

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
 Data File : VX029690.D
 Acq On : 22 Jun 2022 11:44
 Operator : JC/MD
 Sample : N3286-02 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029690.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.746	103	108	117	rBV	70721	96349	3.26%	0.656%
2	1.953	137	142	151	rVB	26777	38738	1.31%	0.264%
3	2.947	299	305	319	rVB	29076	71789	2.43%	0.489%
4	3.105	319	331	338	rBV2	15948	37481	1.27%	0.255%
5	4.306	516	528	542	rVB	53090	147633	4.99%	1.005%
6	5.385	692	705	715	rBV	148130	438578	14.84%	2.985%
7	5.556	723	733	761	rVB	277958	810267	27.41%	5.514%
8	5.958	789	799	814	rBV	155615	421253	14.25%	2.867%
9	6.763	921	931	952	rVB	417097	998956	33.80%	6.799%
10	8.653	1234	1241	1249	rBV	835125	1314706	44.48%	8.947%
11	10.055	1461	1471	1483	rBV	851179	1123313	38.00%	7.645%
12	10.195	1489	1494	1502	rBV	578437	733914	24.83%	4.995%
13	10.305	1506	1512	1526	rVB	2146004	2955771	100.00%	20.116%
14	10.646	1562	1568	1576	rBV	104772	144218	4.88%	0.981%
15	10.963	1615	1620	1627	rBV	35836	45639	1.54%	0.311%
16	11.085	1634	1640	1653	rBV	621200	815031	27.57%	5.547%
17	11.305	1671	1676	1683	rBV	76053	93048	3.15%	0.633%
18	11.378	1683	1688	1696	rBV	394304	676877	22.90%	4.607%
19	11.451	1696	1700	1708	rVB	178302	220745	7.47%	1.502%
20	11.616	1721	1727	1735	rVB	215247	272701	9.23%	1.856%
21	11.756	1744	1750	1756	rVB	805439	1016532	34.39%	6.918%
22	12.024	1788	1794	1800	rBV	826902	1025367	34.69%	6.978%
23	12.085	1800	1804	1810	rVB	257390	320521	10.84%	2.181%
24	12.244	1825	1830	1838	rBV	259612	328191	11.10%	2.234%
25	12.323	1838	1843	1850	rVB2	26963	43402	1.47%	0.295%
26	12.616	1886	1891	1894	rBV	30817	36580	1.24%	0.249%
27	12.701	1900	1905	1912	rBV2	27142	36613	1.24%	0.249%
28	12.963	1945	1948	1953	rVB	30283	35044	1.19%	0.238%
29	13.292	1995	2002	2007	rBV2	54306	71955	2.43%	0.490%
30	13.774	2076	2081	2090	rBV	247900	322470	10.91%	2.195%

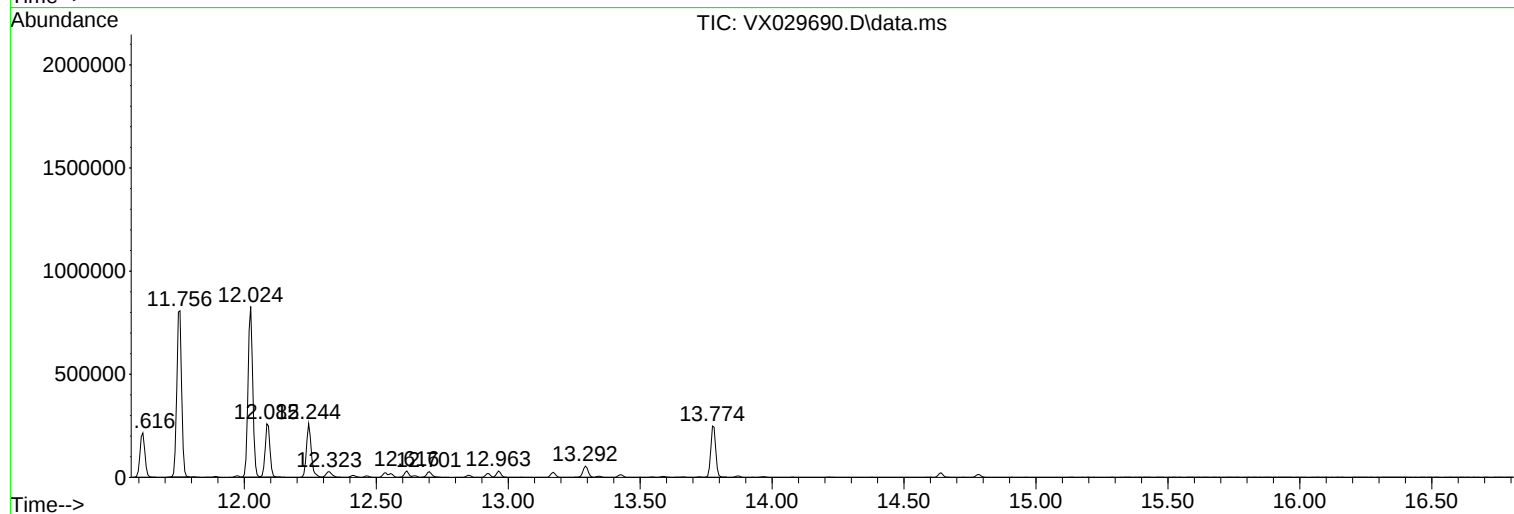
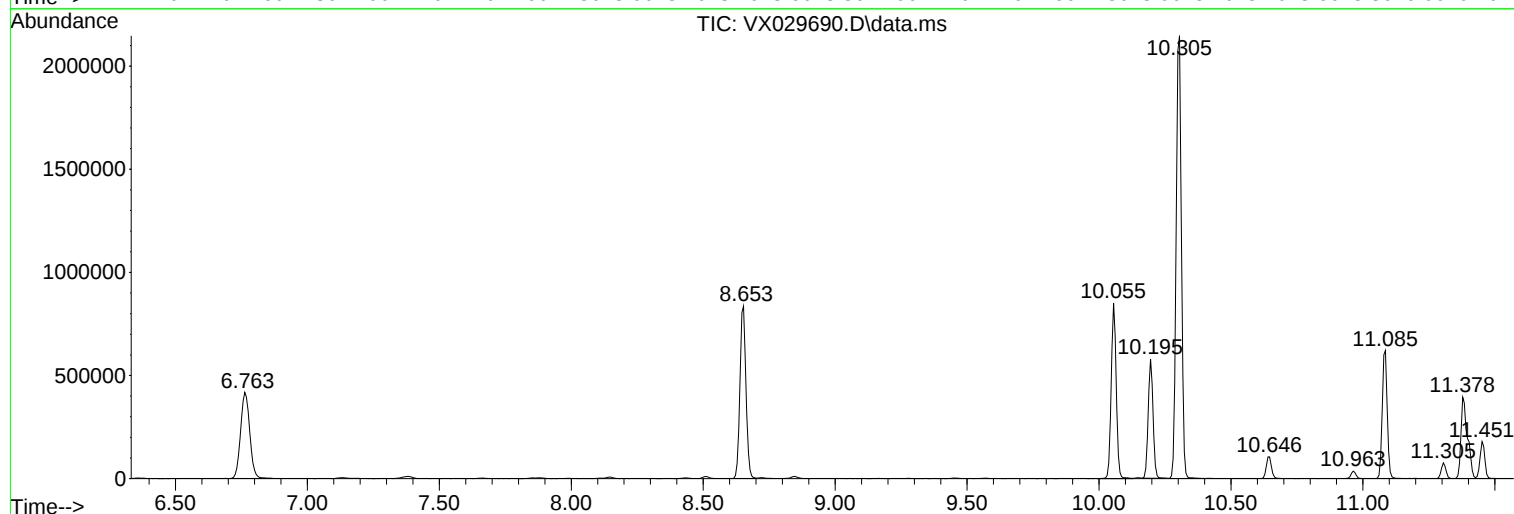
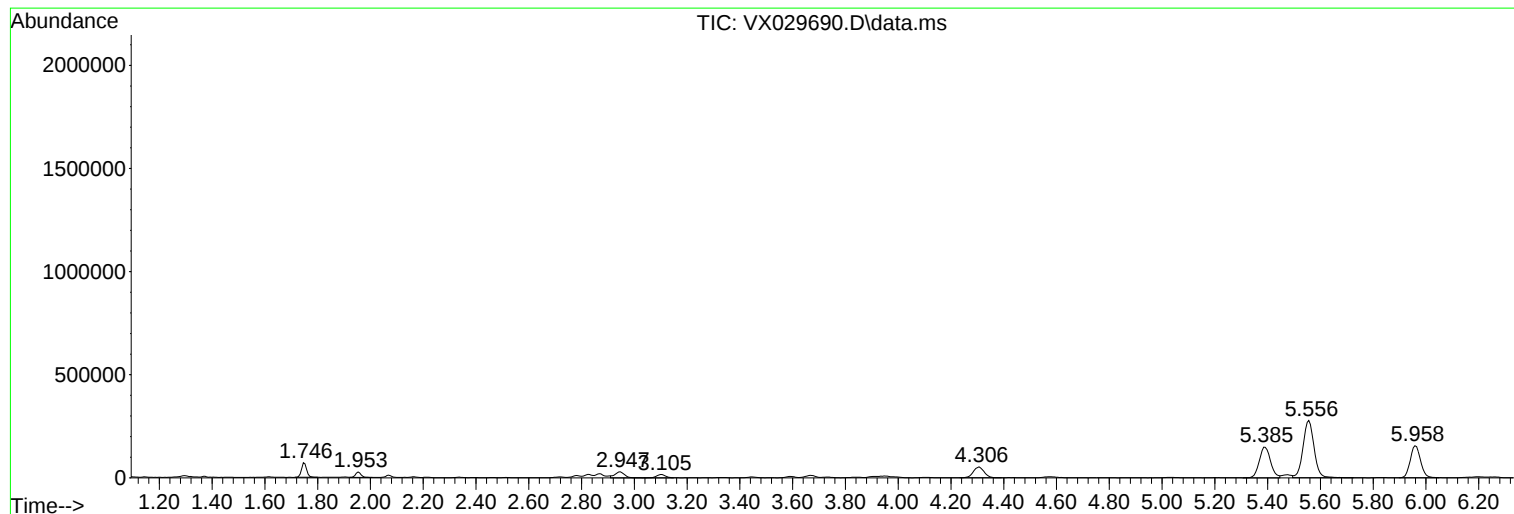
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Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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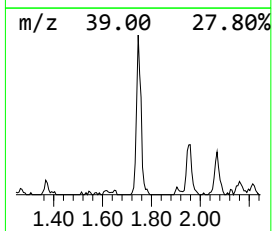
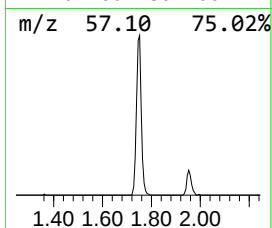
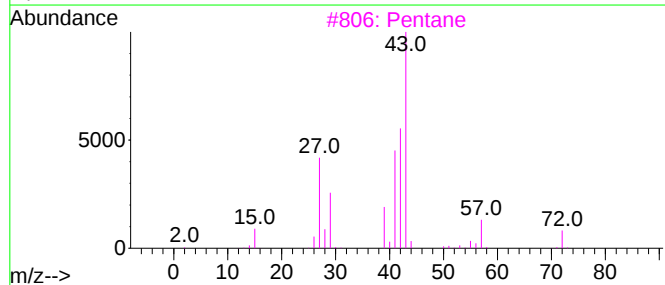
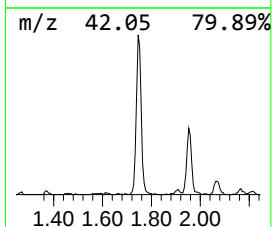
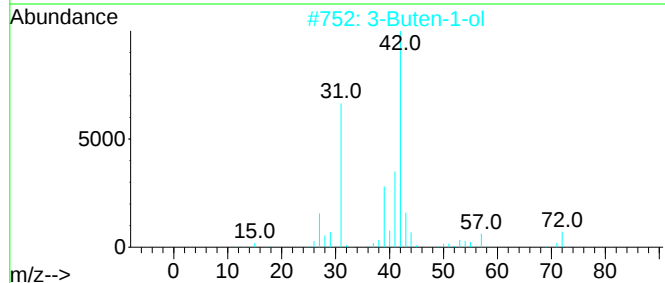
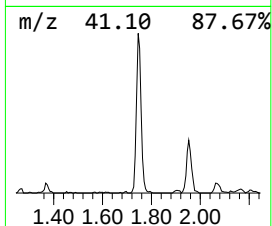
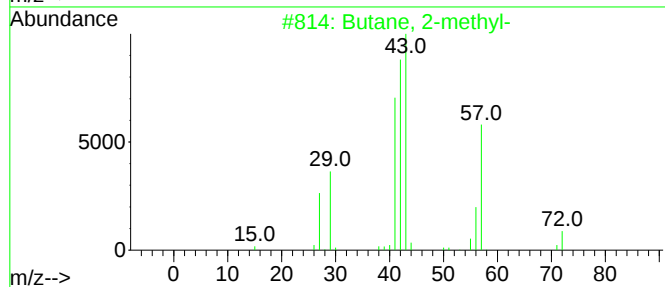
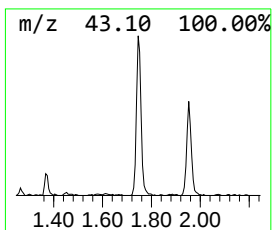
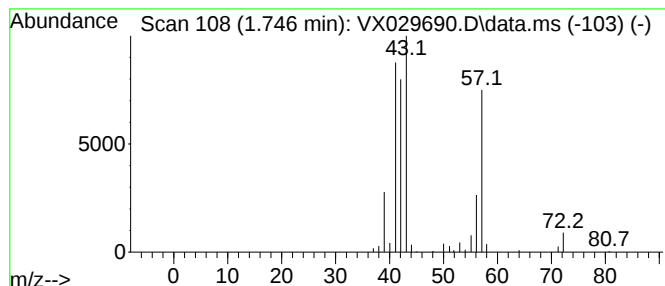
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Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	5.95 ug/l	96349	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Pentane	72	C5H12	000109-66-0	42
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5			1-Butene	56	C4H8	000106-98-9	10



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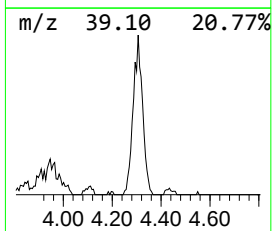
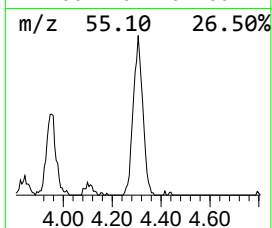
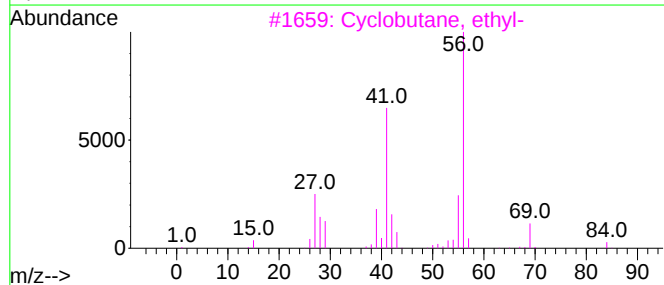
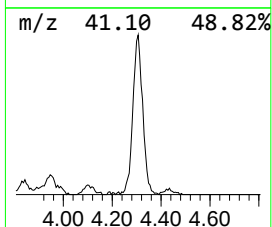
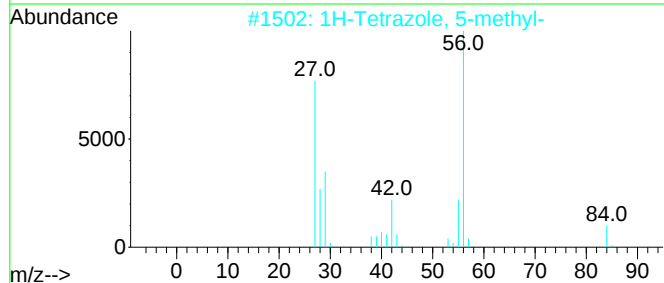
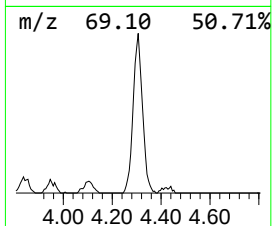
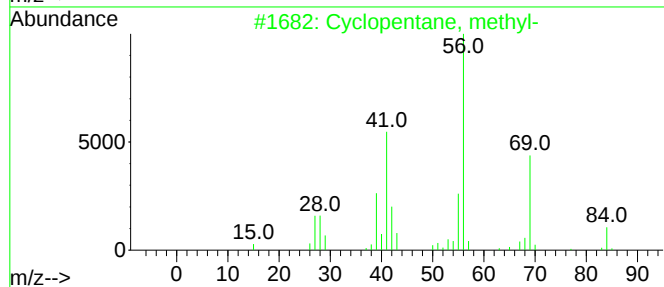
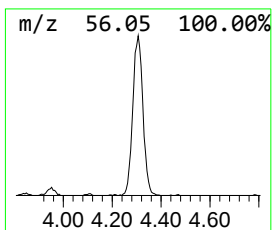
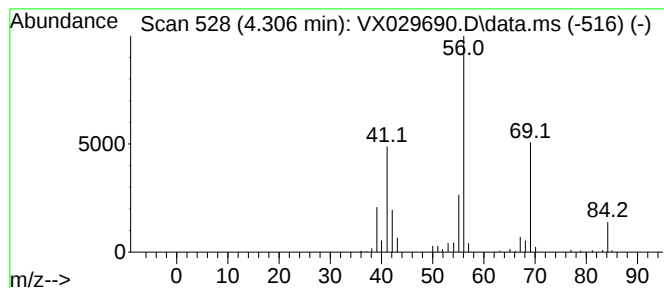
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	9.11 ug/l	147633	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	53
5			Cyclohexane	84	C6H12	000110-82-7	52



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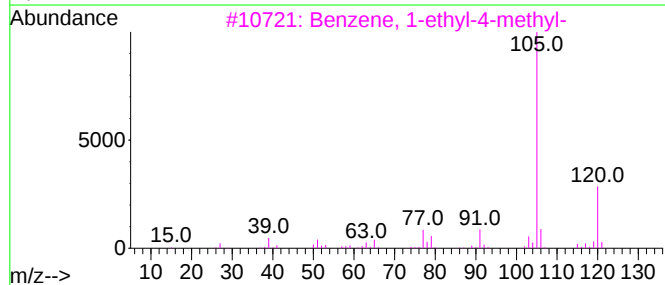
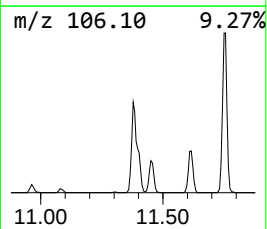
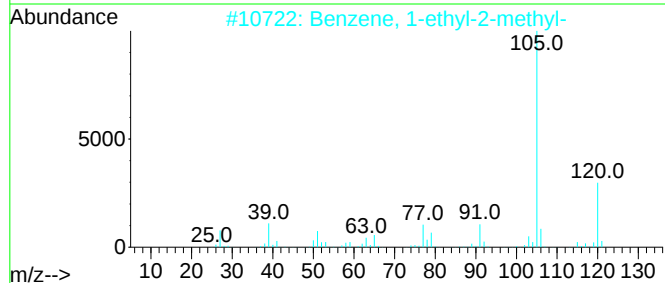
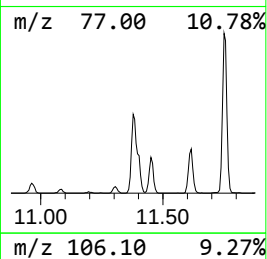
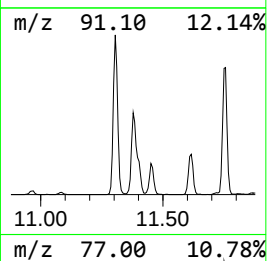
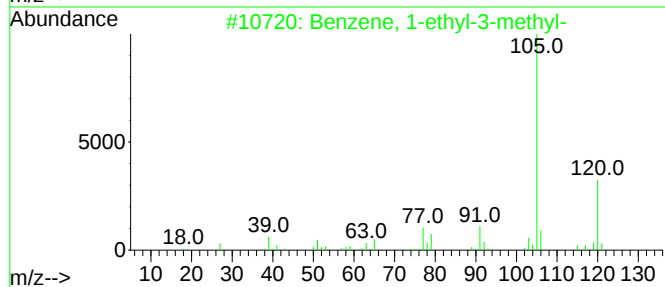
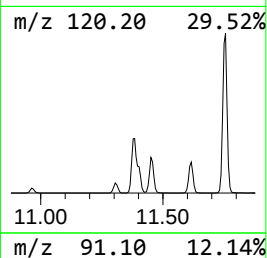
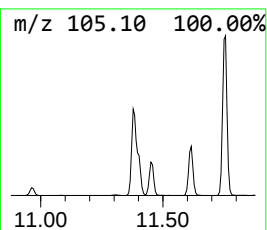
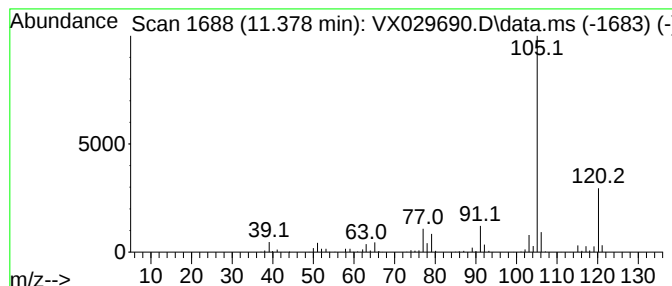
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	33.01 ug/l	676877	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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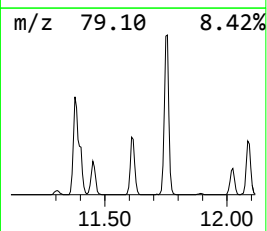
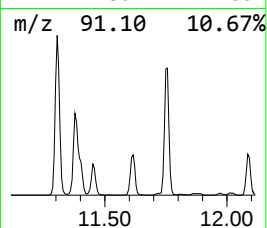
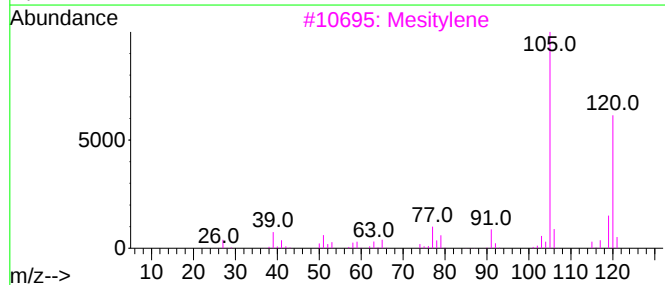
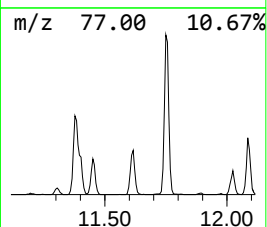
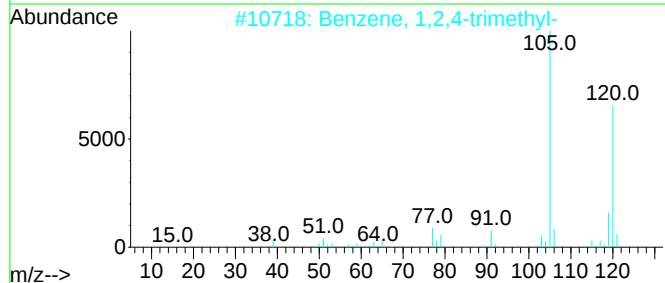
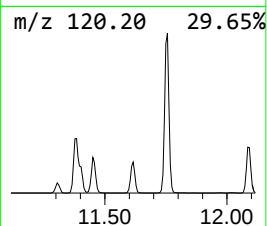
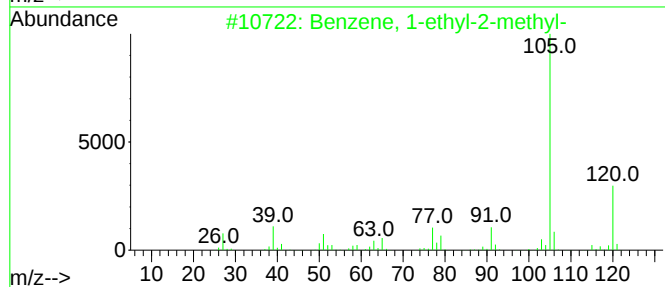
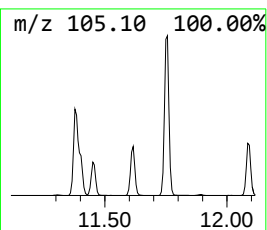
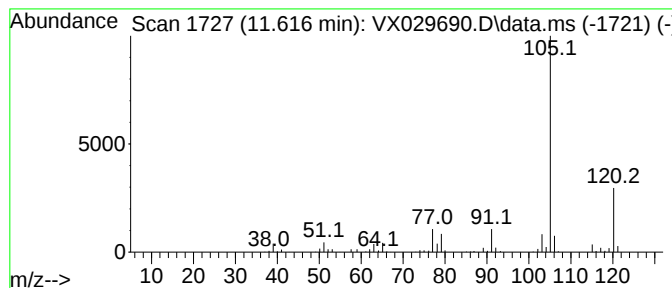
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	13.30 ug/l	272701	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
3			Mesitylene	120	C9H12	000108-67-8	90
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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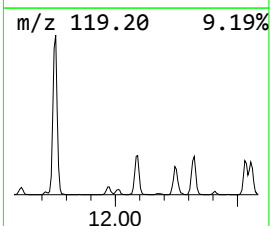
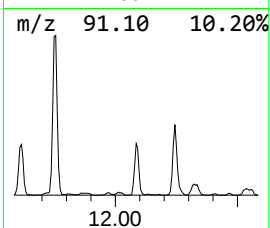
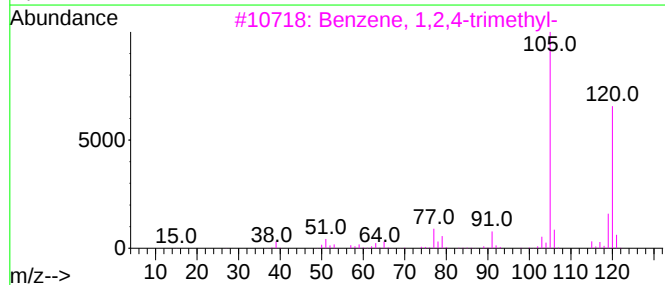
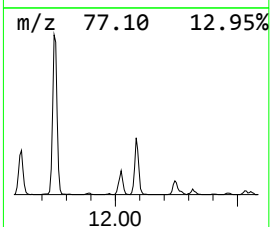
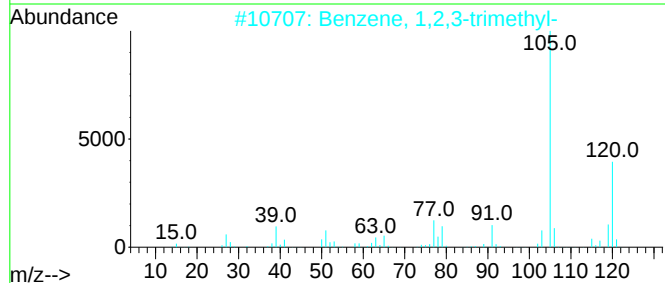
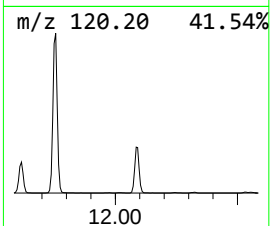
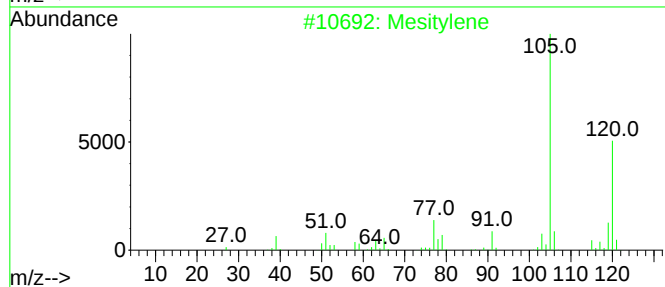
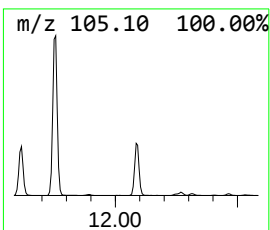
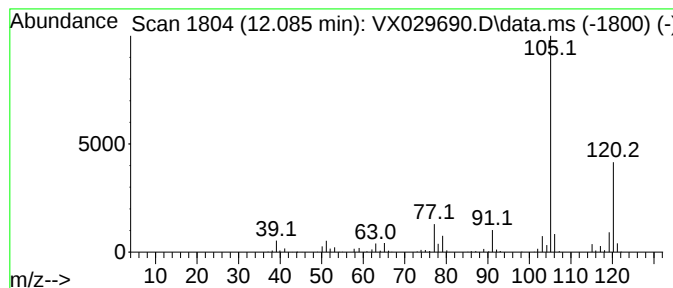
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	15.63 ug/l	320521	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87



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MW-2

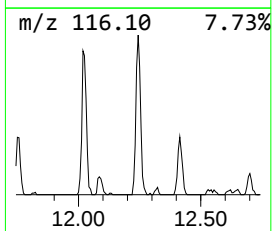
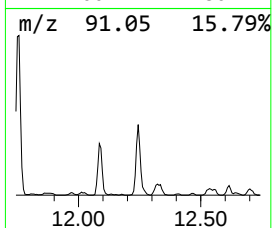
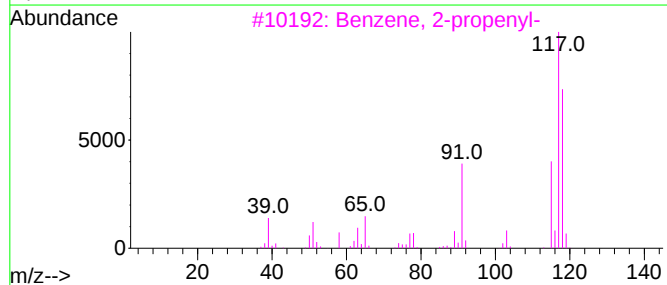
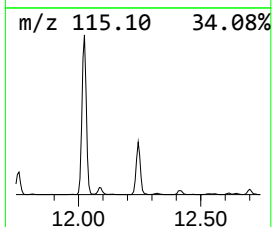
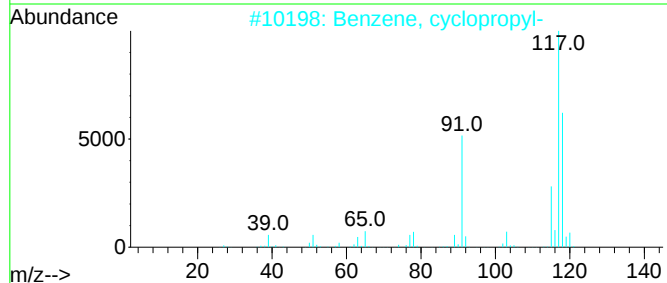
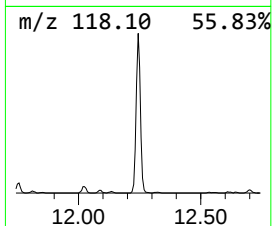
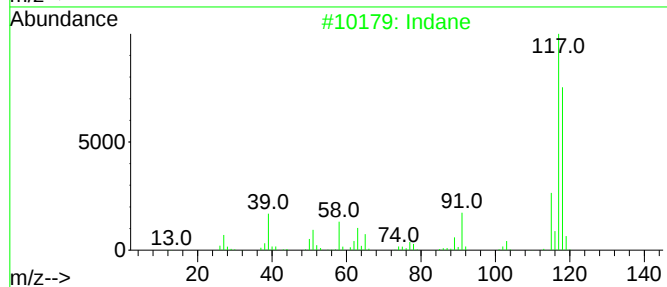
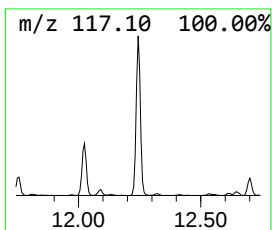
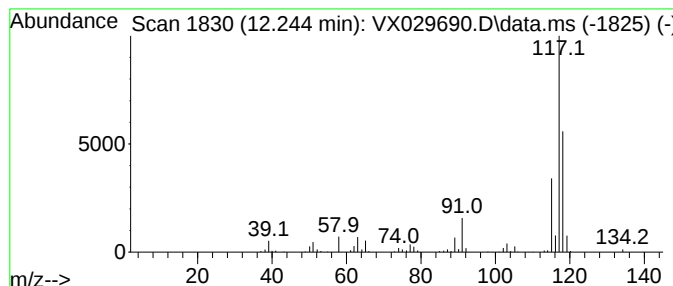
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	16.00 ug/l	328191	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062222\
Data File : VX029690.D
Acq On : 22 Jun 2022 11:44
Operator : JC/MD
Sample : N3286-02 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.746	6.0	ug/l	96349	1	5.556	810267	50.0
Cyclopentane, m...	4.306	9.1	ug/l	147633	1	5.556	810267	50.0
Benzene, 1-ethy...	11.378	33.0	ug/l	676877	4	12.024	1025370	50.0
Benzene, 1-ethy...	11.616	13.3	ug/l	272701	4	12.024	1025370	50.0
Benzene, 1,2,3-...	12.085	15.6	ug/l	320521	4	12.024	1025370	50.0
Indane	12.244	16.0	ug/l	328191	4	12.024	1025370	50.0