

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
 Data File : VX031586.D
 Acq On : 22 Sep 2022 21:24
 Operator : JC/MD
 Sample : N4614-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-41

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: VX031586.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	40	rBV	717751	686463	1.43%	0.289%
2	1.368	40	46	53	rVV	2939471	3109719	6.47%	1.310%
3	1.429	53	56	63	rVV	473078	526494	1.10%	0.222%
4	1.496	63	67	78	rVB	463393	480836	1.00%	0.203%
5	1.746	103	108	121	rVB	4913589	6261494	13.03%	2.637%
6	1.904	129	134	138	rBV	587044	773578	1.61%	0.326%
7	1.953	138	142	155	rVV2	1911011	2849068	5.93%	1.200%
8	2.069	155	161	169	rVV	2027630	2681042	5.58%	1.129%
9	2.160	170	176	181	rVV	1167647	1762614	3.67%	0.742%
10	2.215	181	185	196	rVB	1601369	2181637	4.54%	0.919%
11	2.752	258	273	281	rBV2	438943	1253273	2.61%	0.528%
12	2.825	281	285	288	rVV	372557	727397	1.51%	0.306%
13	2.867	288	292	306	rVB2	545367	1247085	2.60%	0.525%
14	3.105	320	331	352	rVB2	306911	722741	1.50%	0.304%
15	4.306	517	528	540	rVB	695522	1914646	3.98%	0.806%
16	5.477	711	720	728	rBV	222905	655434	1.36%	0.276%
17	6.050	803	814	826	rVB	7325092	18582784	38.67%	7.827%
18	6.251	842	847	858	rVB2	216428	630113	1.31%	0.265%
19	7.379	1020	1032	1040	rBV4	239269	630442	1.31%	0.266%
20	8.653	1235	1241	1246	rVB	505095	775051	1.61%	0.326%
21	8.726	1246	1253	1260	rBV	10561509	16114947	33.54%	6.787%
22	10.055	1461	1471	1476	rBV	345249	510251	1.06%	0.215%
23	10.202	1489	1495	1500	rBV	9096802	12251889	25.50%	5.160%
24	10.317	1506	1514	1519	rVB	31255269	48051932	100.00%	20.239%
25	10.647	1562	1568	1574	rVB	13409740	17166691	35.73%	7.230%
26	10.964	1613	1620	1626	rVB	588777	737600	1.54%	0.311%
27	11.079	1634	1639	1645	rBV	677792	883020	1.84%	0.372%
28	11.305	1668	1676	1683	rBV	1562711	1915300	3.99%	0.807%
29	11.384	1683	1689	1696	rBV	9262590	16063032	33.43%	6.766%
30	11.451	1696	1700	1706	rVB	4425591	5493211	11.43%	2.314%
31	11.616	1721	1727	1736	rBV	4246521	5305644	11.04%	2.235%
32	11.756	1744	1750	1755	rBV	15585079	18752354	39.03%	7.898%
33	12.024	1789	1794	1799	rVB2	623551	852218	1.77%	0.359%
34	12.091	1799	1805	1810	rBV	4596432	5755647	11.98%	2.424%
35	12.244	1824	1830	1838	rBV2	4107782	6052813	12.60%	2.549%
36	12.317	1838	1842	1850	rVB2	1623273	2268378	4.72%	0.955%

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37	12.463	1862	1866	1872	rVB	453962	531027	1.11%	0.224%
38	12.530	1872	1877	1879	rBV	955112	1184196	2.46%	0.499%
39	12.555	1879	1881	1886	rVB	904442	964128	2.01%	0.406%
40	12.616	1886	1891	1894	rBV	1545908	1871284	3.89%	0.788%
41	12.701	1900	1905	1913	rBV2	1117676	1633426	3.40%	0.688%
42	12.847	1924	1929	1934	rVB	510640	633223	1.32%	0.267%
43	12.921	1934	1941	1945	rBV	936843	1161651	2.42%	0.489%
44	12.963	1945	1948	1954	rVB	1456255	1637840	3.41%	0.690%
45	13.171	1978	1982	1986	rVB	1105450	1305063	2.72%	0.550%
46	13.292	1997	2002	2007	rVB2	2445739	3177944	6.61%	1.339%
47	13.420	2019	2023	2031	rVB	643188	840841	1.75%	0.354%
48	13.774	2074	2081	2089	rBV	4507020	5999294	12.49%	2.527%
49	14.225	2149	2155	2163	rBV3	313441	628688	1.31%	0.265%
50	14.640	2210	2223	2233	rBV	3164137	4214209	8.77%	1.775%
51	14.780	2240	2246	2255	rBV	2185470	2771350	5.77%	1.167%
52	15.475	2354	2360	2366	rBV	444397	725022	1.51%	0.305%
53	15.615	2374	2383	2386	rBV	627495	972516	2.02%	0.410%
54	15.652	2386	2389	2397	rVB	384131	544736	1.13%	0.229%

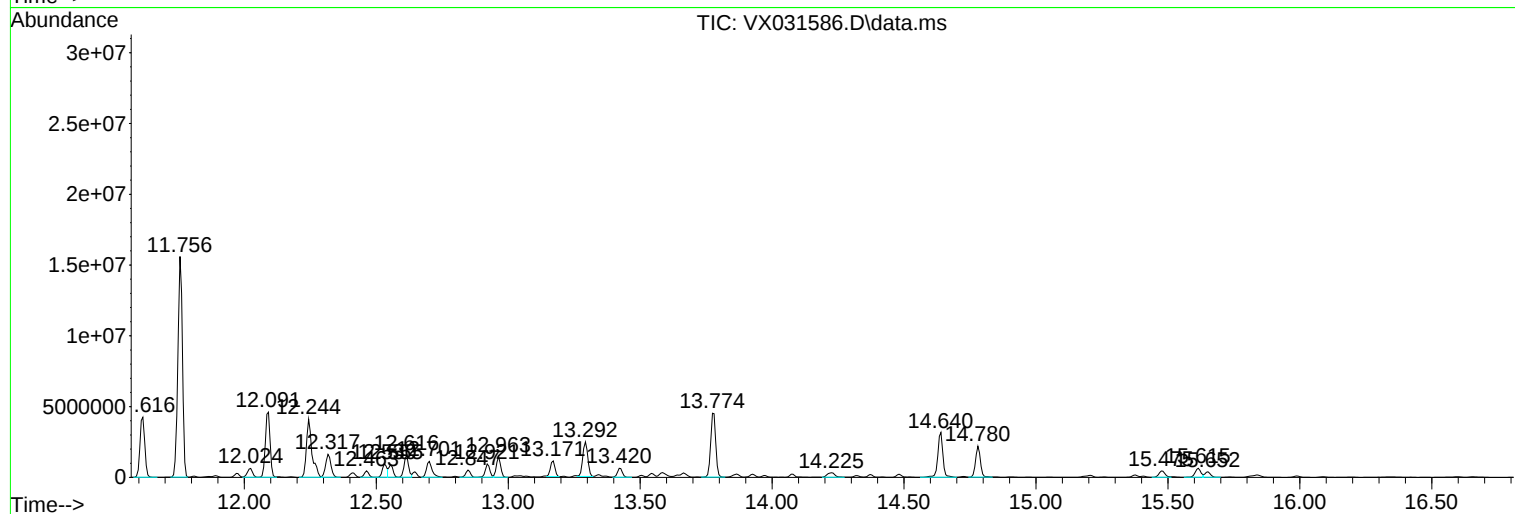
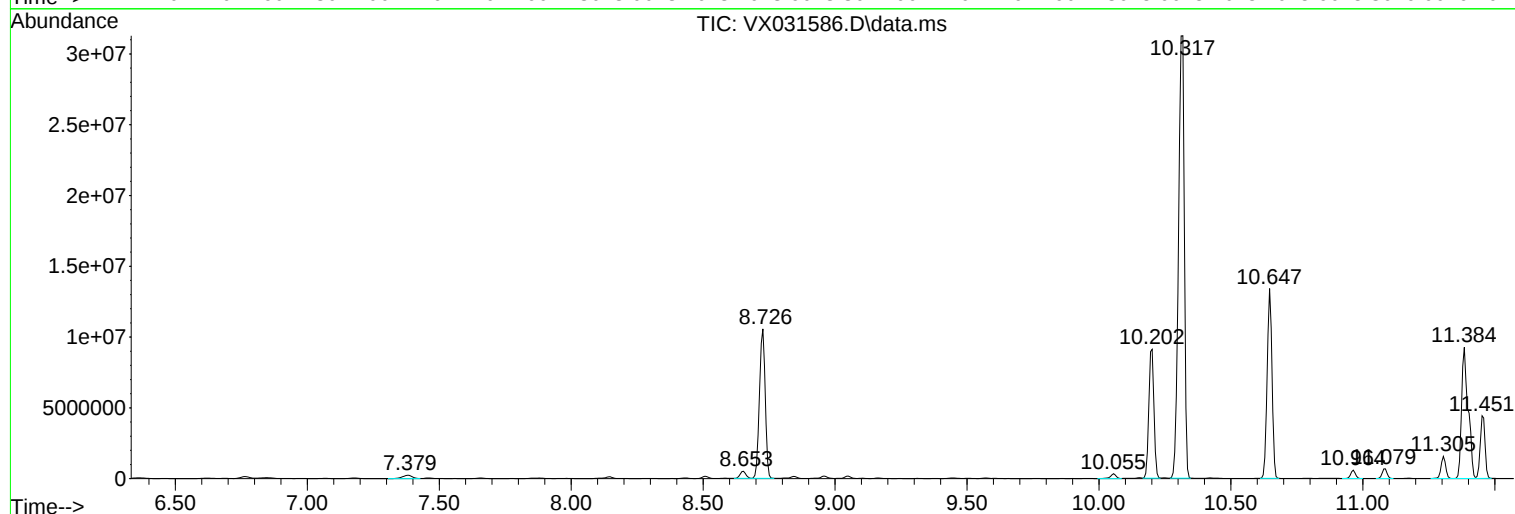
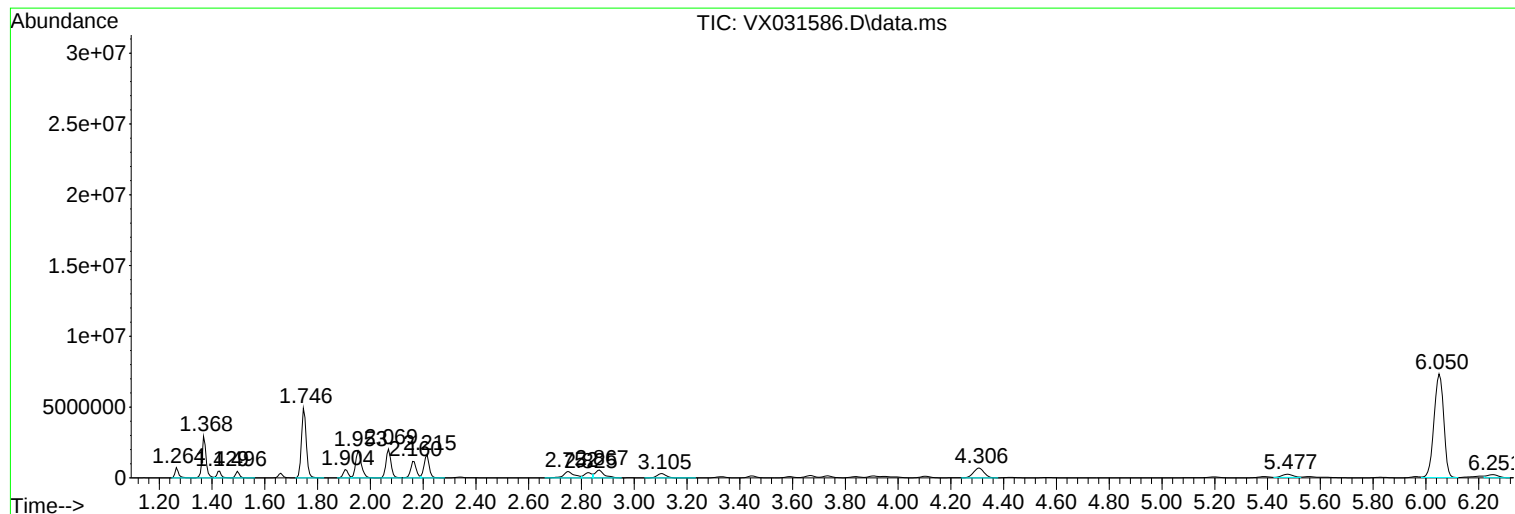
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Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
MW-41

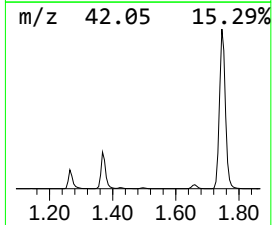
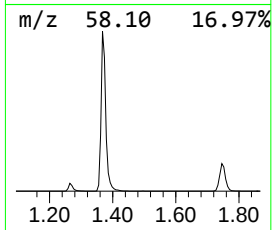
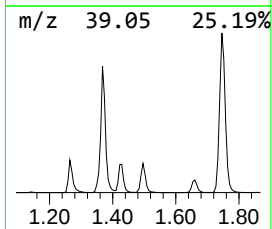
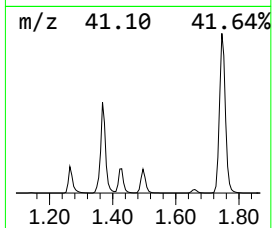
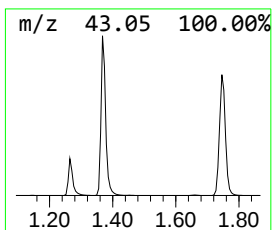
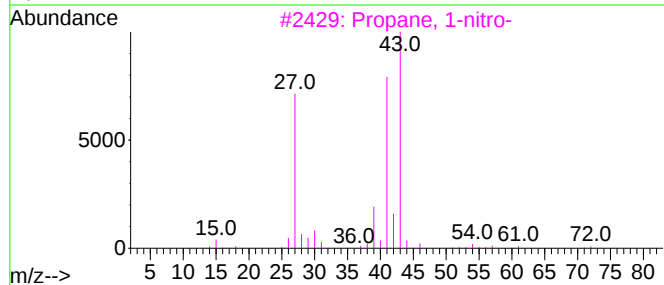
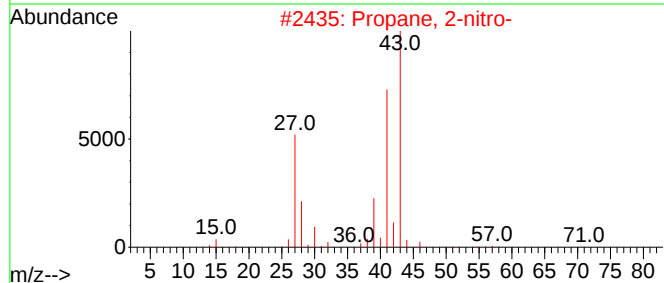
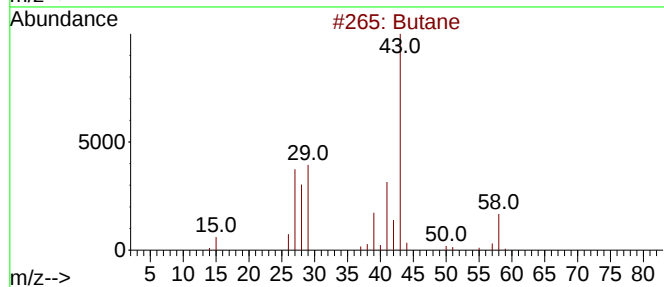
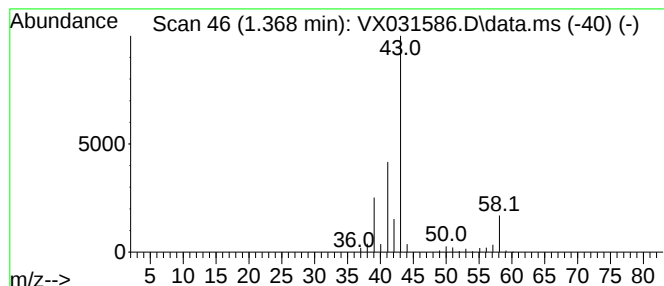
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Quant Title : SW846 8260

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.
1.368	237.23 ug/l	3109720	Pentafluorobenzene	5.556

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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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-41

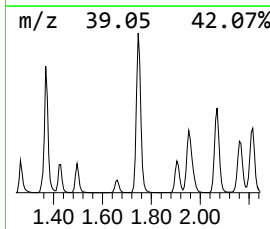
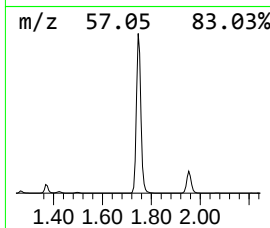
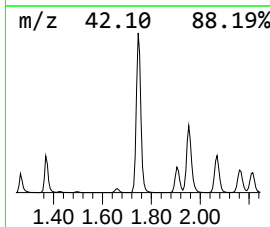
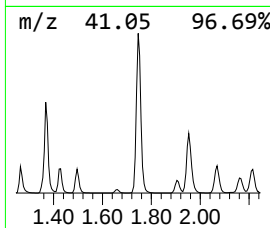
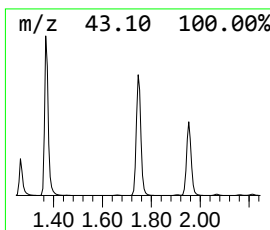
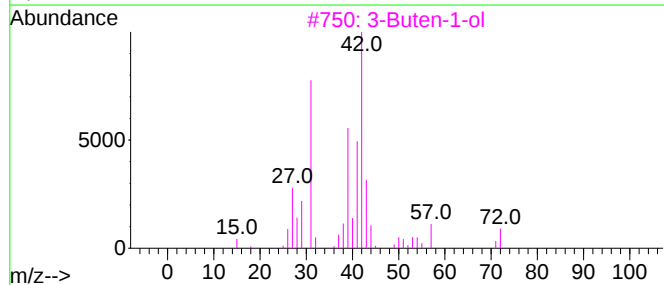
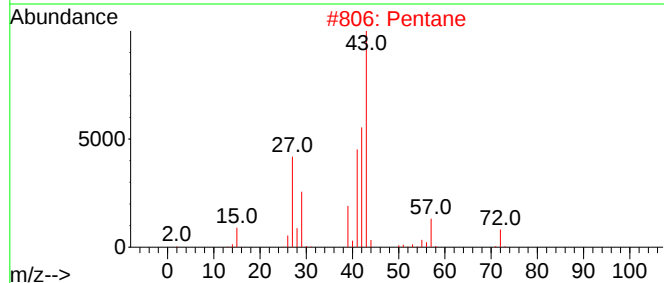
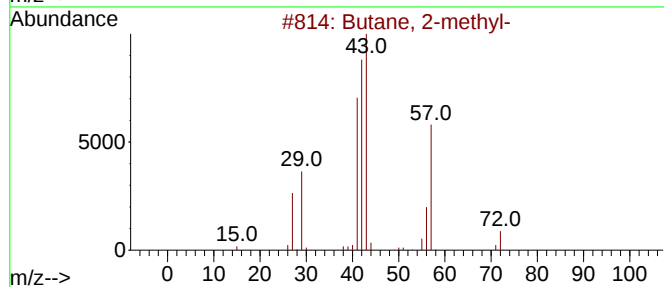
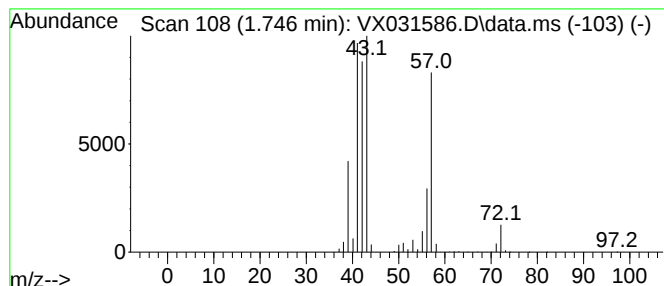
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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.
1.746	477.66 ug/l	6261490	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	33
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
5			Oxirane, trimethyl-	86	C5H10O	005076-19-7	25



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

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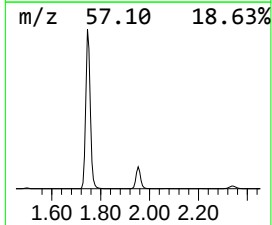
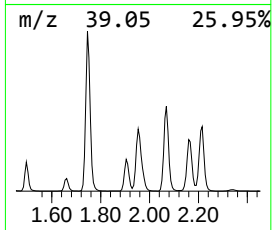
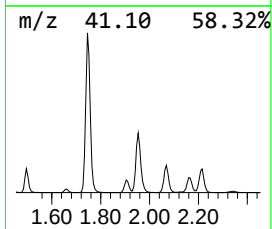
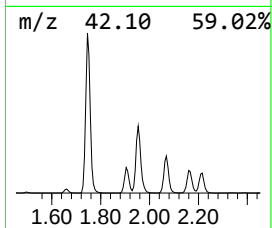
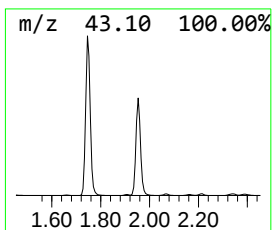
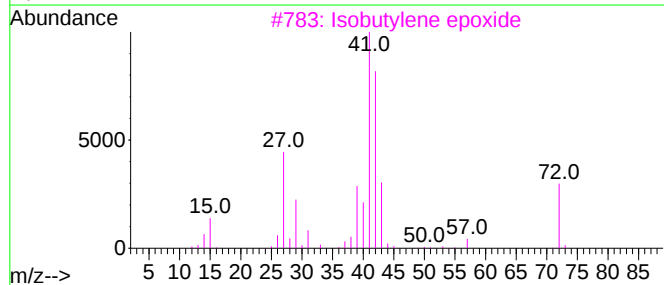
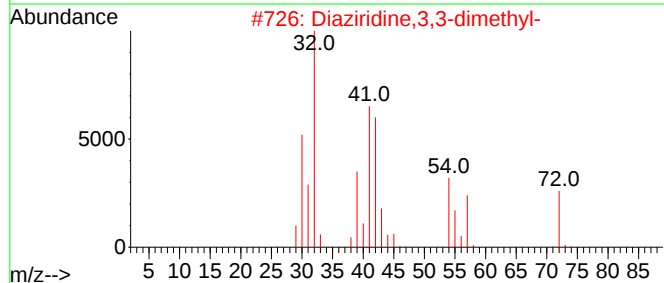
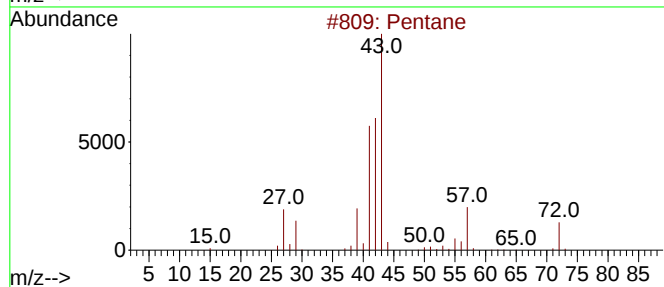
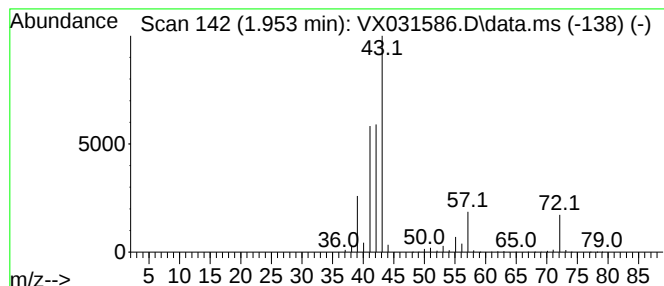
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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	217.34 ug/l	2849070	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Diaziridine,3,3-dimethyl-			72	C3H8N2	004901-76-2	53
3	Isobutylene epoxide			72	C4H8O	000558-30-5	47
4	Oxirane, ethyl-			72	C4H8O	000106-88-7	40
5	Tetrahydrofuran			72	C4H8O	000109-99-9	37



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-41

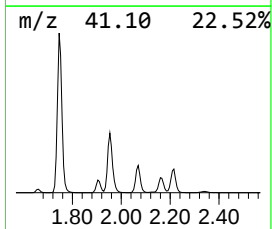
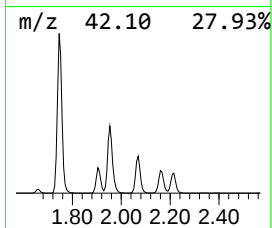
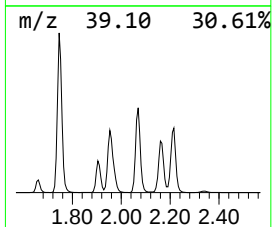
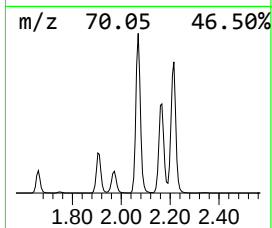
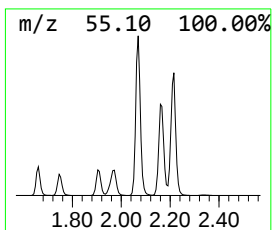
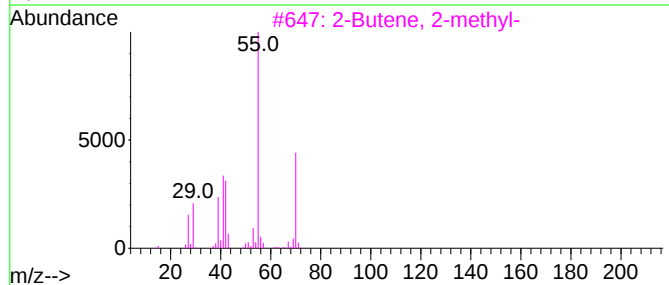
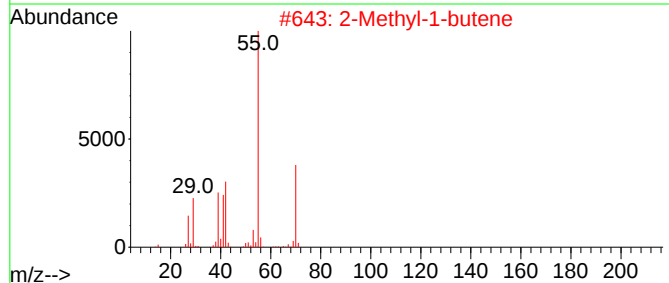
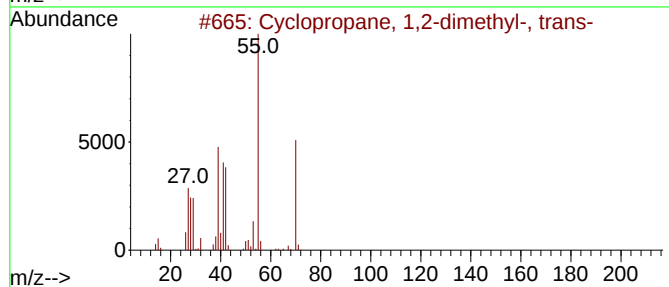
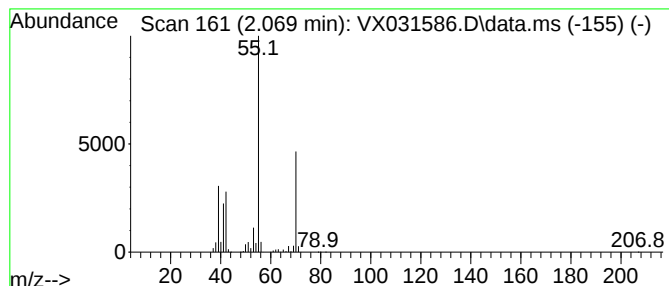
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	204.52 ug/l	2681040	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
2			2-Methyl-1-butene	70	C5H10	000563-46-2	87
3			2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
4			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72



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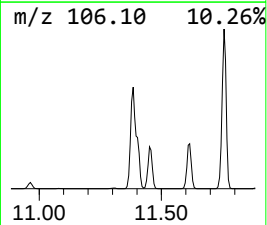
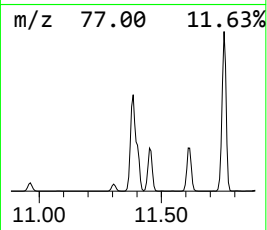
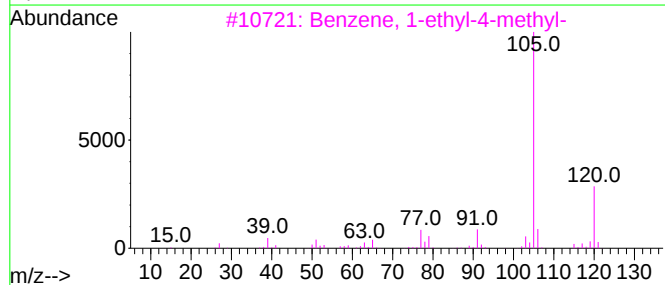
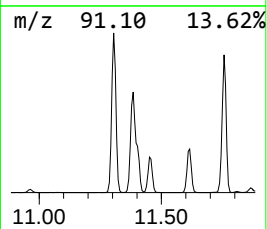
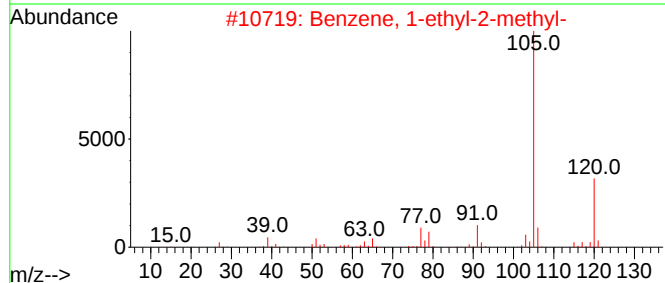
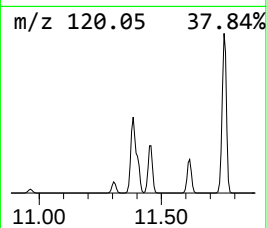
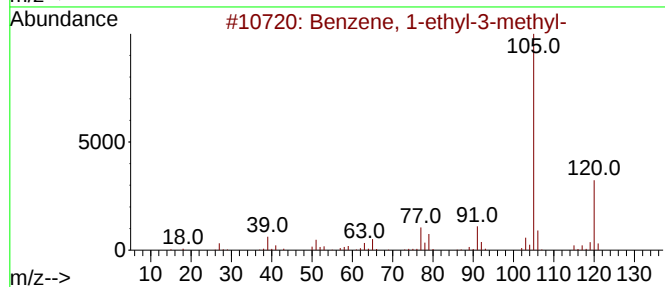
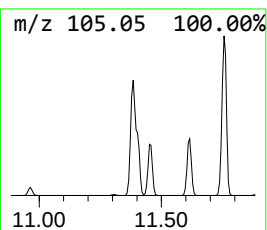
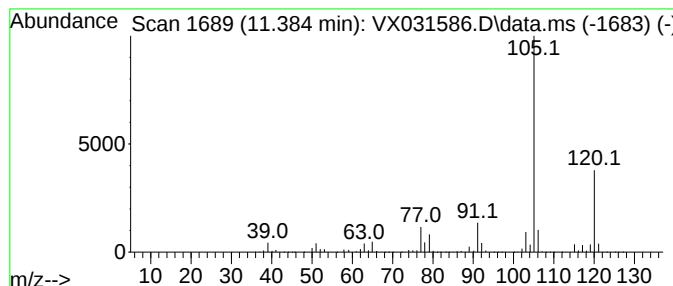
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Quant Title : SW846 8260

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	942.42 ug/l	16063000	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-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

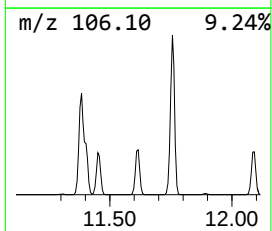
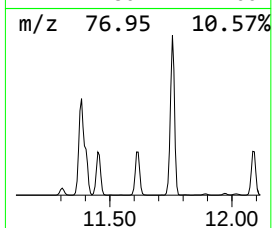
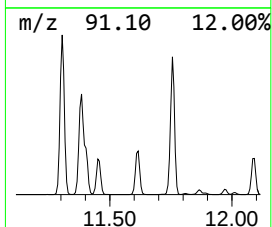
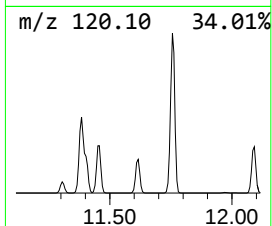
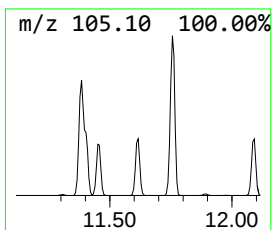
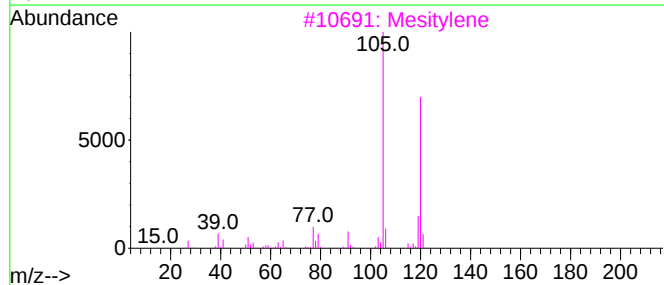
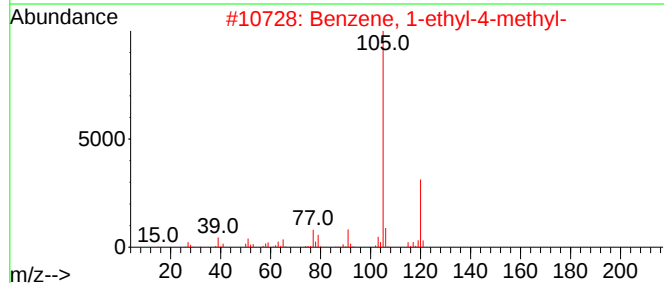
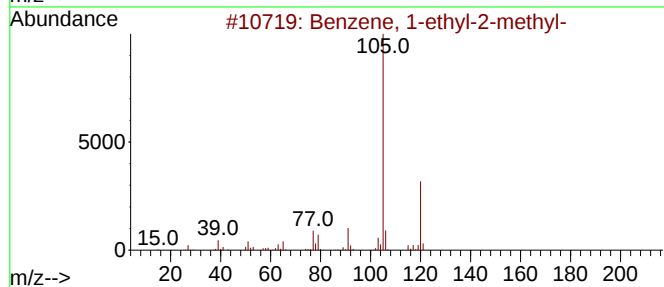
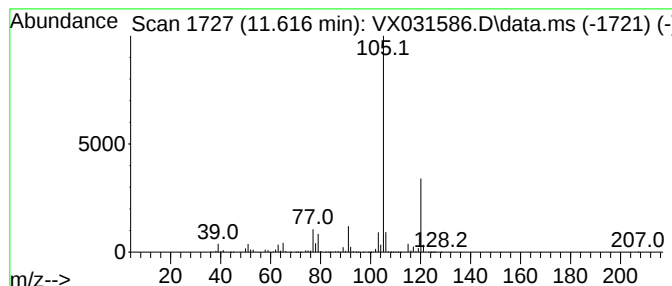
Instrument :
MSVOA_X
ClientSampleId :
MW-41

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 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.616	311.28 ug/l	5305640	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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-41

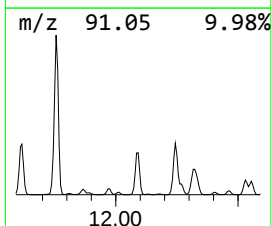
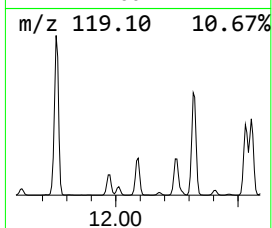
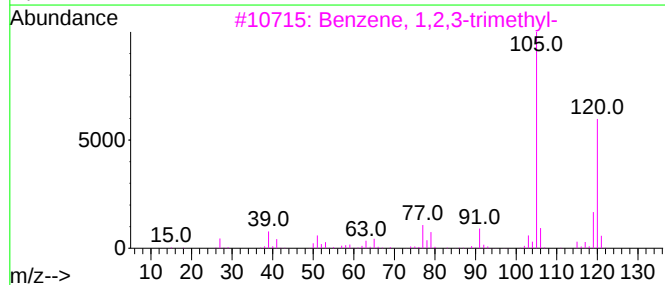
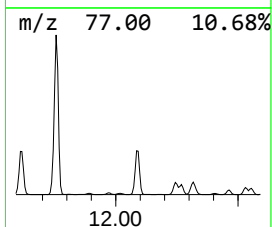
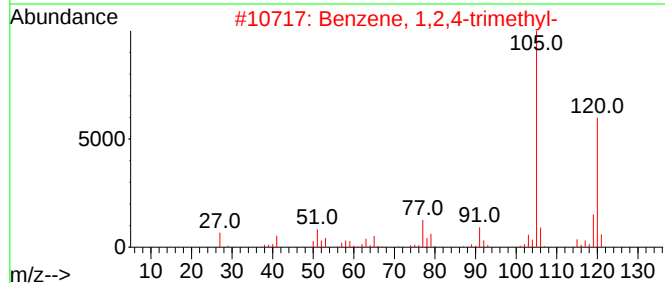
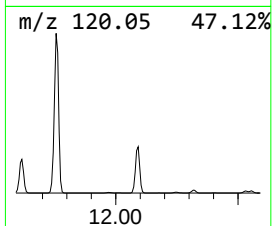
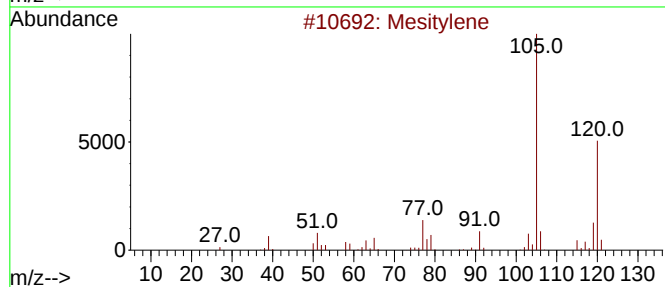
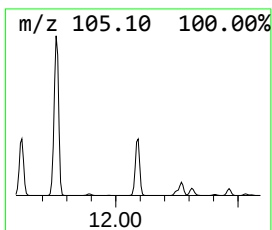
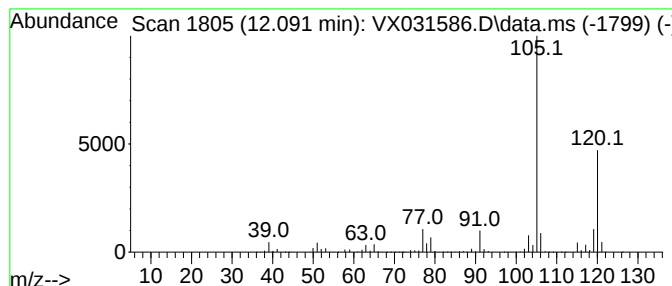
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	337.69 ug/l	5755650	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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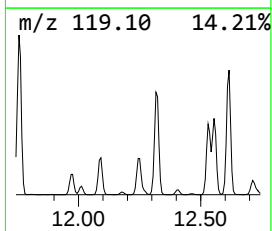
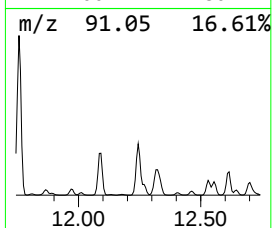
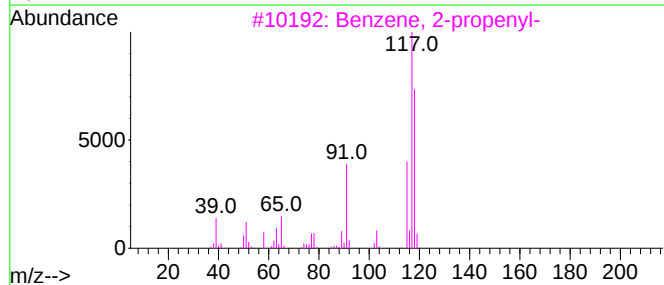
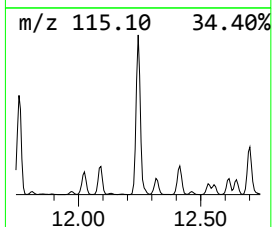
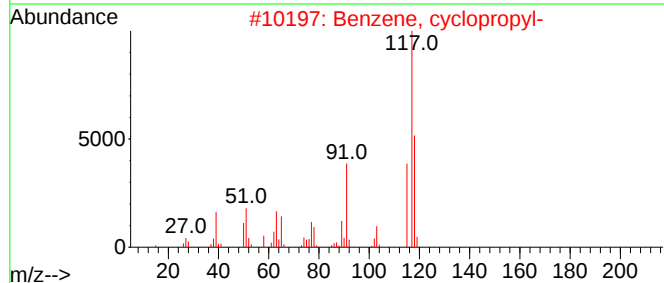
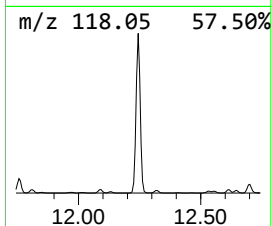
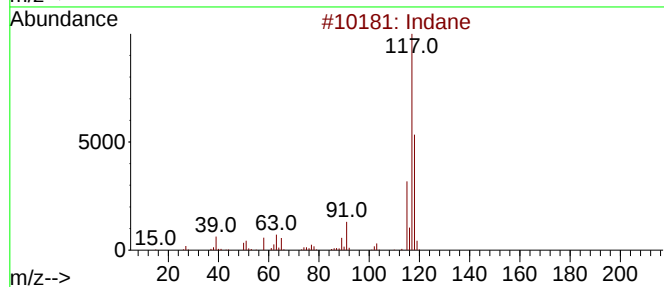
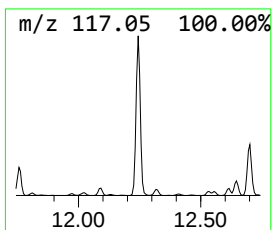
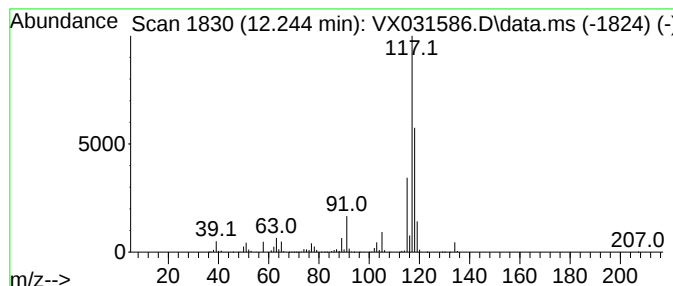
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	355.12 ug/l	6052810	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5			Benzeneethanol, .beta.-ethenyl-....	162	C11H14O	040596-14-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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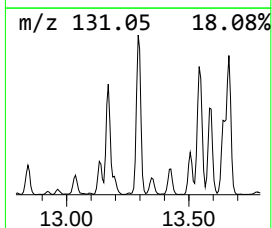
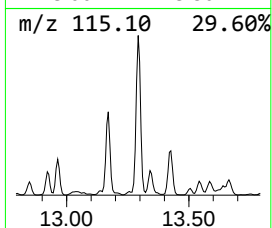
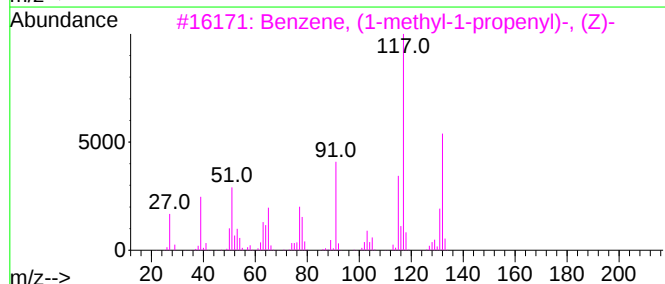
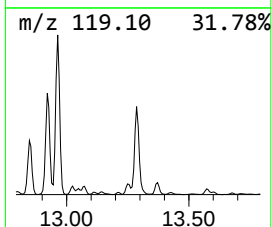
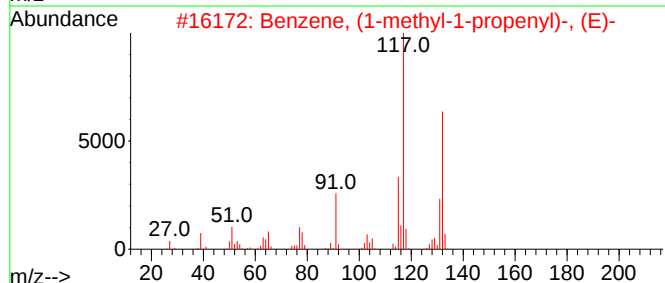
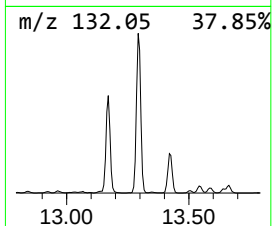
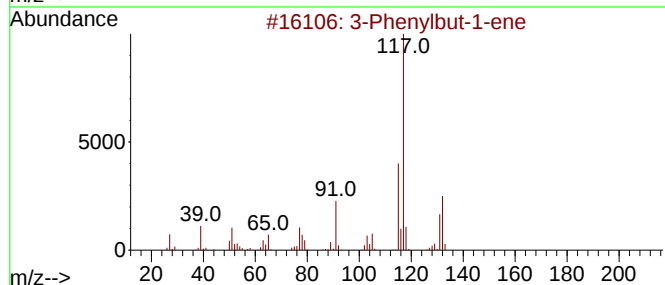
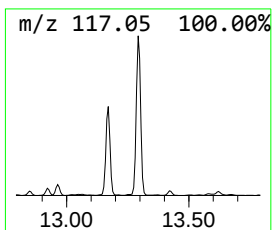
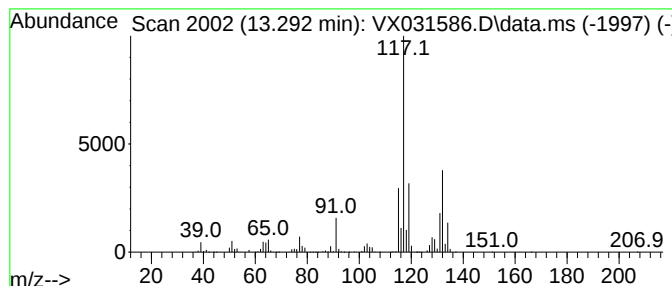
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Quant Title : SW846 8260

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

Peak Number 9 3-Phenylbut-1-ene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	186.45 ug/l	3177940	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	83
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			Indan, 1-methyl-	132	C10H12	000767-58-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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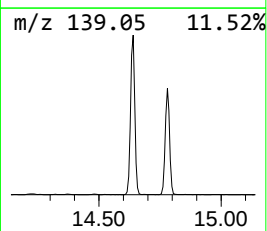
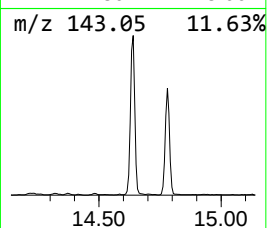
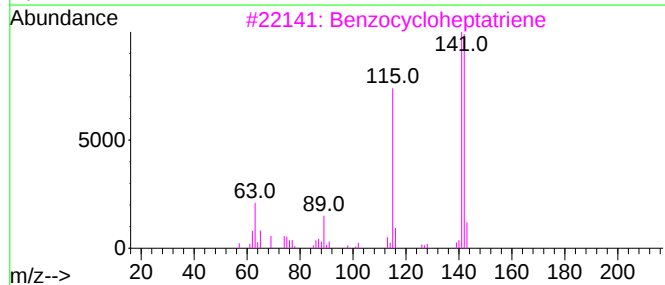
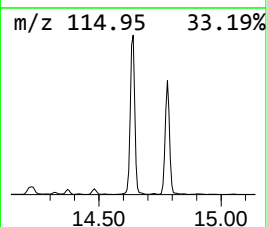
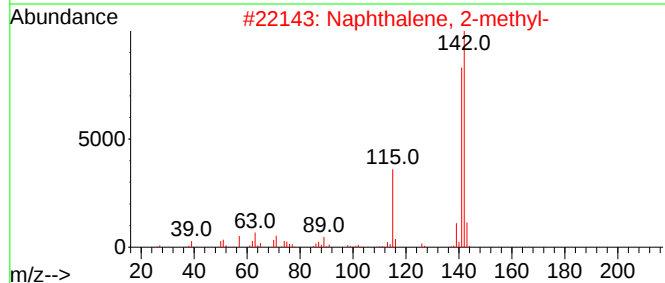
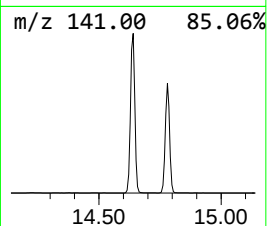
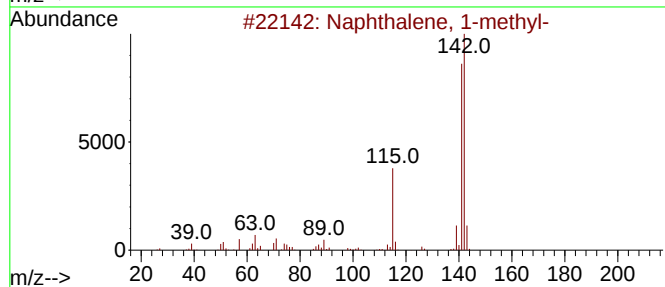
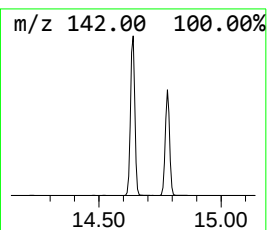
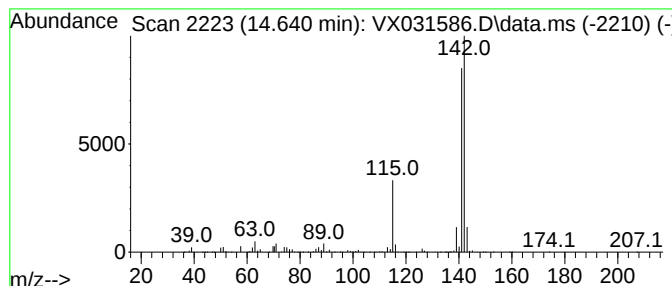
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	247.25 ug/l	4214210	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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 : VX031586.D
Acq On : 22 Sep 2022 21:24
Operator : JC/MD
Sample : N4614-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-41

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-	1.746	477.7	ug/l	6261490	1	5.556	655434	50.0
Pentane	1.953	217.3	ug/l	2849070	1	5.556	655434	50.0
Cyclopropane, 1...	2.069	204.5	ug/l	2681040	1	5.556	655434	50.0
Benzene, 1-ethy...	11.384	942.4	ug/l	16063000	4	12.024	852218	50.0
Benzene, 1-ethy...	11.616	311.3	ug/l	5305640	4	12.024	852218	50.0
Benzene, 1,2,4-...	12.091	337.7	ug/l	5755650	4	12.024	852218	50.0
Indane	12.244	355.1	ug/l	6052810	4	12.024	852218	50.0
3-Phenylbut-1-ene	13.292	186.4	ug/l	3177940	4	12.024	852218	50.0
Naphthalene, 1-...	14.640	247.3	ug/l	4214210	4	12.024	852218	50.0