

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
 Data File : VX032636.D
 Acq On : 07 Nov 2022 18:44
 Operator : JC/MD
 Sample : N5497-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-12

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	40	46	52	rBV	77026	80175	1.89%	0.213%
2	1.746	103	108	121	rVB	144825	189002	4.45%	0.503%
3	1.959	138	143	155	rVB3	71382	142374	3.35%	0.379%
4	2.069	155	161	172	rVV	39578	59414	1.40%	0.158%
5	2.215	180	185	194	rVB	58225	89614	2.11%	0.238%
6	2.752	261	273	276	rBV	24093	56886	1.34%	0.151%
7	2.825	281	285	288	rVV	35164	67780	1.60%	0.180%
8	2.867	288	292	305	rVB2	43729	96082	2.26%	0.255%
9	3.105	323	331	342	rVB2	32084	77744	1.83%	0.207%
10	4.306	517	528	540	rVB2	47690	137688	3.24%	0.366%
11	5.196	663	674	682	rBV3	20732	62584	1.47%	0.166%
12	5.385	694	705	713	rBV	68706	202204	4.76%	0.538%
13	5.477	713	720	725	rVV2	22009	63708	1.50%	0.169%
14	5.550	725	732	743	rVB	109530	299123	7.04%	0.795%
15	5.958	789	799	804	rBV	74972	193866	4.56%	0.515%
16	6.044	804	813	826	rVB	524082	1389798	32.72%	3.696%
17	6.196	828	838	846	rBV2	19476	60383	1.42%	0.161%
18	6.763	922	931	941	rBV	176339	433378	10.20%	1.152%
19	7.379	1021	1032	1042	rBV4	25522	68582	1.61%	0.182%
20	8.507	1209	1217	1224	rVB2	25213	46600	1.10%	0.124%
21	8.647	1234	1240	1246	rBV	370565	573208	13.49%	1.524%
22	8.720	1246	1252	1261	rVB	1222556	1852291	43.61%	4.925%
23	8.958	1282	1291	1297	rBV	82476	128996	3.04%	0.343%
24	9.049	1297	1306	1312	rVB2	89687	151207	3.56%	0.402%
25	10.055	1462	1471	1476	rBV	382305	511012	12.03%	1.359%
26	10.195	1488	1494	1500	rBV	3162333	4030114	94.87%	10.716%
27	10.305	1504	1512	1520	rVB	2519441	3059986	72.04%	8.137%
28	10.646	1562	1568	1578	rVB	3186713	4247833	100.00%	11.295%
29	10.963	1614	1620	1625	rVB	111863	139595	3.29%	0.371%
30	11.079	1634	1639	1645	rBV	353724	461585	10.87%	1.227%
31	11.305	1671	1676	1681	rVV	201536	237710	5.60%	0.632%
32	11.402	1681	1692	1696	rVV	466846	679085	15.99%	1.806%
33	11.451	1696	1700	1711	rVB	952981	1103517	25.98%	2.934%
34	11.616	1721	1727	1737	rBV	1606727	2051998	48.31%	5.456%
35	11.756	1744	1750	1755	rVB	2701166	3361952	79.15%	8.940%
36	12.024	1789	1794	1798	rVV	425745	538555	12.68%	1.432%

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Stop Thrs : 0

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

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37	12.085	1798	1804	1809	rVB	2141844	2630248	61.92%	6.994%
38	12.244	1824	1830	1838	rBV	2596744	3177324	74.80%	8.449%
39	12.317	1838	1842	1849	rVB2	1935550	269234	6.34%	0.716%
40	12.414	1852	1858	1862	rBV	252774	323921	7.63%	0.861%
41	12.463	1862	1866	1872	rVB	65711	80758	1.90%	0.215%
42	12.530	1872	1877	1880	rBV	157951	214669	5.05%	0.571%
43	12.555	1880	1881	1886	rVB	76652	57840	1.36%	0.154%
44	12.616	1886	1891	1894	rBV	259837	330115	7.77%	0.878%
45	12.646	1894	1896	1900	rVB	75390	75208	1.77%	0.200%
46	12.701	1900	1905	1913	rBV2	285807	389946	9.18%	1.037%
47	12.847	1924	1929	1935	rVB	99489	121883	2.87%	0.324%
48	12.920	1935	1941	1945	rBV	150101	186045	4.38%	0.495%
49	12.963	1945	1948	1954	rVB	174427	202543	4.77%	0.539%
50	13.170	1977	1982	1987	rVB	191635	224502	5.29%	0.597%
51	13.292	1997	2002	2007	rVV2	546366	692917	16.31%	1.842%
52	13.341	2007	2010	2019	rVB3	46317	66129	1.56%	0.176%
53	13.426	2019	2024	2032	rVB	110505	146851	3.46%	0.390%
54	13.774	2076	2081	2090	rBV	893166	1101288	25.93%	2.928%
55	13.865	2091	2096	2102	rVB	187762	236372	5.56%	0.629%
56	14.780	2241	2246	2252	rBV	100297	134119	3.16%	0.357%

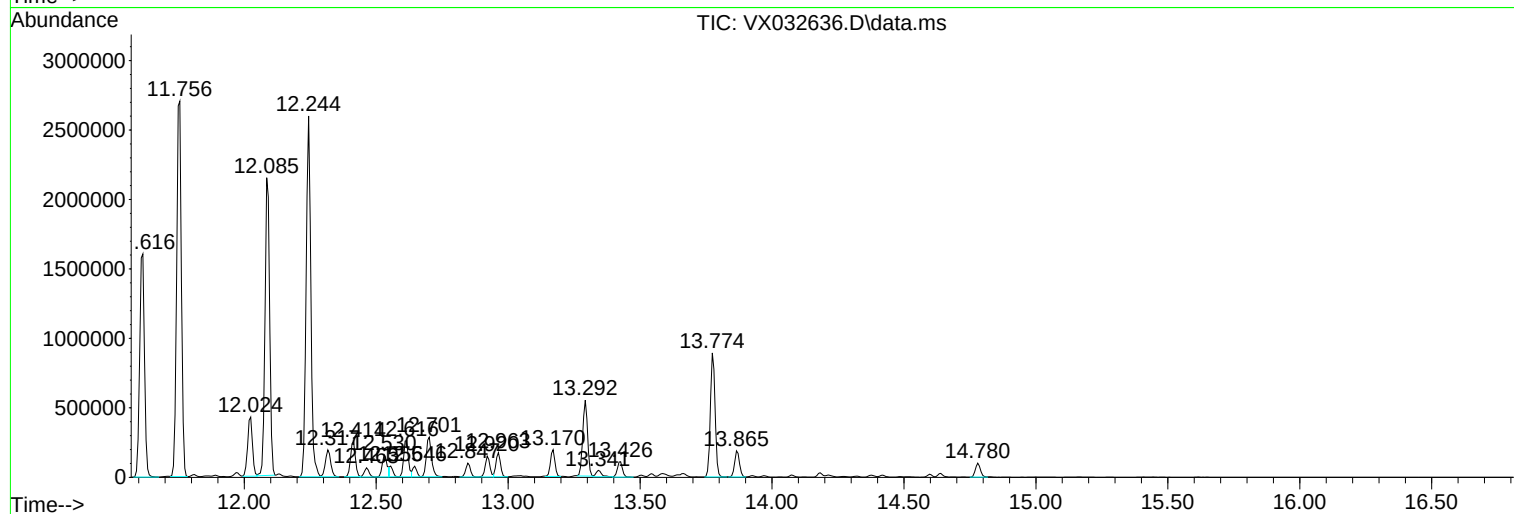
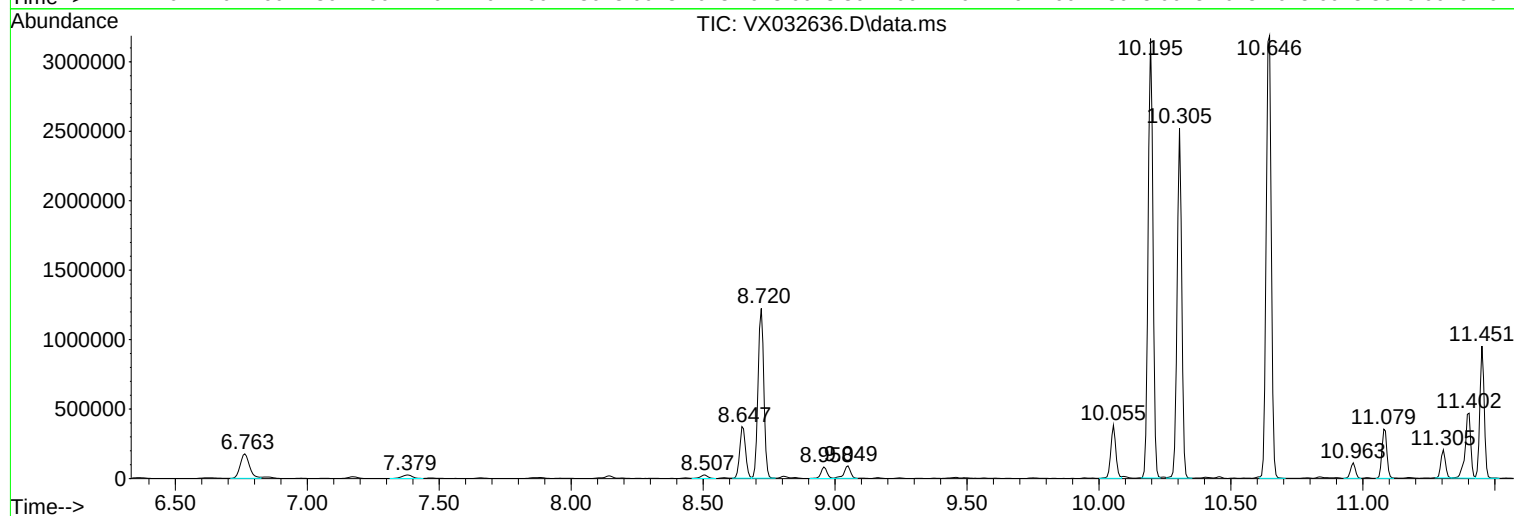
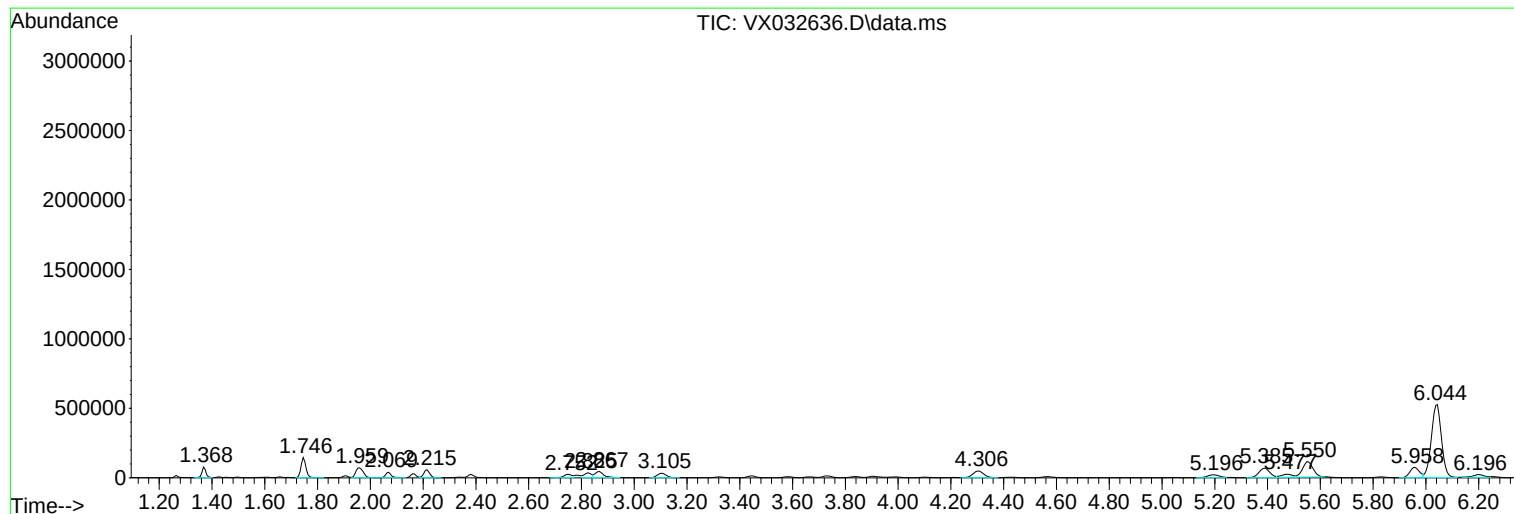
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Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
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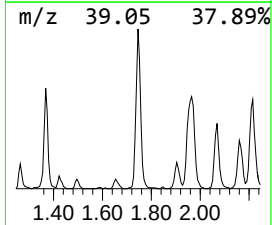
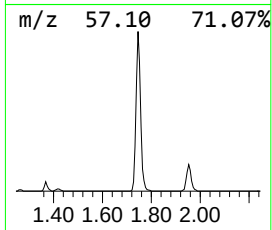
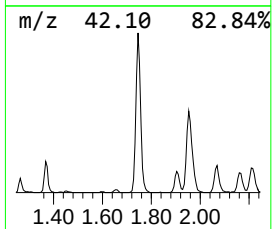
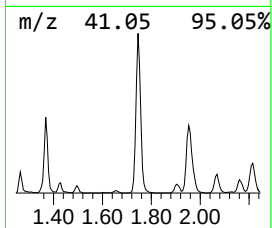
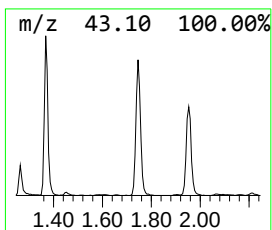
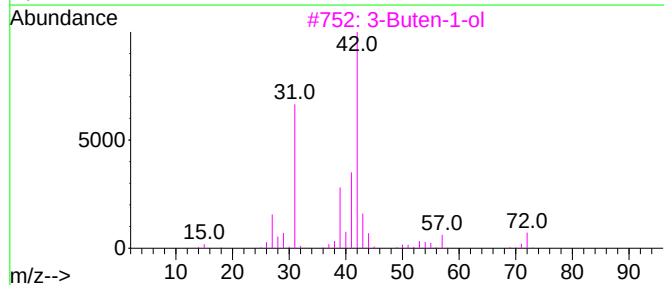
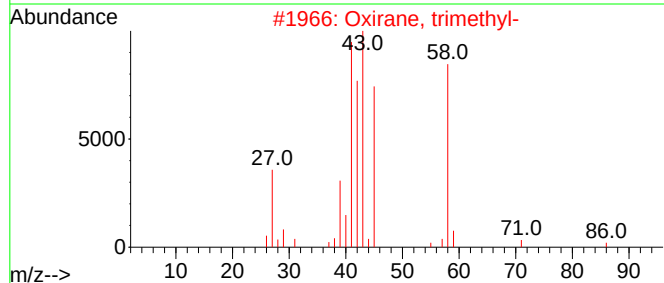
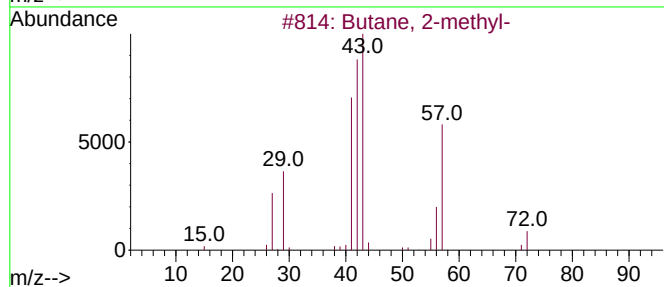
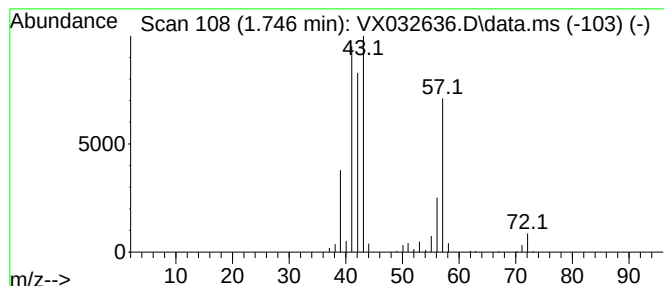
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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	31.59 ug/l	189002	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
3			3-Buten-1-ol	72	C4H8O	000627-27-0	37
4			Pentane	72	C5H12	000109-66-0	33
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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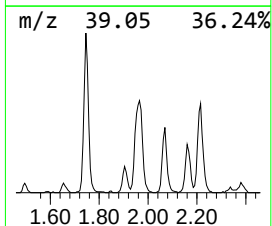
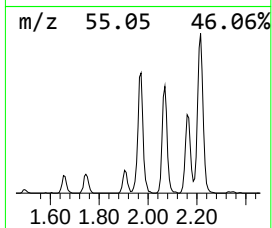
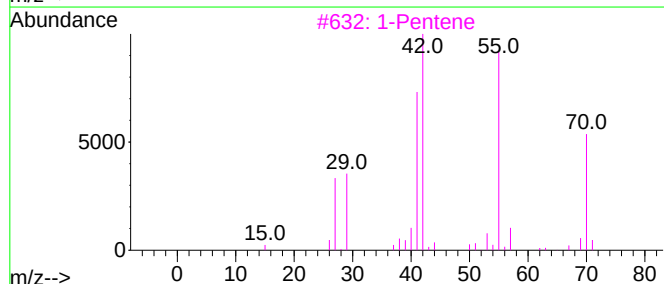
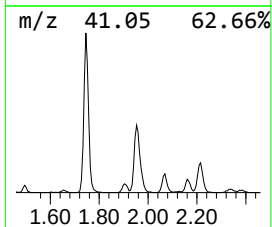
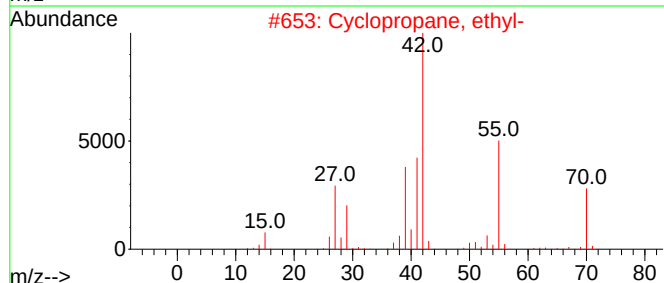
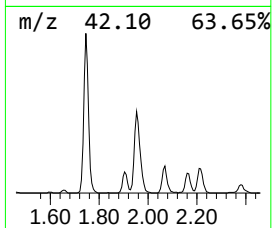
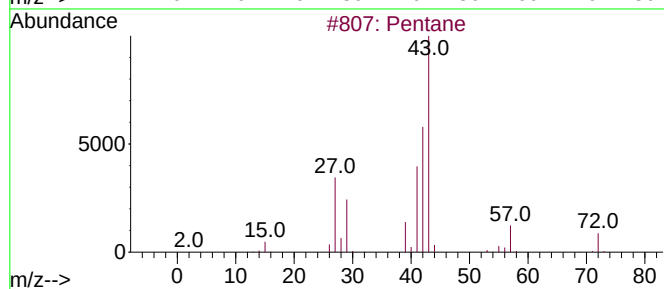
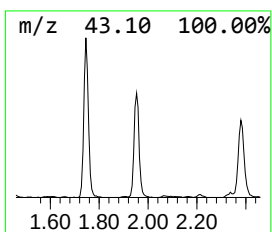
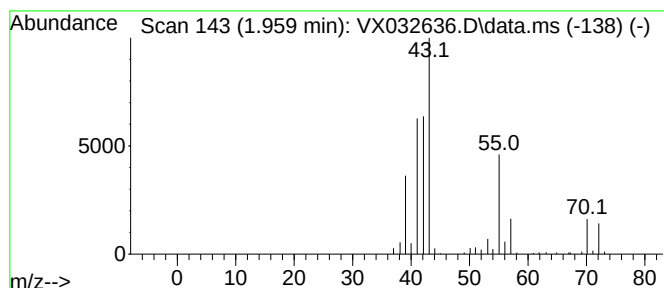
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	23.80 ug/l	142374	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	59
2			Cyclopropane, ethyl-	70	C5H10	001191-96-4	49
3			1-Pentene	70	C5H10	000109-67-1	43
4			Cyclobutanone	70	C4H6O	001191-95-3	35
5			Oxirane, ethyl-	72	C4H8O	000106-88-7	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
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Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

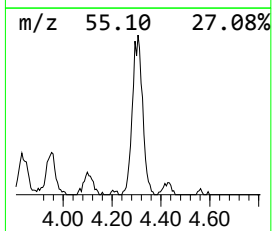
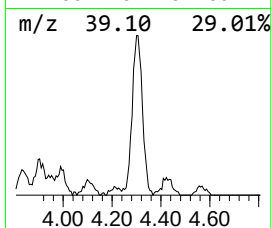
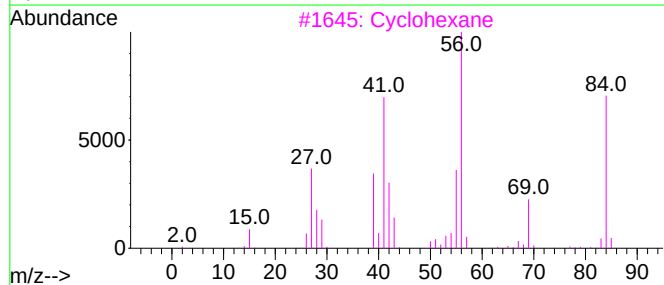
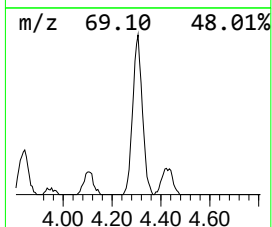
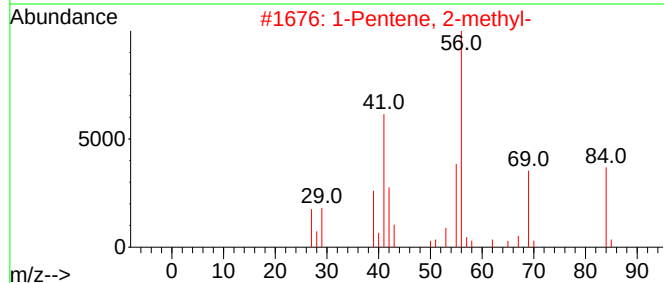
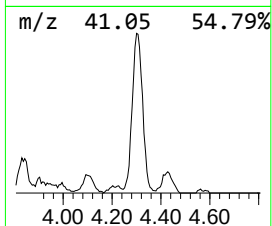
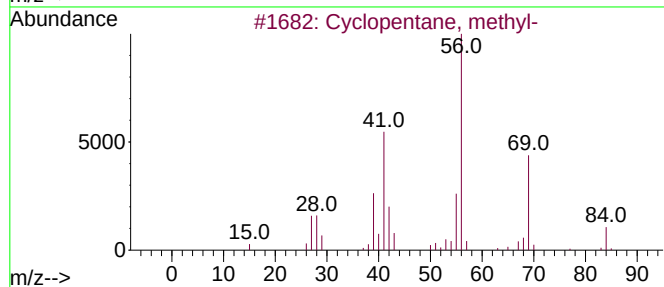
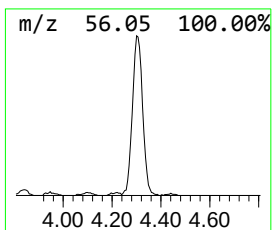
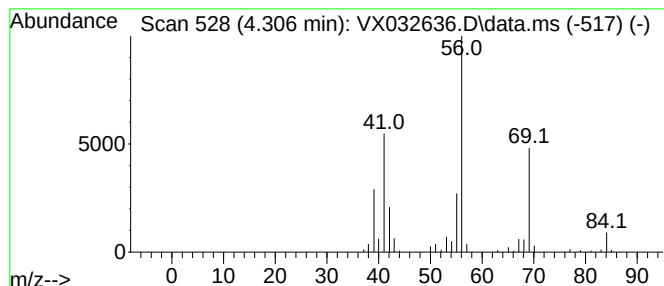
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	23.02 ug/l	137688	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3			Cyclohexane	84	C6H12	000110-82-7	86
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64



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Instrument :
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ClientSampleId :
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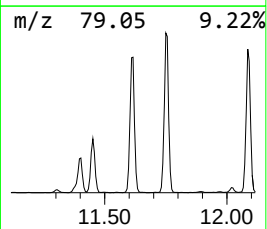
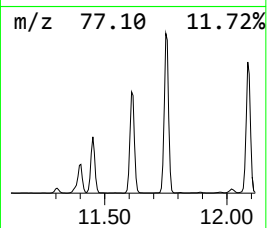
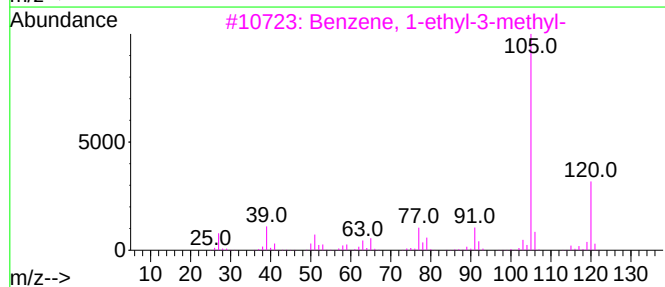
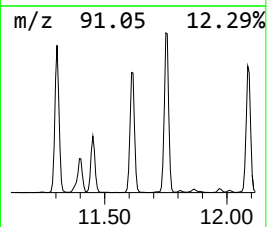
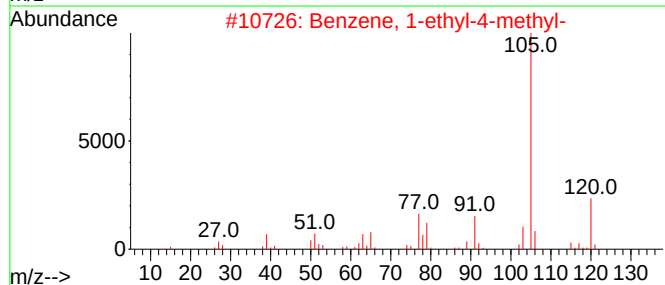
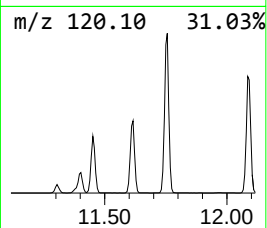
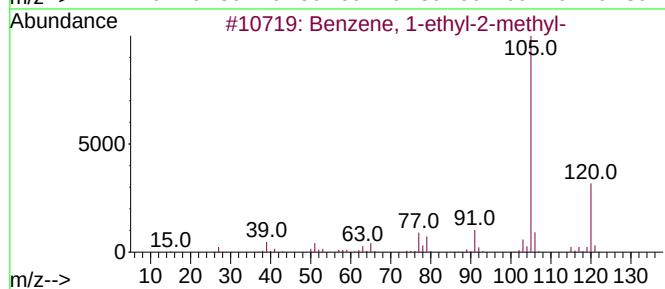
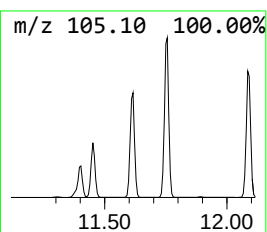
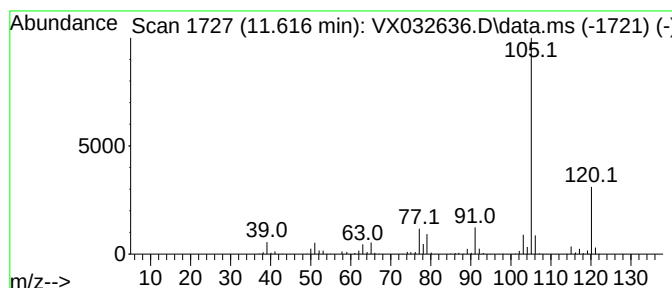
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	190.51 ug/l	2052000	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-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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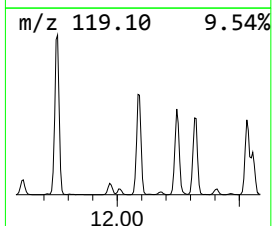
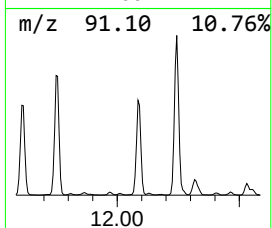
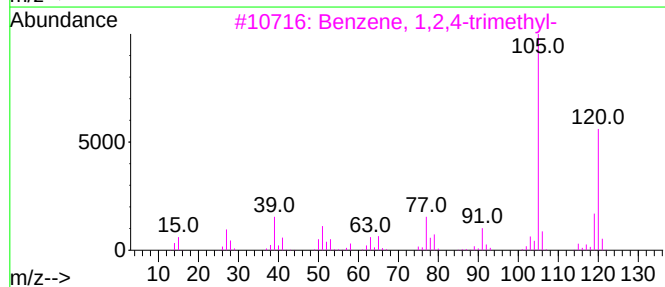
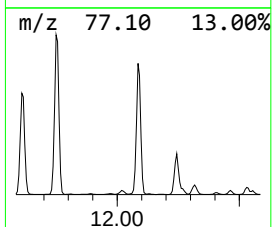
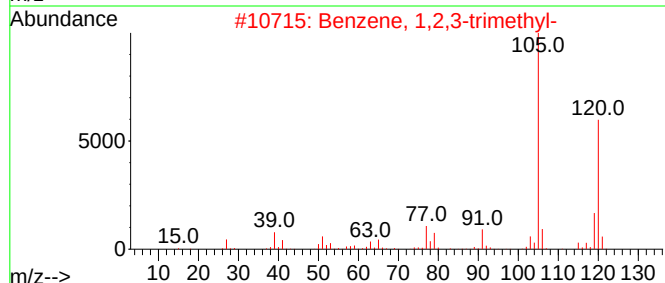
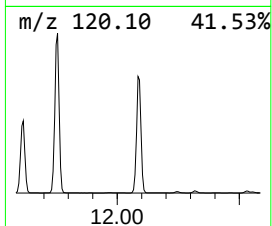
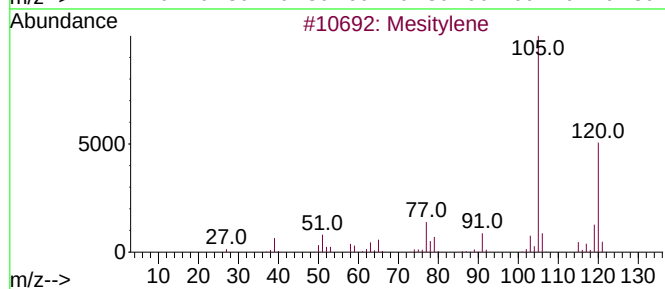
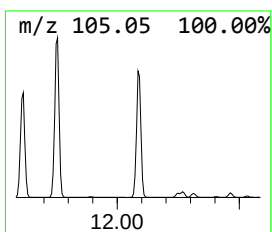
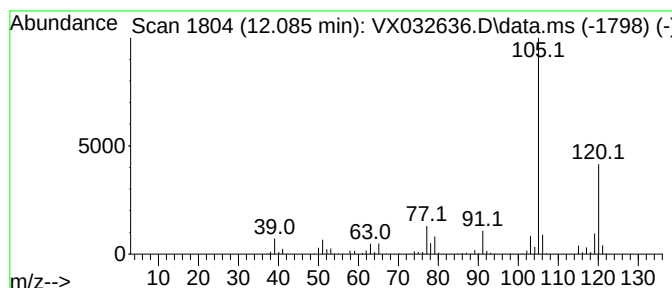
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	244.19 ug/l	2630250	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	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

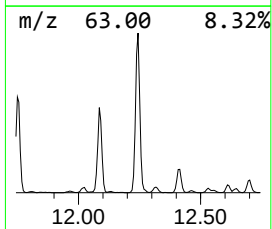
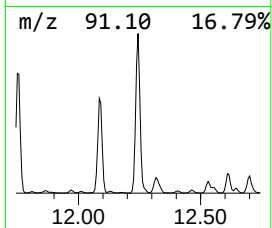
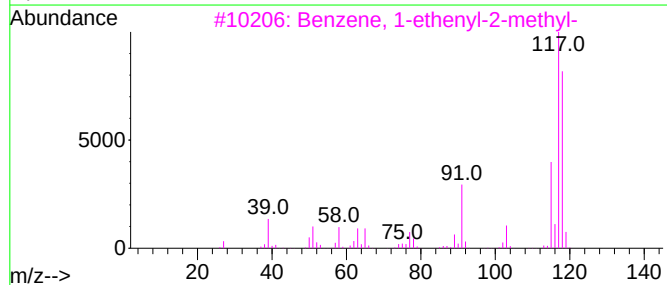
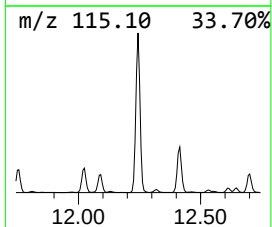
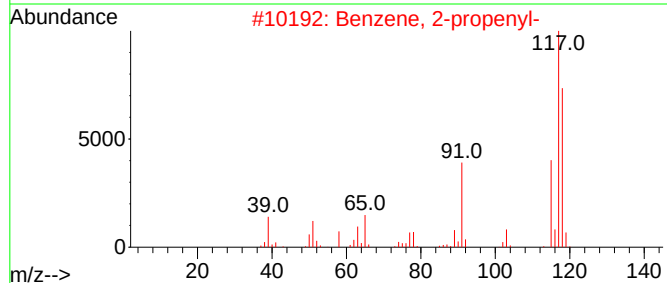
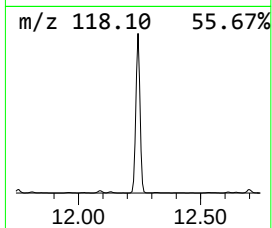
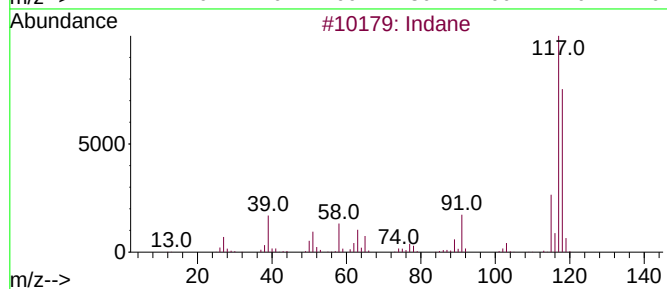
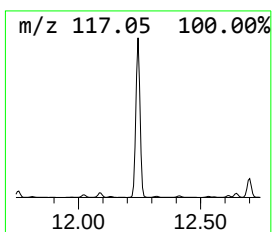
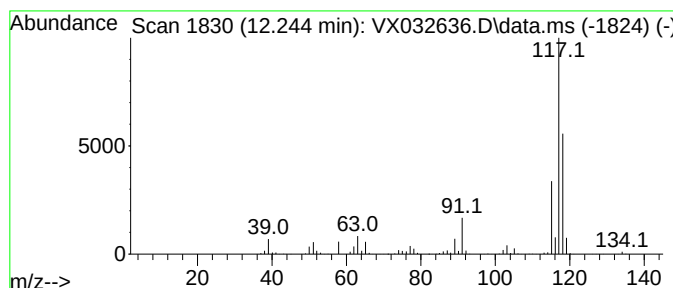
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	294.99 ug/l	3177320	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, 2-propenyl-	118	C9H10	000300-57-2	74
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

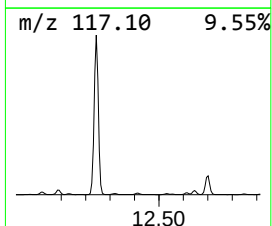
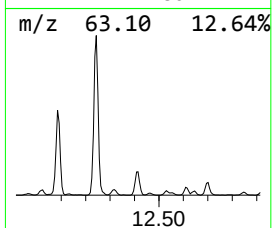
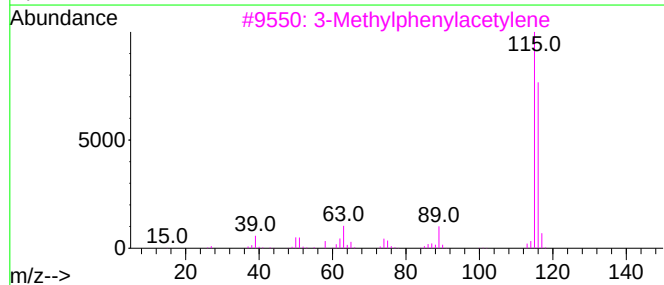
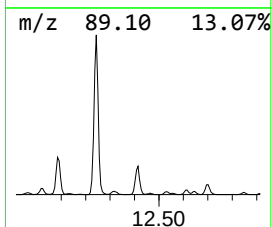
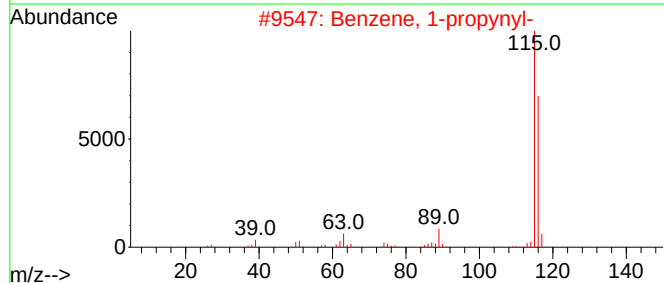
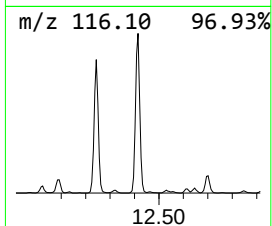
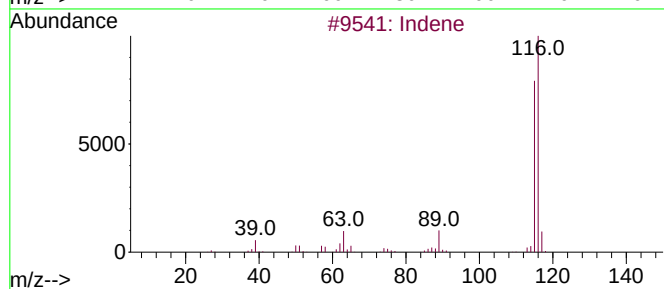
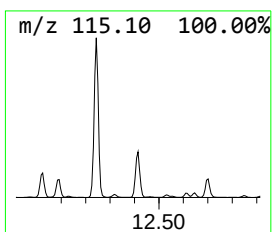
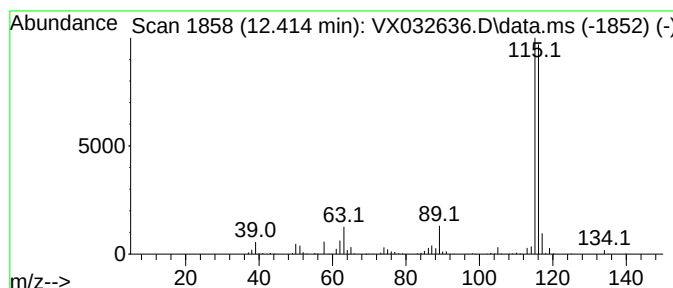
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Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.415	30.07 ug/l	323921	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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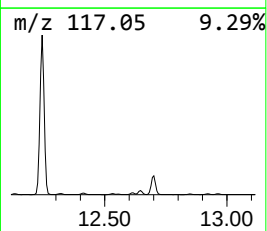
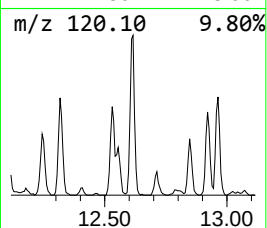
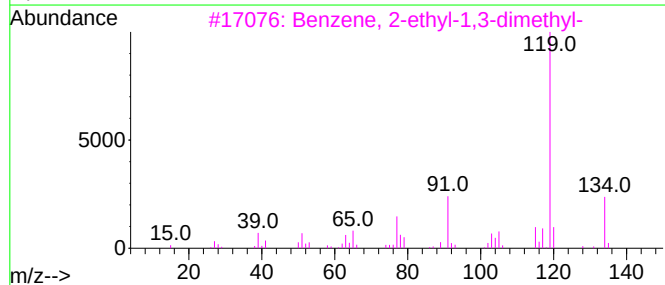
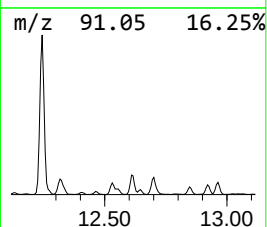
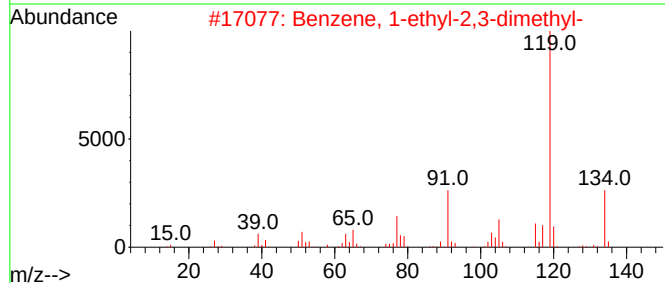
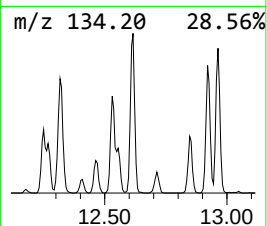
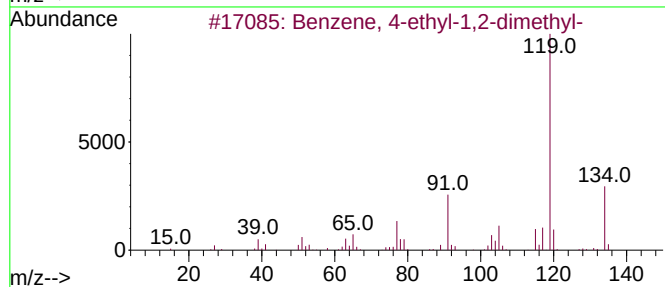
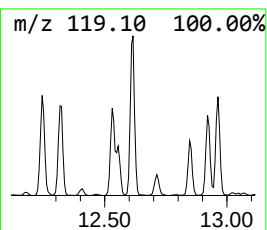
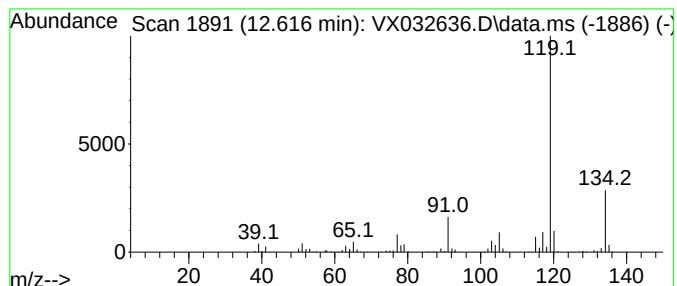
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	30.65 ug/l	330115	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

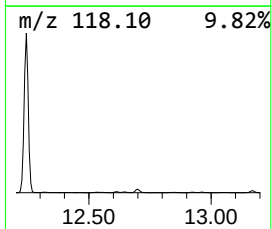
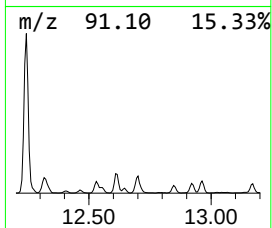
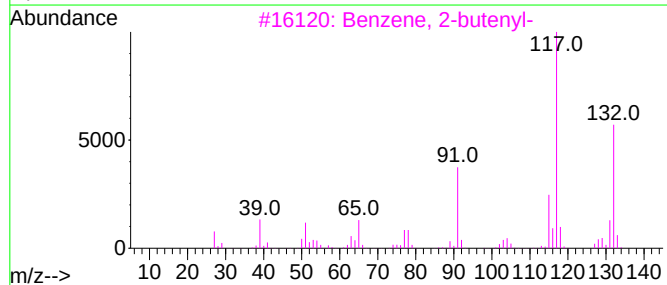
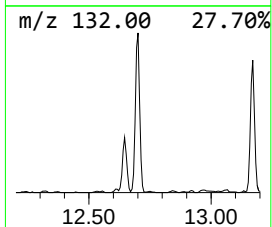
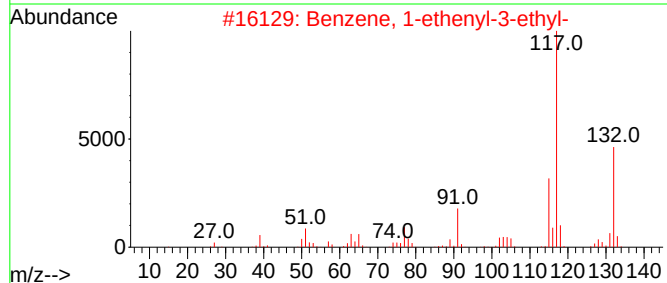
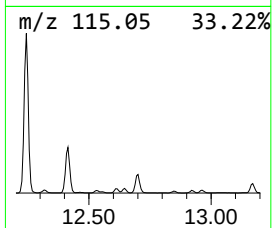
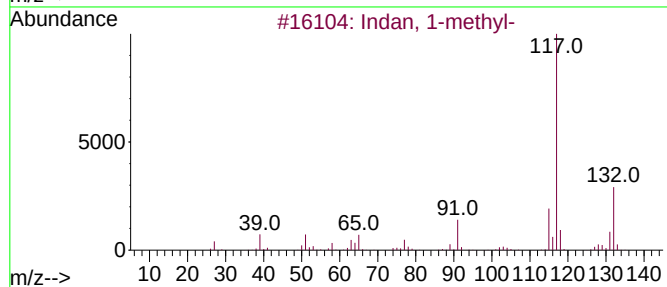
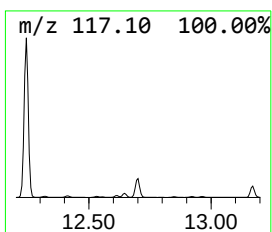
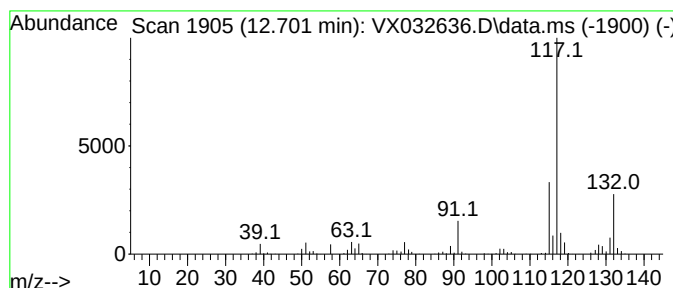
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Quant Title : SW846 8260

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

Peak Number 9 Indan, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	36.20 ug/l	389946	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

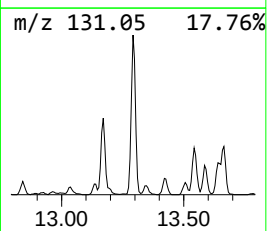
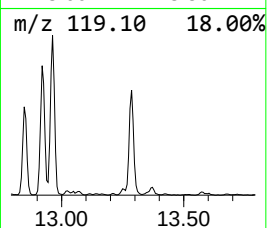
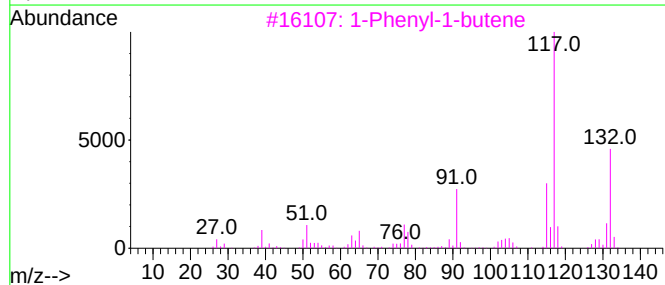
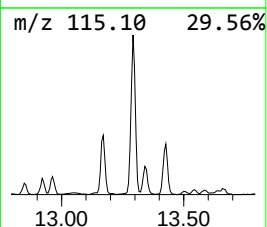
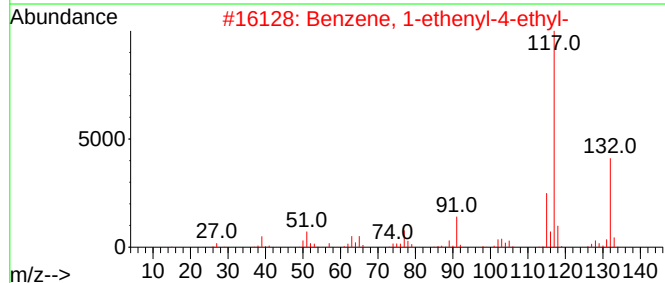
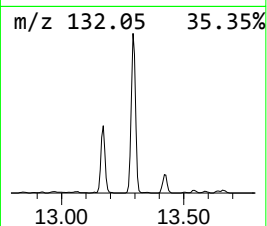
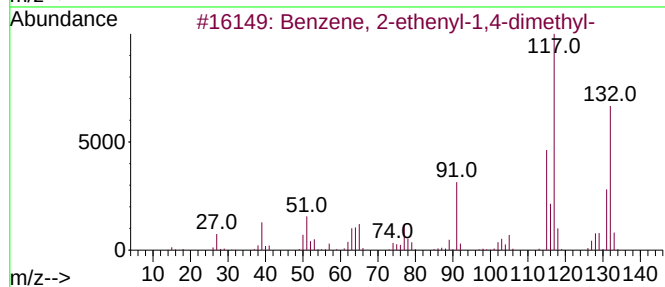
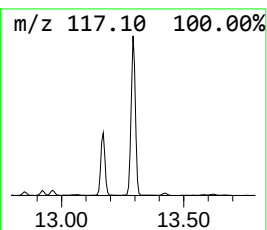
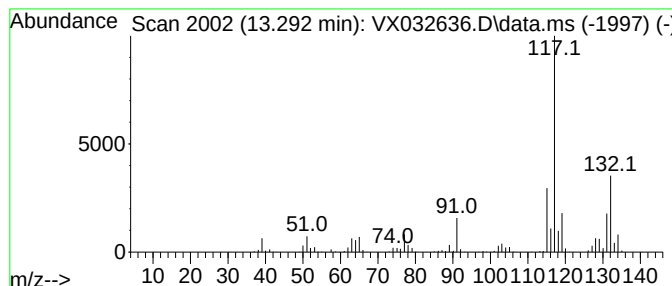
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	64.33 ug/l	692917	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3		1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110722\
Data File : VX032636.D
Acq On : 07 Nov 2022 18:44
Operator : JC/MD
Sample : N5497-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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
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Pentane	1.959	23.8	ug/l	142374	1	5.556	299123	50.0
Cyclopentane, m...	4.306	23.0	ug/l	137688	1	5.556	299123	50.0
Benzene, 1-ethy...	11.616	190.5	ug/l	2052000	4	12.024	538555	50.0
Benzene, 1,2,3-...	12.085	244.2	ug/l	2630250	4	12.024	538555	50.0
Indane	12.244	295.0	ug/l	3177320	4	12.024	538555	50.0
Indene	12.415	30.1	ug/l	323921	4	12.024	538555	50.0
Benzene, 4-ethy...	12.616	30.6	ug/l	330115	4	12.024	538555	50.0
Indan, 1-methyl-	12.701	36.2	ug/l	389946	4	12.024	538555	50.0
Benzene, 2-ethe...	13.292	64.3	ug/l	692917	4	12.024	538555	50.0