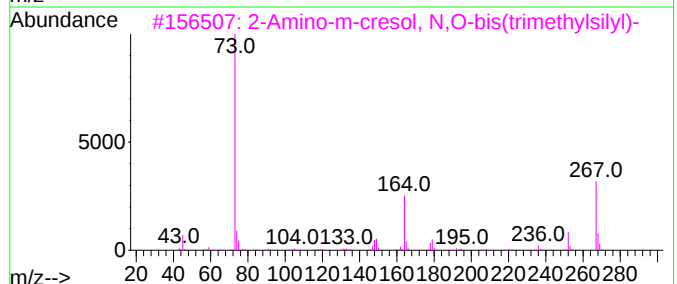
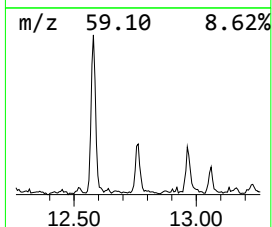
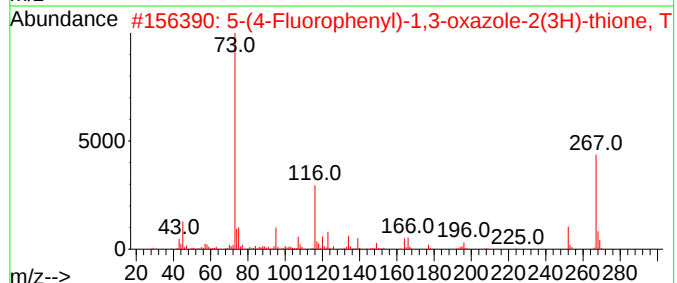
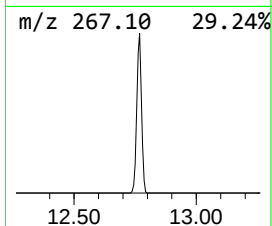
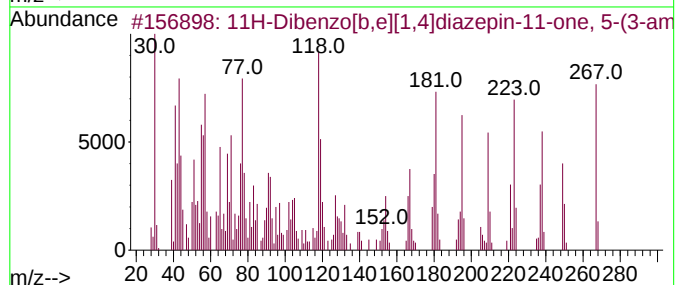
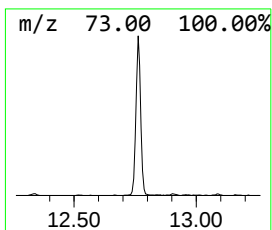
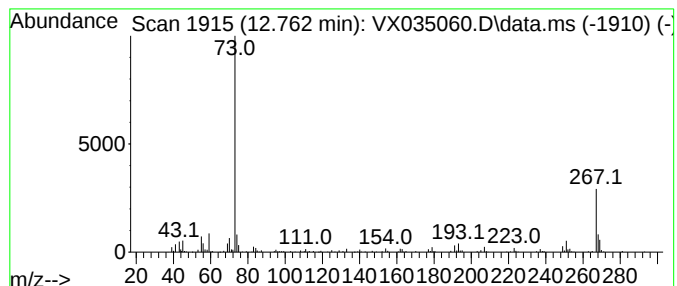
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.762	5.30 ug/l	132520	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	83
2	5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	50
3	2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	50
4	Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	42
5	Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	40



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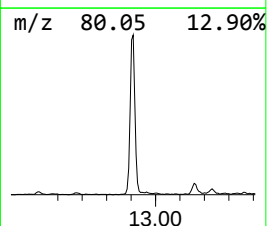
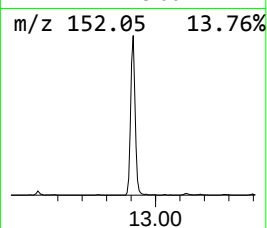
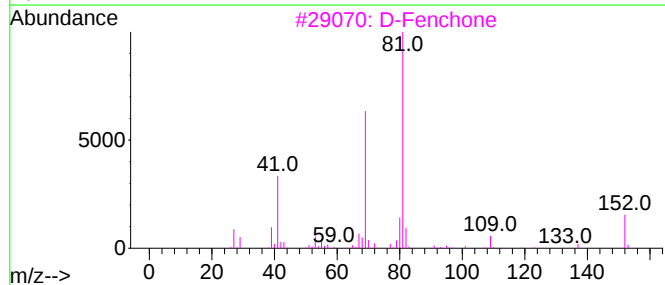
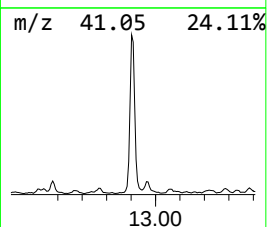
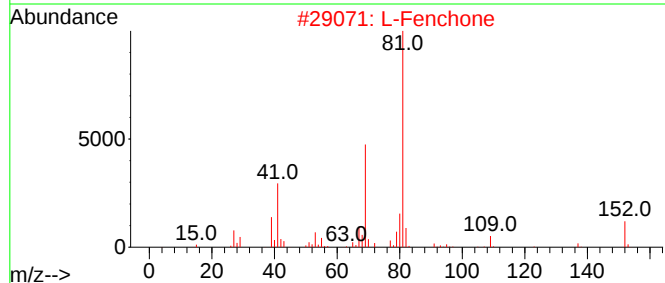
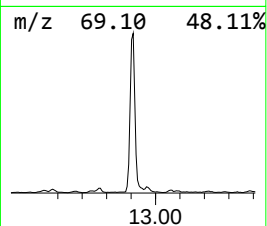
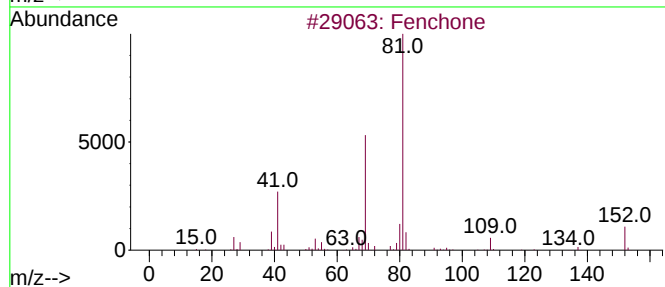
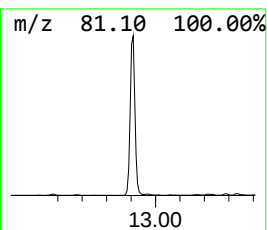
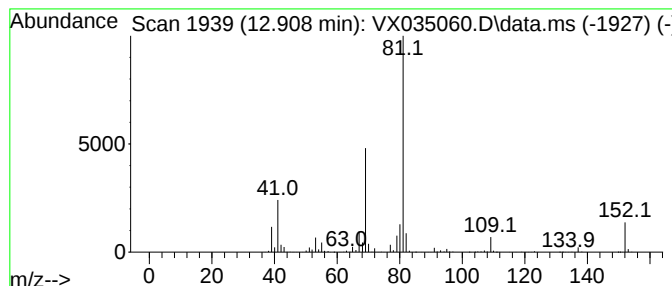
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Quant Title : SW846 8260

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

Peak Number 5 Fenchone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.908	54.54 ug/l	1364230	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	95
3			D-Fenchone	152	C10H16O	004695-62-9	94
4			Ethanone, 1-(2-methyl-2-cyclopenten-1-yl)-	124	C8H12O	001767-84-6	45
5			Cyclohexanone, 5-methyl-2-(1-methylethyl)-	152	C10H16O	015932-80-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
Data File : VX035060.D
Acq On : 13 Apr 2023 13:40
Operator : JC/MD
Sample : 02325-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230412098-02-VOA

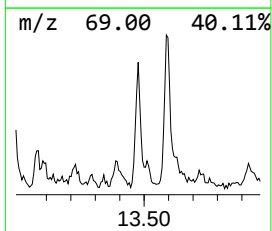
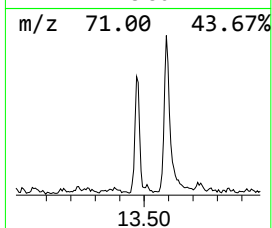
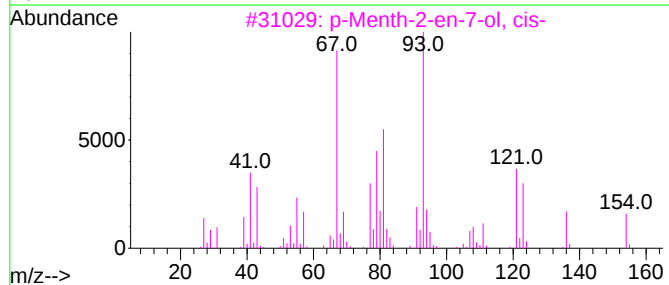
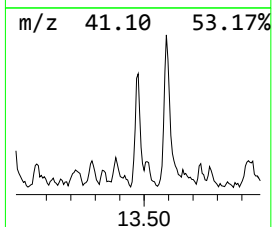
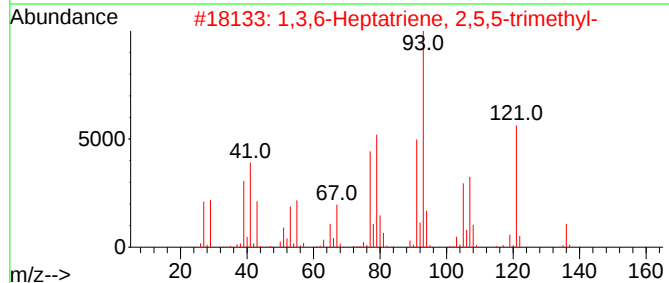
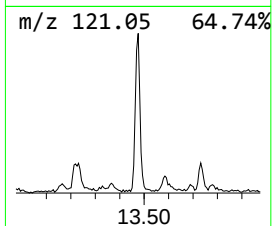
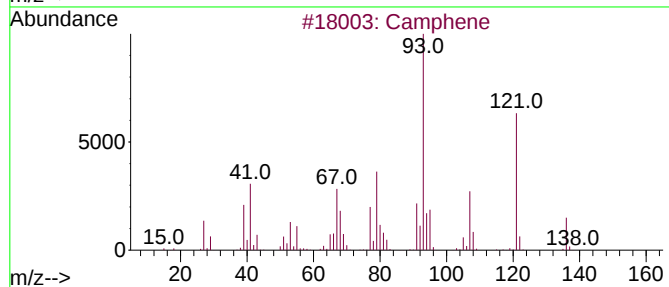
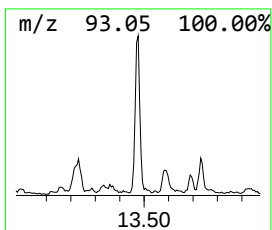
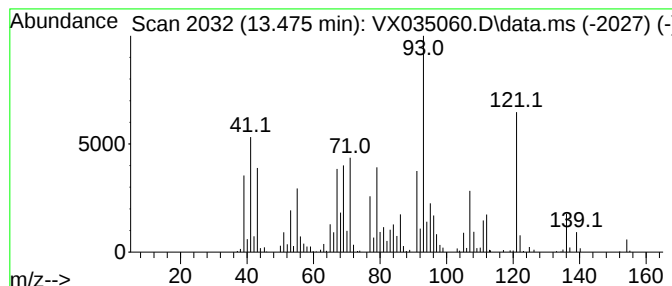
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 6 Camphene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	11.23 ug/l	280930	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	93
2			1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	60
3			p-Menth-2-en-7-ol, cis-	154	C10H18O	019898-86-3	58
4			2-Carene	136	C10H16	000554-61-0	49
5			(+)-4-Carene	136	C10H16	029050-33-7	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041423\
Data File : VX035060.D
Acq On : 13 Apr 2023 13:40
Operator : JC/MD
Sample : 02325-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230412098-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.245	6.6	ug/l	136857	2	6.763	1037680	50.0
3-Pentanone, 2,...	9.378	8.8	ug/l	243211	3	10.055	1374910	50.0
Benzene, 2-prop...	12.244	5.4	ug/l	134394	4	12.024	1250610	50.0
11H-Dibenzo[b,e...	12.762	5.3	ug/l	132520	4	12.024	1250610	50.0
Fenchone	12.908	54.5	ug/l	1364230	4	12.024	1250610	50.0
Camphene	13.475	11.2	ug/l	280930	4	12.024	1250610	50.0