

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
 Data File : VX031610.D
 Acq On : 23 Sep 2022 08:00
 Operator : JC/MD
 Sample : N4614-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DUP091322

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\82X091922W.M
 Title : SW846 8260

Signal : TIC: VX031610.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	41	rBV	692424	703573	1.51%	0.305%
2	1.367	41	46	53	rVV	2732798	3085912	6.63%	1.336%
3	1.428	53	56	63	rVV	476625	497741	1.07%	0.215%
4	1.745	103	108	122	rVB	4864230	6402485	13.76%	2.772%
5	1.910	129	135	138	rBV	554961	745724	1.60%	0.323%
6	1.953	138	142	155	rVV2	1909770	2814204	6.05%	1.218%
7	2.068	155	161	169	rVV	1951189	2580055	5.55%	1.117%
8	2.166	170	177	181	rVV	1114585	1672753	3.60%	0.724%
9	2.215	181	185	196	rVB	1451161	1950520	4.19%	0.844%
10	2.751	256	273	281	rBV2	437962	1261940	2.71%	0.546%
11	2.824	281	285	288	rVV	400802	776035	1.67%	0.336%
12	2.867	288	292	306	rVB2	546525	1275419	2.74%	0.552%
13	3.105	320	331	349	rVB2	327740	758665	1.63%	0.328%
14	4.306	517	528	540	rVB	713021	1988229	4.27%	0.861%
15	5.476	711	720	728	rBV2	225763	674235	1.45%	0.292%
16	6.049	803	814	826	rVB	6978795	17578439	37.79%	7.610%
17	6.251	826	847	858	rVB3	238748	1149211	2.47%	0.498%
18	7.378	1020	1032	1040	rBV4	256171	667156	1.43%	0.289%
19	8.653	1235	1241	1246	rVV	519288	796481	1.71%	0.345%
20	8.726	1246	1253	1260	rVV	10311647	15622323	33.58%	6.763%
21	10.055	1461	1471	1476	rBV	375770	576218	1.24%	0.249%
22	10.201	1489	1495	1500	rBV	8974611	11829872	25.43%	5.121%
23	10.311	1506	1513	1519	rVB	31078106	46520860	100.00%	20.140%
24	10.646	1562	1568	1574	rVB	13083655	16551345	35.58%	7.166%
25	10.963	1614	1620	1626	rVB	591762	727077	1.56%	0.315%
26	11.079	1635	1639	1645	rBV	675828	860139	1.85%	0.372%
27	11.305	1667	1676	1683	rBV	1558865	1880657	4.04%	0.814%
28	11.384	1683	1689	1696	rBV	9163396	15773702	33.91%	6.829%
29	11.451	1696	1700	1707	rVB	4233342	5378469	11.56%	2.328%
30	11.615	1721	1727	1736	rBV	4296816	5193295	11.16%	2.248%
31	11.756	1744	1750	1755	rBV	15194860	18281044	39.30%	7.914%
32	12.024	1789	1794	1799	rVB2	646910	852920	1.83%	0.369%
33	12.091	1799	1805	1810	rBV	4718879	5628391	12.10%	2.437%
34	12.243	1825	1830	1833	rBV	3933203	5050262	10.86%	2.186%
35	12.317	1838	1842	1852	rVB2	1628119	2250329	4.84%	0.974%
36	12.463	1862	1866	1872	rVB	446136	523190	1.12%	0.227%

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Peak Location: TOP

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Peak separation: 5

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37	12.530	1872	1877	1879	rBV	924773	1141649	2.45%	0.494%
38	12.554	1879	1881	1886	rVB	878509	968826	2.08%	0.419%
39	12.615	1886	1891	1894	rBV	1559652	1839891	3.95%	0.797%
40	12.701	1900	1905	1913	rBV2	1122702	1593347	3.43%	0.690%
41	12.847	1925	1929	1934	rVB2	492240	618129	1.33%	0.268%
42	12.920	1934	1941	1945	rBV	890896	1145391	2.46%	0.496%
43	12.963	1945	1948	1954	rVB	1426346	1612244	3.47%	0.698%
44	13.170	1978	1982	1986	rVB	1096516	1271917	2.73%	0.551%
45	13.292	1998	2002	2007	rVB2	2405020	3080496	6.62%	1.334%
46	13.426	2019	2024	2032	rVB	616508	830630	1.79%	0.360%
47	13.585	2046	2050	2056	rVV3	292522	540487	1.16%	0.234%
48	13.780	2074	2082	2090	rBV	4469468	5830999	12.53%	2.524%
49	14.225	2149	2155	2163	rBV3	297185	626609	1.35%	0.271%
50	14.639	2210	2223	2233	rBV	3224950	4136830	8.89%	1.791%
51	14.780	2241	2246	2255	rBV	2072091	2656175	5.71%	1.150%
52	15.475	2354	2360	2366	rBV	435670	710951	1.53%	0.308%
53	15.615	2374	2383	2386	rBV	637555	958887	2.06%	0.415%
54	15.651	2386	2389	2397	rVB	385355	542912	1.17%	0.235%

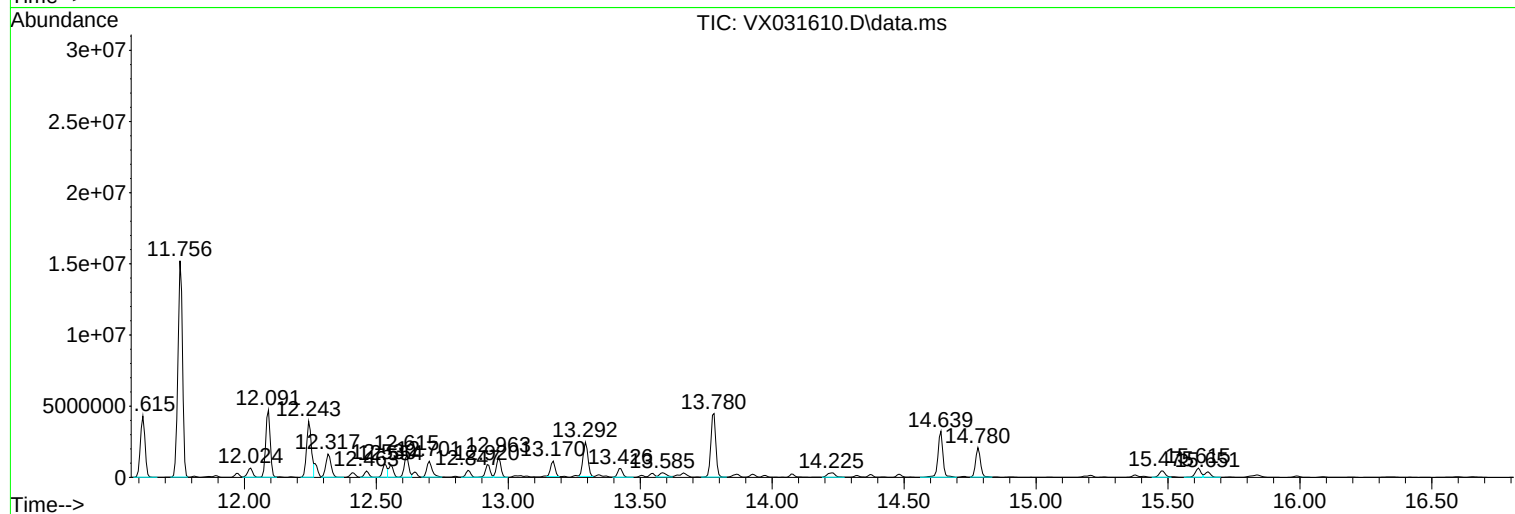
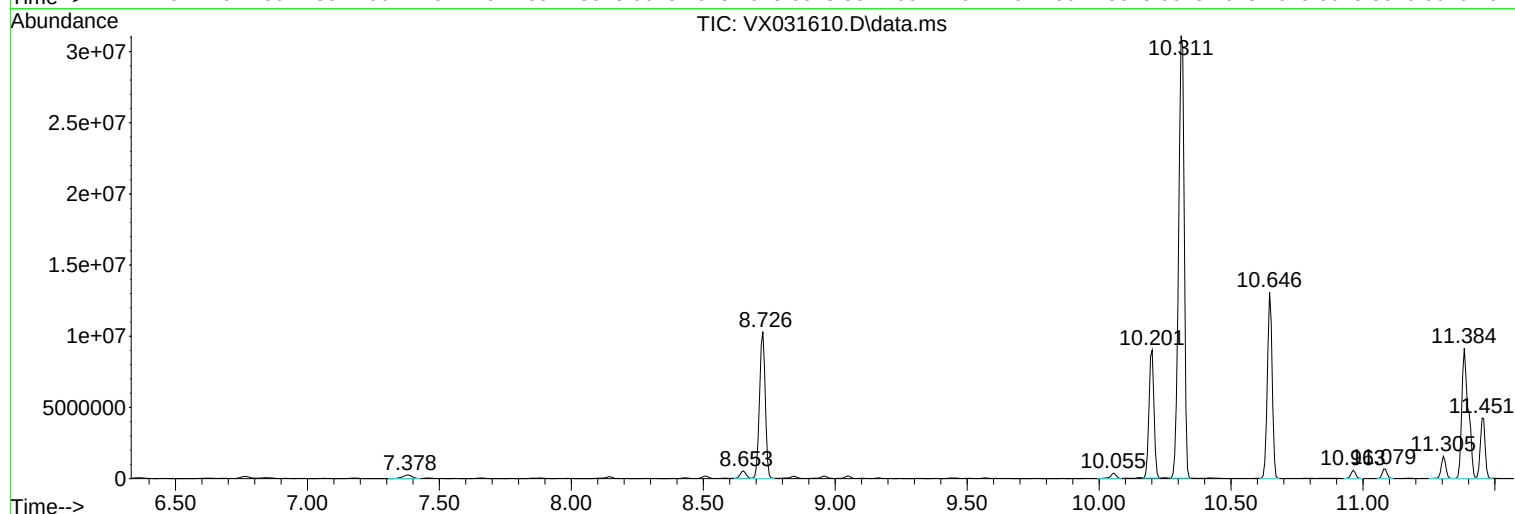
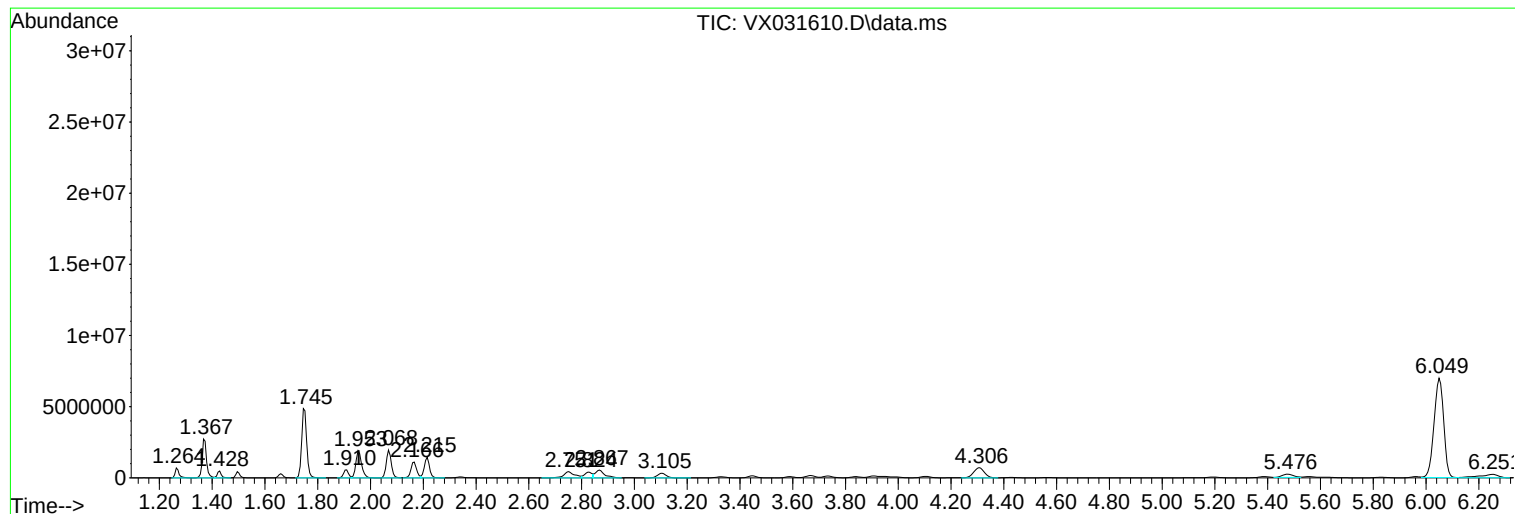
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Quant Title : SW846 8260

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



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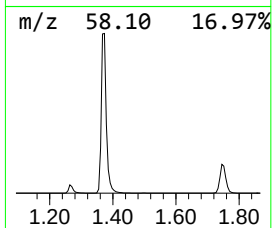
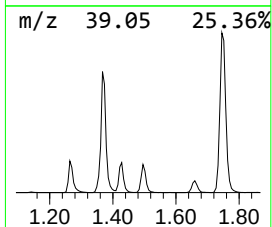
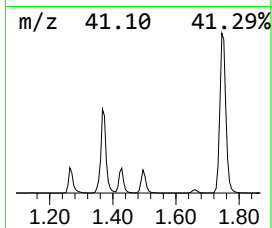
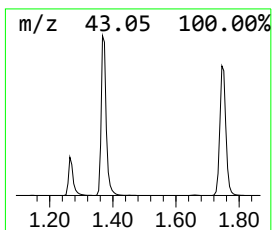
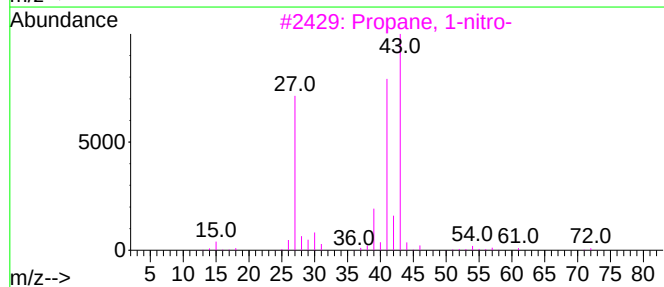
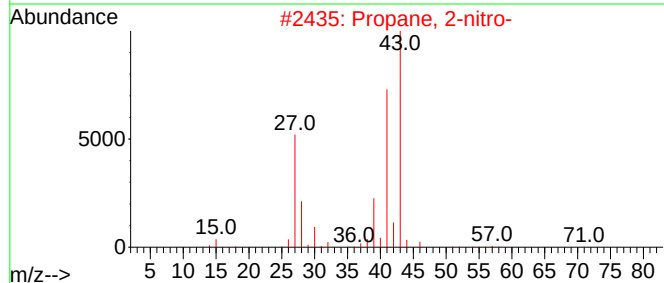
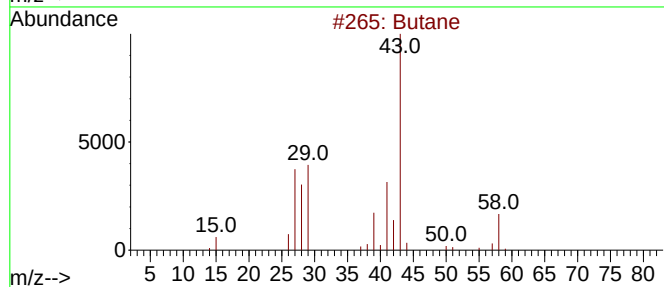
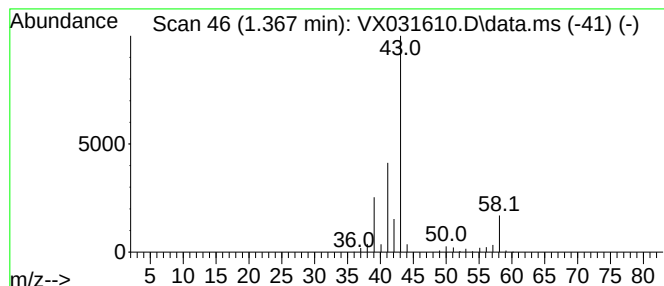
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	228.85 ug/l	3085910	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
4			Acetone	58	C3H6O	000067-64-1	7
5			Isobutane	58	C4H10	000075-28-5	4



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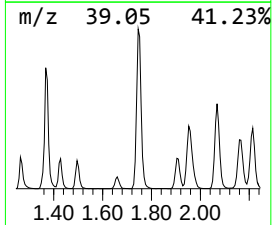
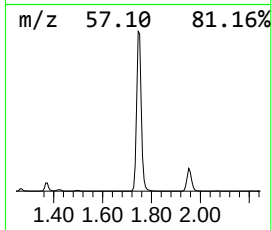
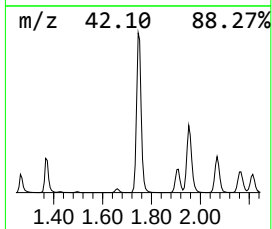
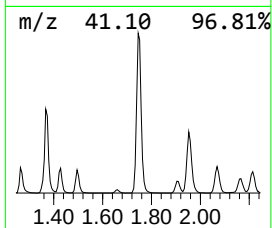
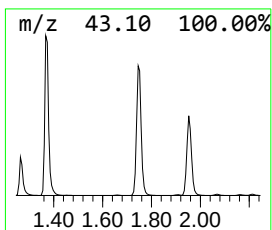
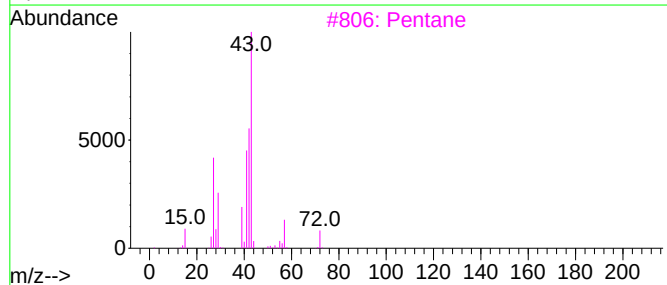
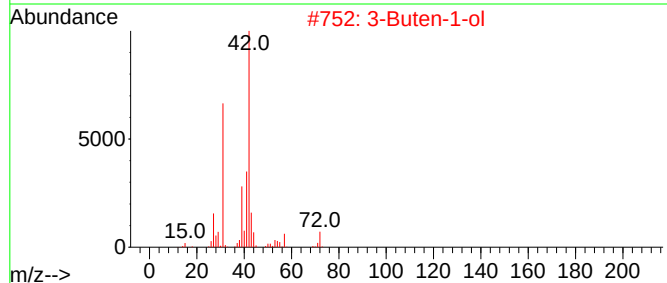
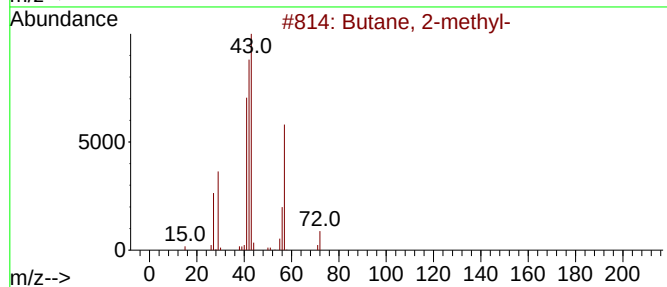
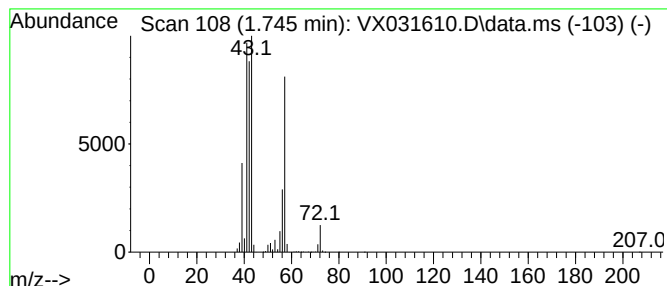
Instrument :
MSVOA_X
ClientSampleId :
DUP091322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.745	474.80 ug/l	6402490	Pentafluorobenzene	5.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Pentane	72	C5H12	000109-66-0	36
4	1-Butene	56	C4H8	000106-98-9	27
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
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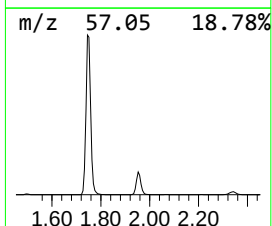
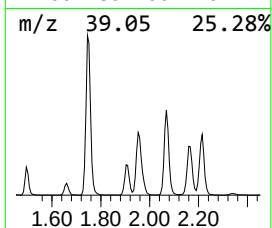
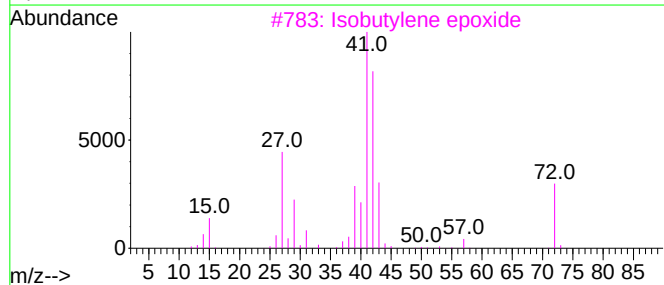
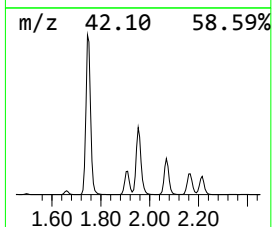
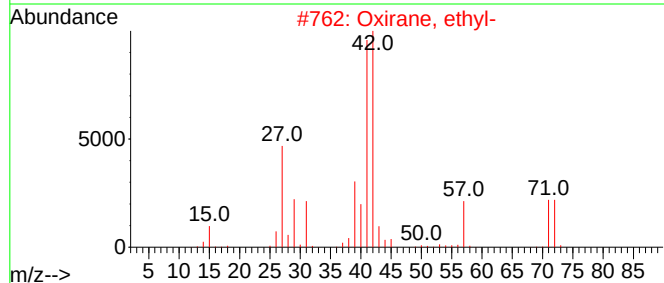
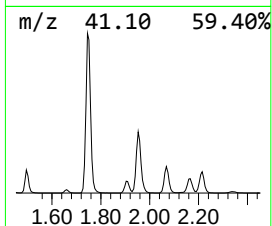
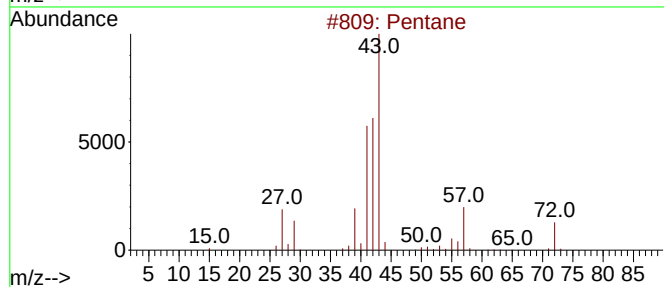
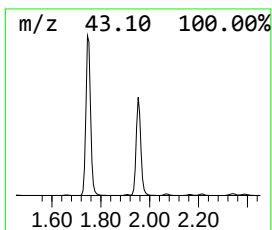
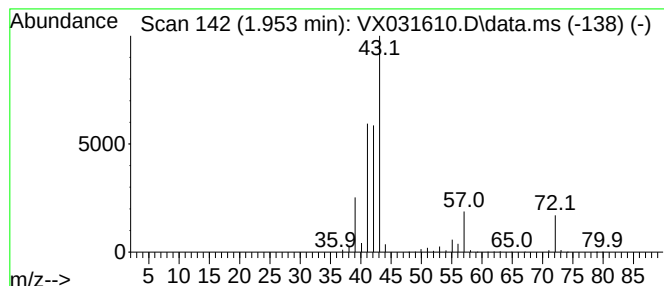
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	208.70 ug/l	2814200	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3			Isobutylene epoxide	72	C4H8O	000558-30-5	47
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
5			1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	25



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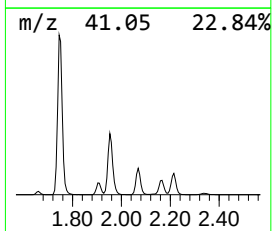
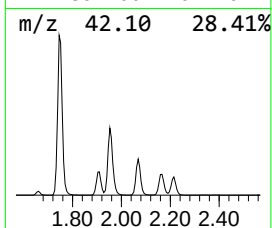
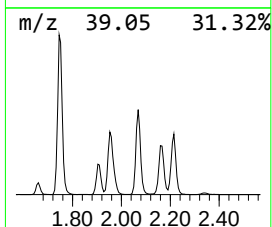
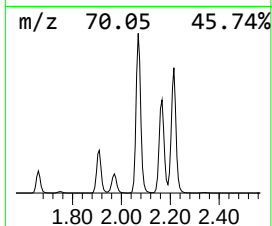
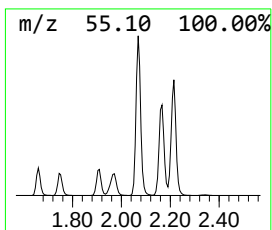
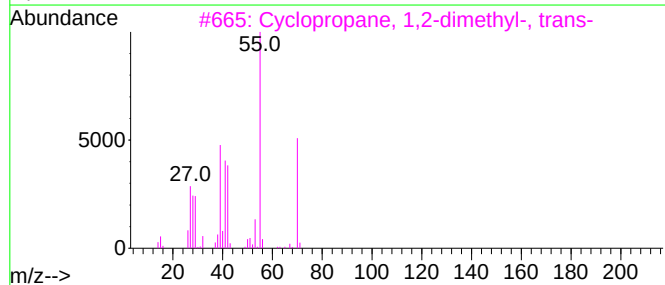
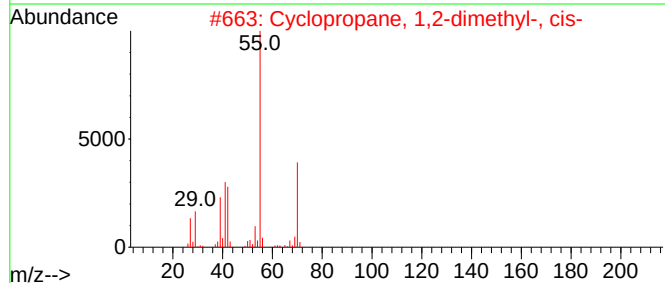
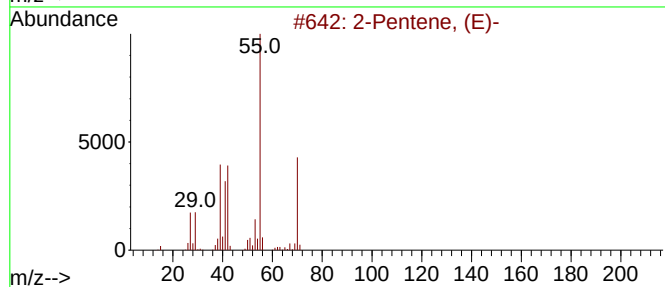
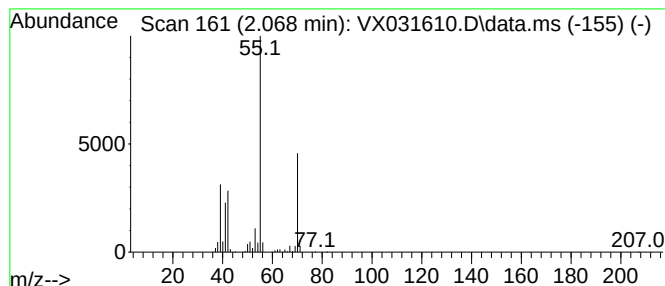
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.068	191.33 ug/l	2580060	Pentafluorobenzene	5.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4	2-Methyl-1-butene	70	C5H10	000563-46-2	87
5	2-Pentene	70	C5H10	000109-68-2	78



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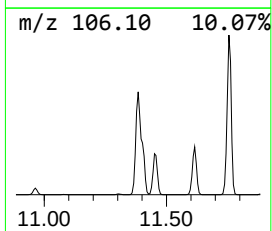
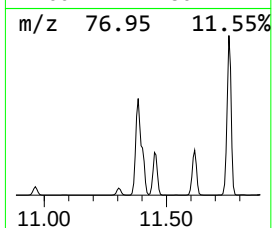
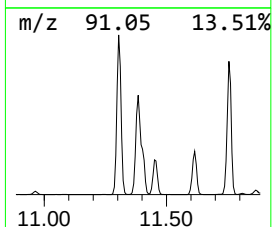
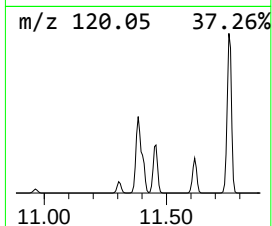
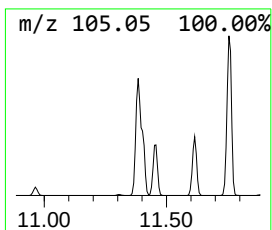
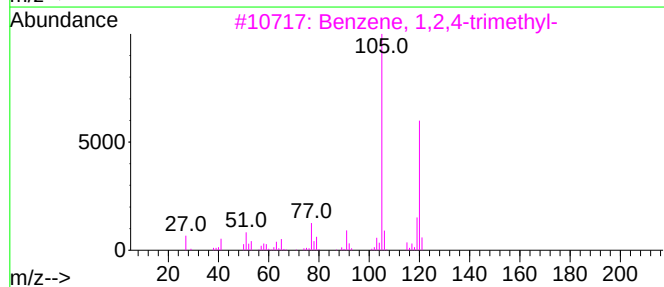
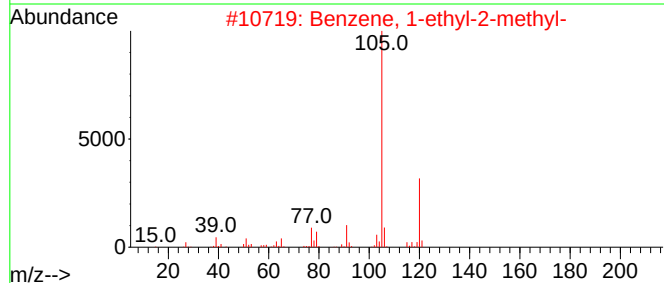
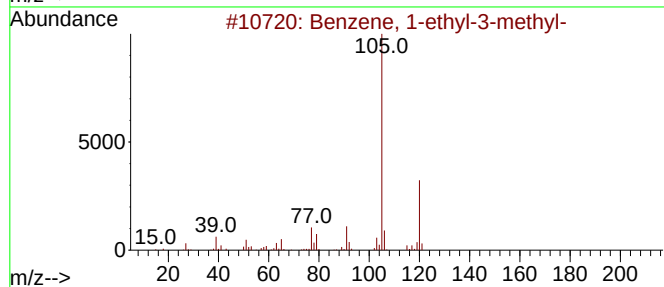
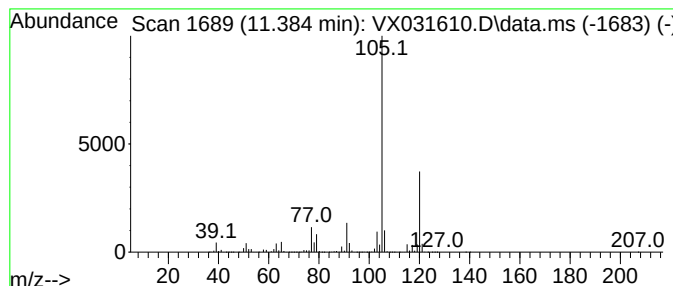
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	924.69 ug/l	15773700	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	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

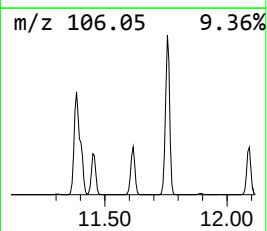
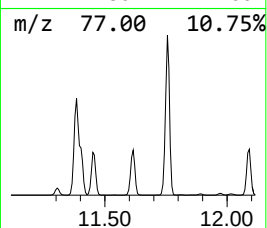
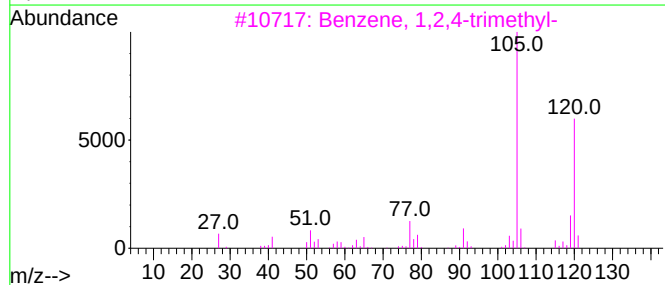
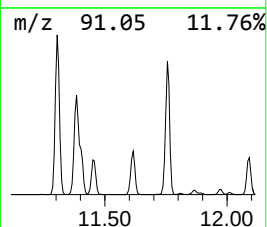
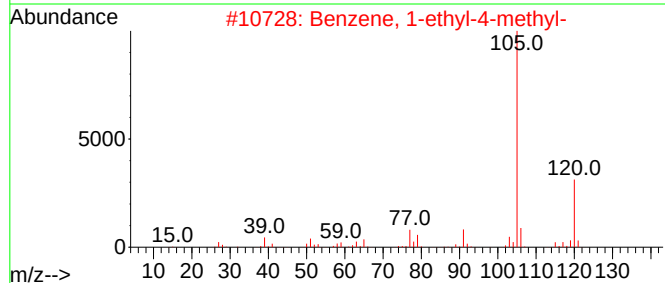
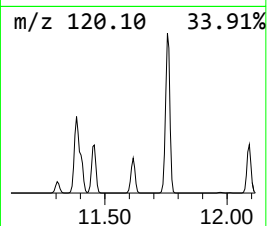
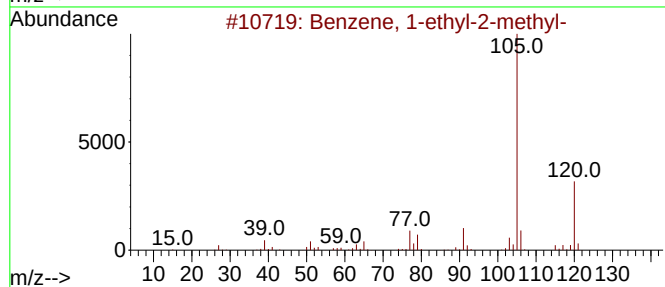
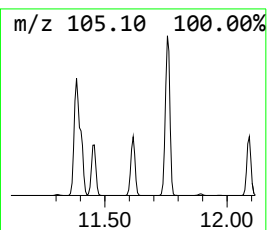
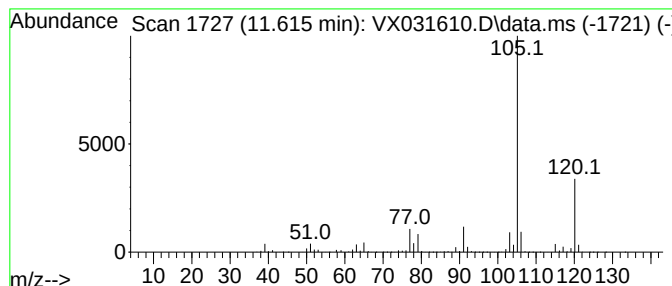
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.615	304.44 ug/l	5193300	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	91
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			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

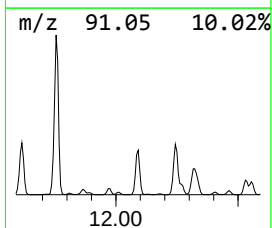
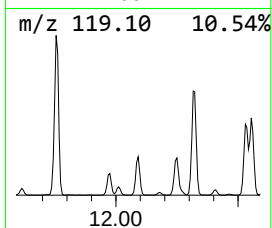
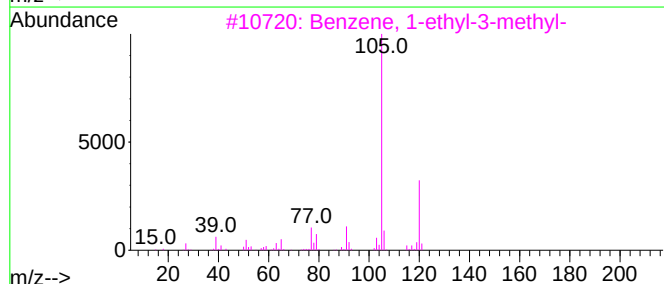
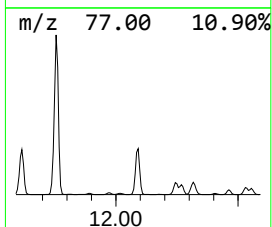
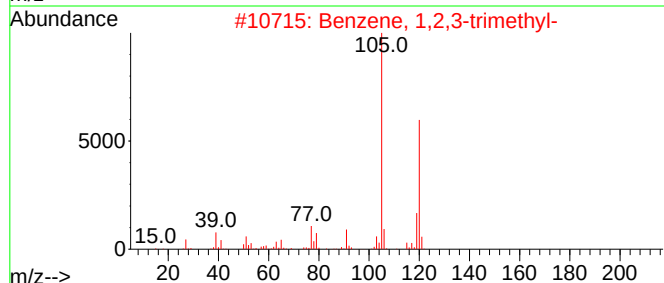
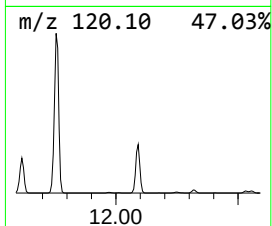
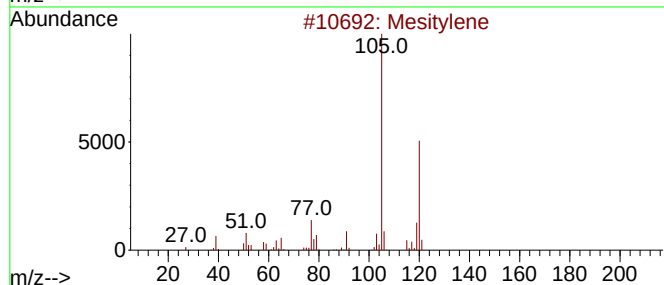
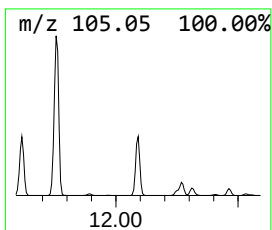
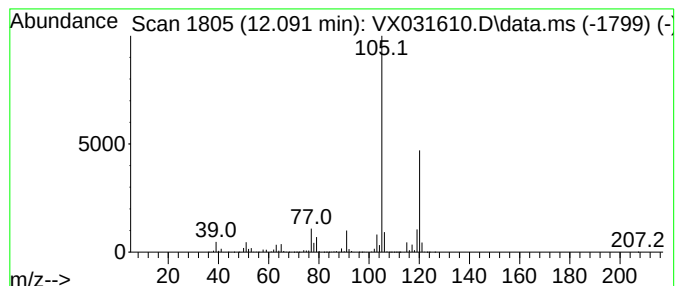
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	329.95 ug/l	5628390	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-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

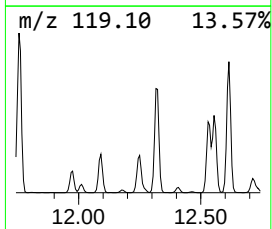
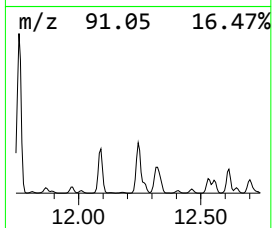
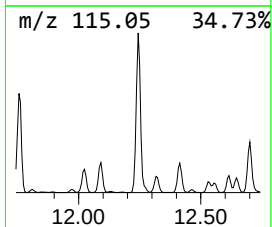
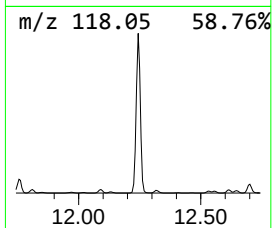
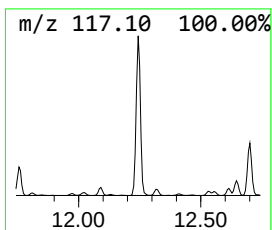
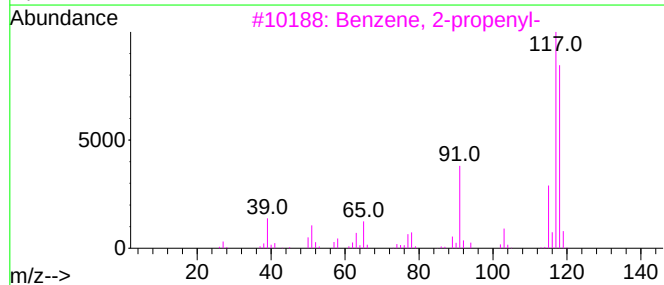
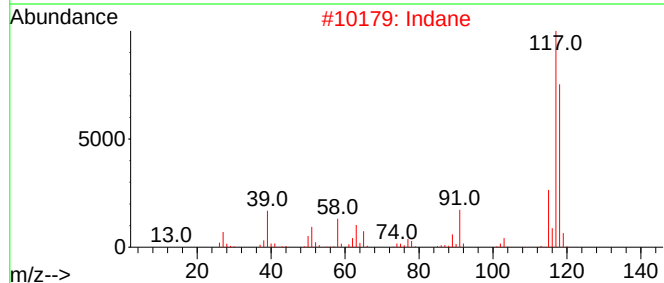
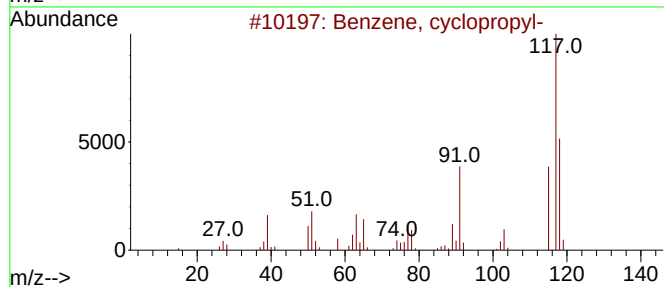
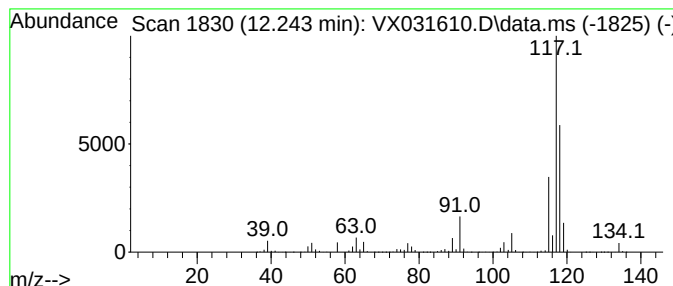
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, cyclopropyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	296.06 ug/l	5050260	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5			Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

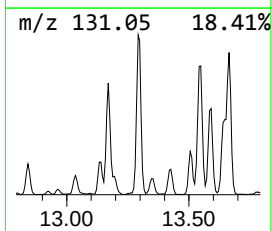
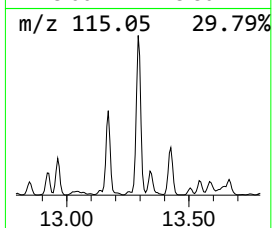
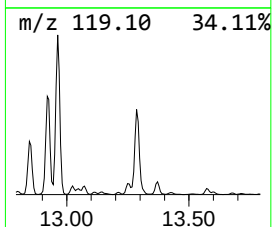
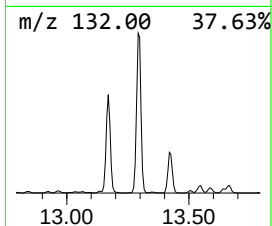
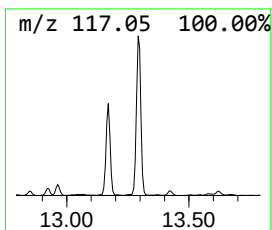
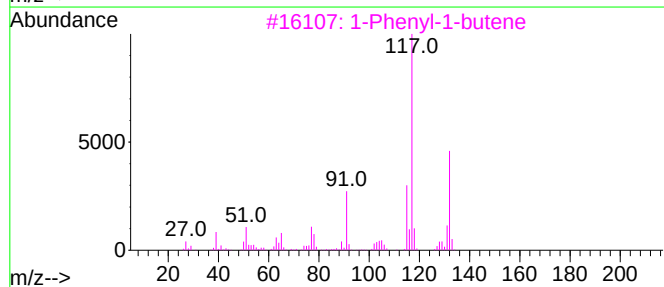
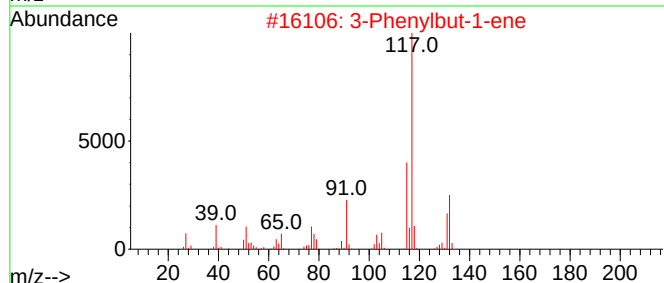
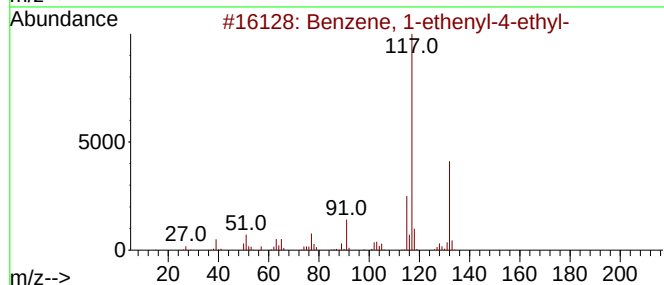
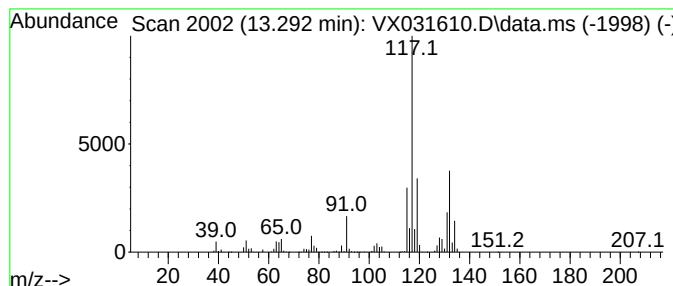
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	180.59 ug/l	3080500	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

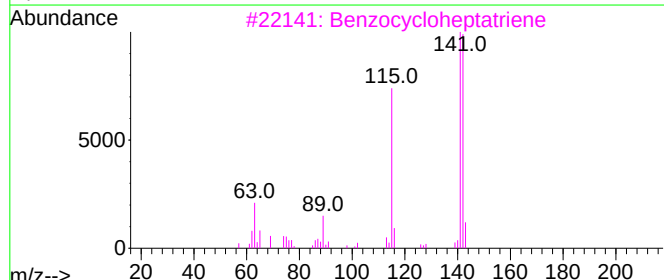
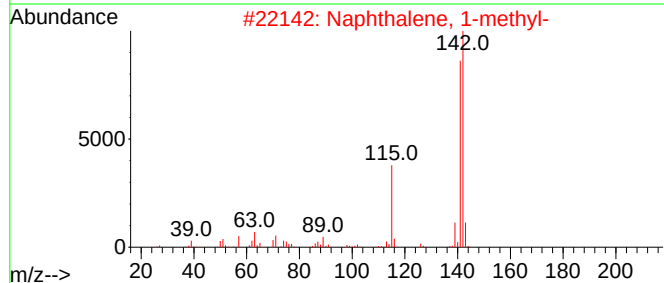
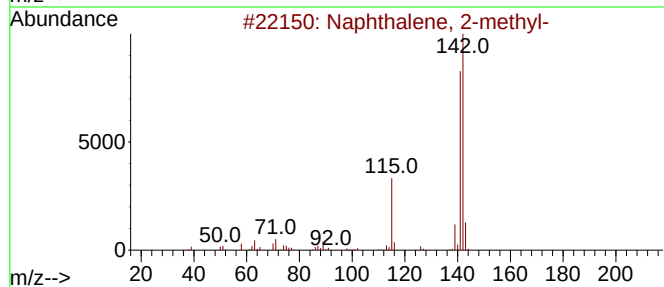
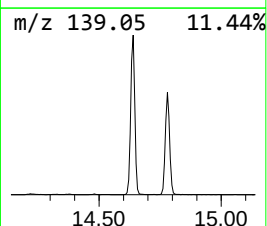
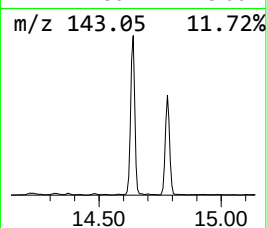
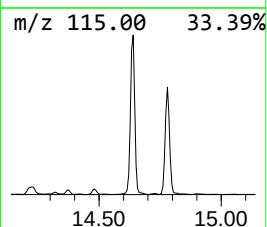
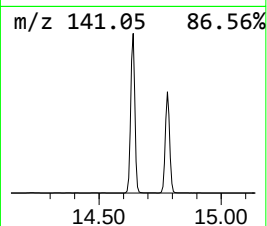
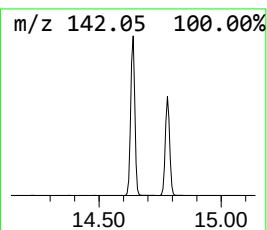
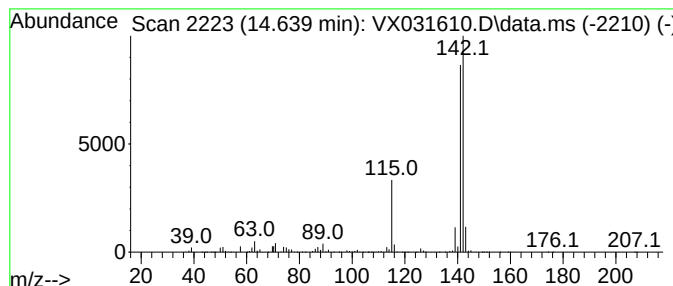
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	242.51 ug/l	4136830	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031610.D
Acq On : 23 Sep 2022 08:00
Operator : JC/MD
Sample : N4614-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 54 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DUP091322

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.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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Butane, 2-methyl-	1.745	474.8	ug/l	6402490	1	5.562	674235	50.0
Pentane	1.953	208.7	ug/l	2814200	1	5.562	674235	50.0
2-Pentene, (E)-	2.068	191.3	ug/l	2580060	1	5.562	674235	50.0
Benzene, 1-ethy...	11.384	924.7	ug/l	15773700	4	12.024	852920	50.0
Benzene, 1-ethy...	11.615	304.4	ug/l	5193300	4	12.024	852920	50.0
Benzene, 1,2,3-...	12.091	329.9	ug/l	5628390	4	12.024	852920	50.0
Benzene, cyclop...	12.243	296.1	ug/l	5050260	4	12.024	852920	50.0
Benzene, 1-ethe...	13.292	180.6	ug/l	3080500	4	12.024	852920	50.0
Naphthalene, 1-...	14.639	242.5	ug/l	4136830	4	12.024	852920	50.0