

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
 Data File : VX033154.D
 Acq On : 01 Dec 2022 11:42
 Operator : JC/MD
 Sample : N5815-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-04

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033154.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	36	rBV	54604	55296	5.40%	0.682%
2	1.374	43	47	52	rBV	251033	257059	25.11%	3.173%
3	1.752	104	109	123	rVB	776574	1023595	100.00%	12.633%
4	1.959	137	143	153	rVB2	69763	114045	11.14%	1.408%
5	2.215	180	185	196	rVB	53237	85660	8.37%	1.057%
6	2.343	199	206	221	rVB	29129	59423	5.81%	0.733%
7	2.782	270	278	283	rBV	79200	179294	17.52%	2.213%
8	2.831	283	286	288	rVV	43760	69828	6.82%	0.862%
9	2.867	288	292	310	rVB2	69352	162636	15.89%	2.007%
10	3.105	320	331	344	rVB	69699	155885	15.23%	1.924%
11	3.324	359	367	374	rBV3	6660	15095	1.47%	0.186%
12	3.733	424	434	443	rBV3	15347	36860	3.60%	0.455%
13	3.843	443	452	458	rBV2	19619	49548	4.84%	0.612%
14	3.904	458	462	472	rVB3	4641	10955	1.07%	0.135%
15	4.105	484	495	504	rVV3	12694	31834	3.11%	0.393%
16	4.214	504	513	518	rVV3	5197	14671	1.43%	0.181%
17	4.306	518	528	540	rVV	127519	364078	35.57%	4.493%
18	4.428	540	548	559	rVB4	9359	28526	2.79%	0.352%
19	5.190	667	673	686	rVB3	16223	49409	4.83%	0.610%
20	5.385	694	705	713	rBV	62650	186414	18.21%	2.301%
21	5.470	713	719	725	rVV2	24503	64347	6.29%	0.794%
22	5.556	725	733	741	rVV	120250	323869	31.64%	3.997%
23	5.842	770	780	789	rBV4	4696	14793	1.45%	0.183%
24	5.958	789	799	807	rVV	67214	178142	17.40%	2.199%
25	6.043	807	813	824	rVV2	20892	58647	5.73%	0.724%
26	6.165	824	833	842	rVV6	10020	43673	4.27%	0.539%
27	6.257	842	848	857	rVV4	16356	48101	4.70%	0.594%
28	6.354	857	864	875	rVB4	8196	23287	2.28%	0.287%
29	6.763	921	931	942	rBV	204439	499293	48.78%	6.162%
30	6.854	942	946	959	rVB4	11306	27773	2.71%	0.343%
31	7.171	991	998	1009	rVB3	16636	37118	3.63%	0.458%
32	7.379	1018	1032	1045	rBV4	19510	58554	5.72%	0.723%
33	7.982	1122	1131	1142	rVB3	6783	16466	1.61%	0.203%
34	8.104	1145	1151	1154	rBV	14214	28172	2.75%	0.348%
35	8.141	1154	1157	1163	rVB	21513	36409	3.56%	0.449%
36	8.506	1210	1217	1223	rVB	17129	28222	2.76%	0.348%

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Integrator: RTE

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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	8.647	1234	1240	1248	rVV	307991	479743	46.87%	5.921%
38	8.720	1248	1252	1258	rVB	6440	11005	1.08%	0.136%
39	9.165	1319	1325	1334	rBV	7145	11235	1.10%	0.139%
40	10.055	1465	1471	1480	rBV	406359	548742	53.61%	6.773%
41	10.195	1489	1494	1500	rVV	135454	175492	17.14%	2.166%
42	10.305	1504	1512	1519	rVB	14284	19886	1.94%	0.245%
43	10.963	1615	1620	1626	rVB	21119	26303	2.57%	0.325%
44	11.079	1634	1639	1651	rBV	267059	342516	33.46%	4.227%
45	11.305	1670	1676	1682	rBV	31499	39076	3.82%	0.482%
46	11.616	1721	1727	1736	rVB	155953	200777	19.61%	2.478%
47	11.750	1745	1749	1755	rVB	8302	10474	1.02%	0.129%
48	12.024	1788	1794	1800	rBV	419994	530765	51.85%	6.551%
49	12.085	1800	1804	1815	rVB	186871	231934	22.66%	2.863%
50	12.244	1824	1830	1837	rBV2	304000	371706	36.31%	4.588%
51	12.317	1837	1842	1850	rVV	16886	23915	2.34%	0.295%
52	12.408	1852	1857	1862	rVV3	17055	22671	2.21%	0.280%
53	12.463	1862	1866	1873	rVB	35832	43664	4.27%	0.539%
54	12.615	1886	1891	1894	rBV	72202	89628	8.76%	1.106%
55	12.701	1900	1905	1912	rVB2	74646	106598	10.41%	1.316%
56	12.847	1924	1929	1935	rVB	24627	29263	2.86%	0.361%
57	12.920	1935	1941	1945	rBV	54760	66763	6.52%	0.824%
58	13.170	1978	1982	1992	rVB	38907	47834	4.67%	0.590%
59	13.292	1992	2002	2007	rBV2	126212	166612	16.28%	2.056%
60	13.426	2019	2024	2030	rVB2	15168	20507	2.00%	0.253%
61	13.585	2046	2050	2055	rVB2	6926	10287	1.00%	0.127%
62	13.774	2077	2081	2090	rBV	20351	26962	2.63%	0.333%
63	14.780	2242	2246	2251	rBV	9192	11117	1.09%	0.137%

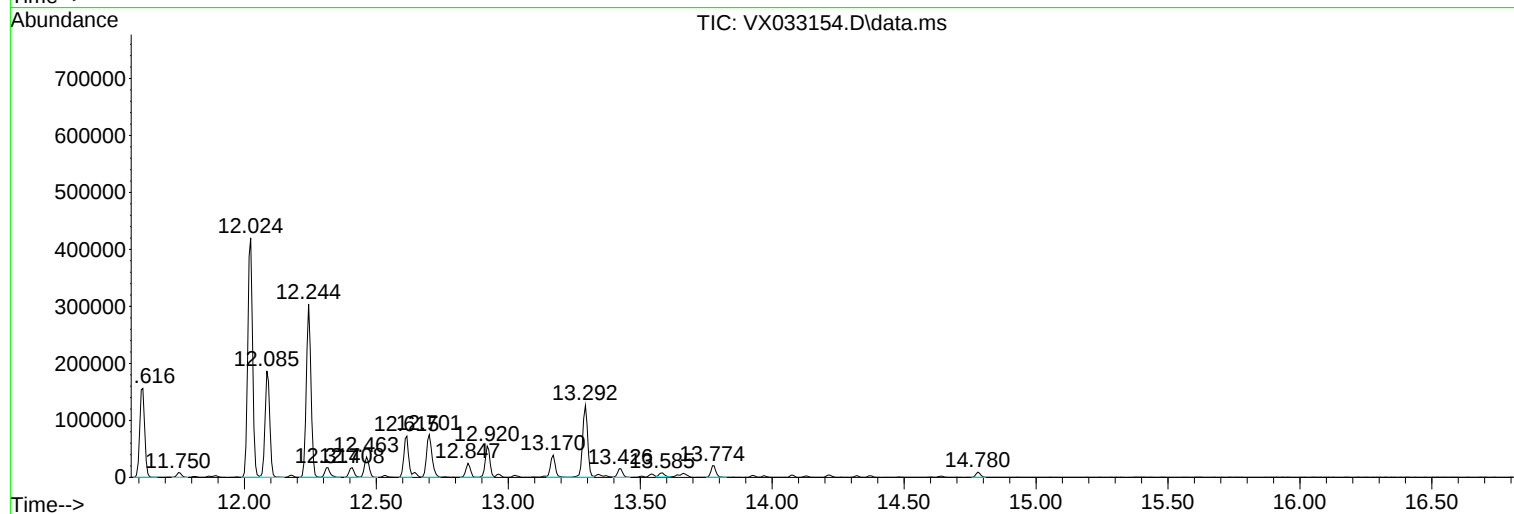
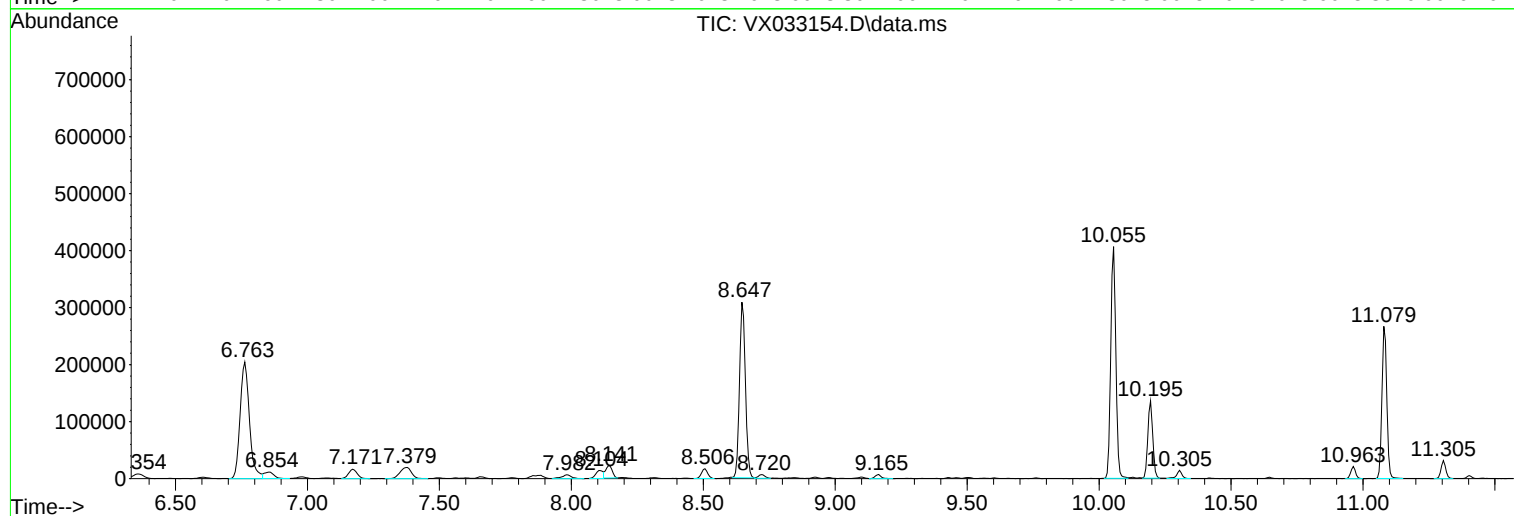
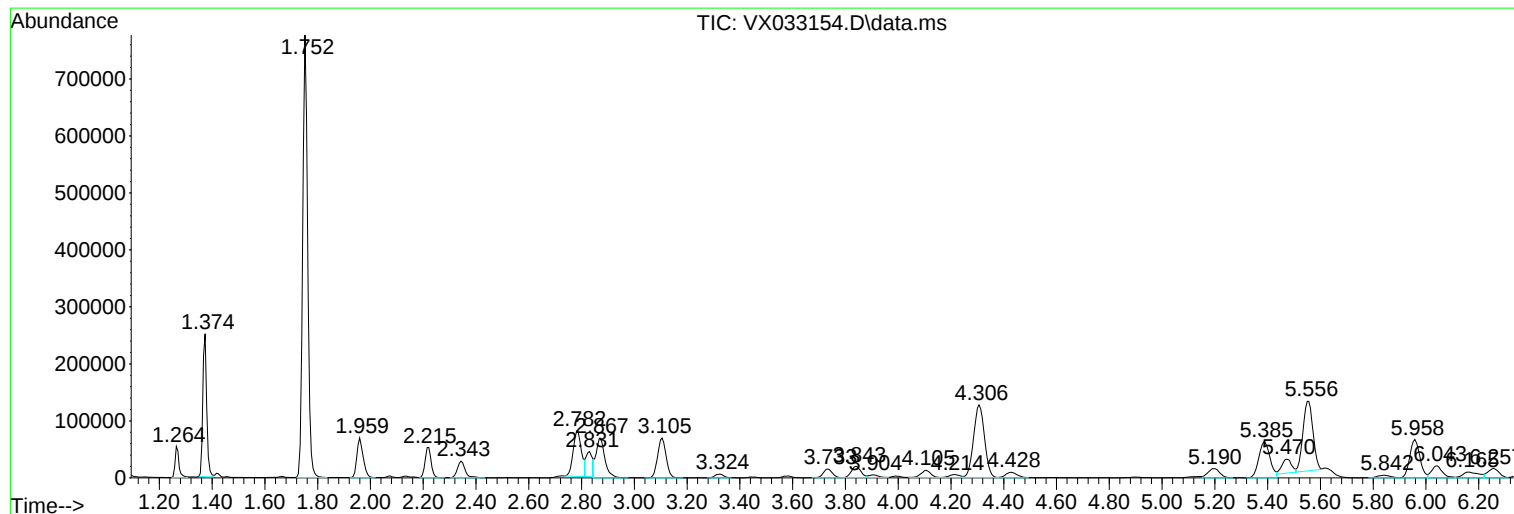
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ClientSampleId :
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
MW-04

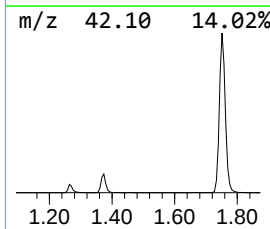
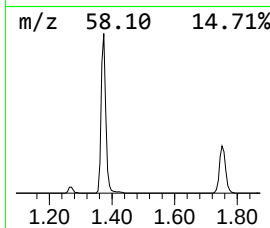
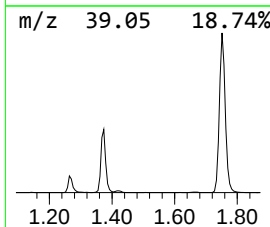
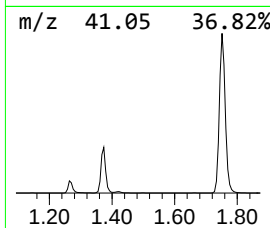
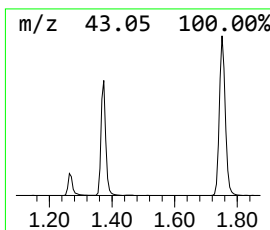
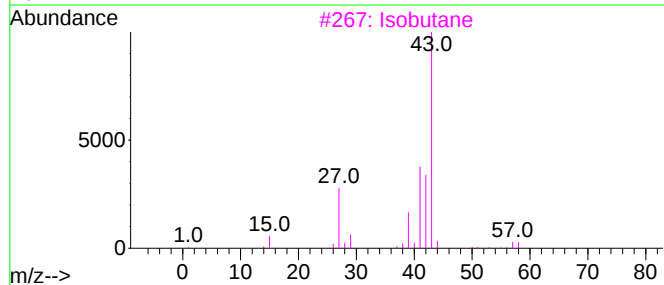
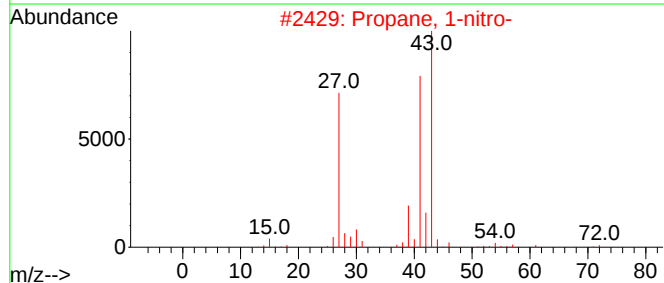
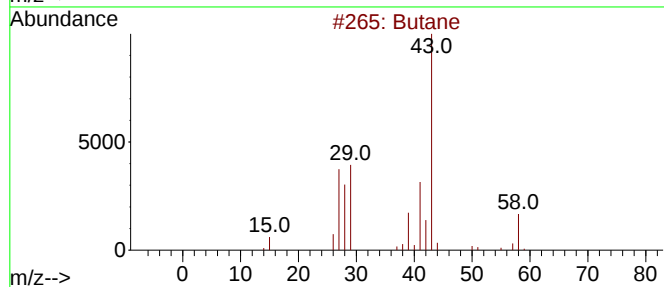
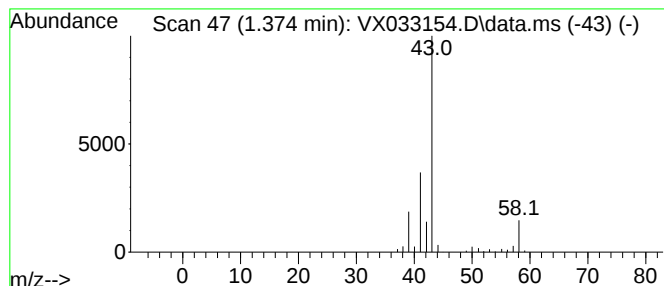
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	39.69 ug/l	257059	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	72
2	Propane, 1-nitro-			89	C3H7NO2	000108-03-2	9
3	Isobutane			58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
5	Acetone			58	C3H6O	000067-64-1	4



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Instrument :
MSVOA_X
ClientSampleId :
MW-04

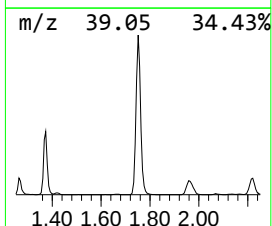
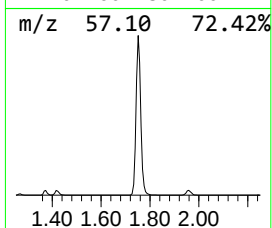
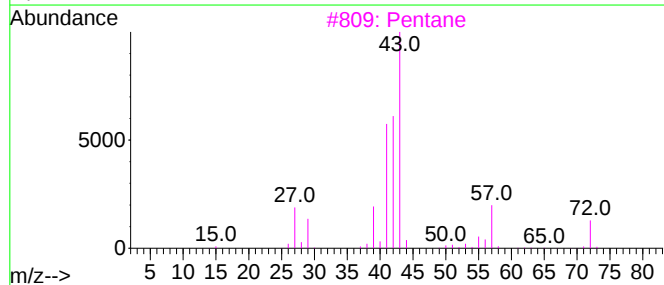
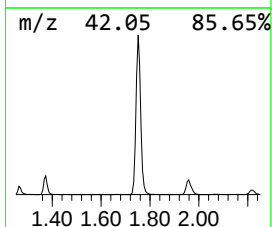
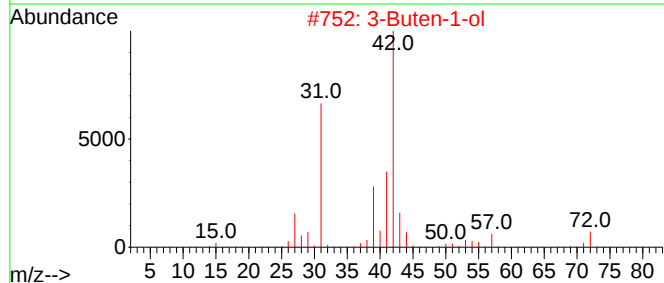
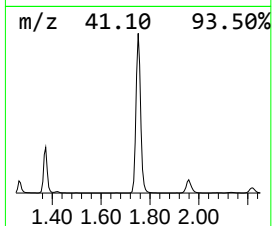
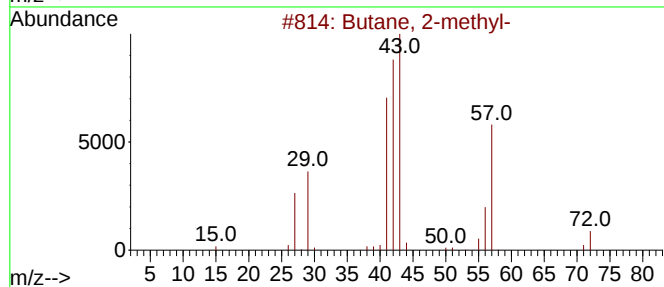
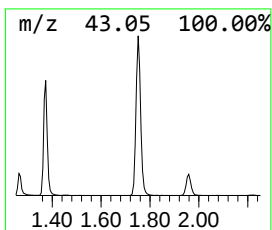
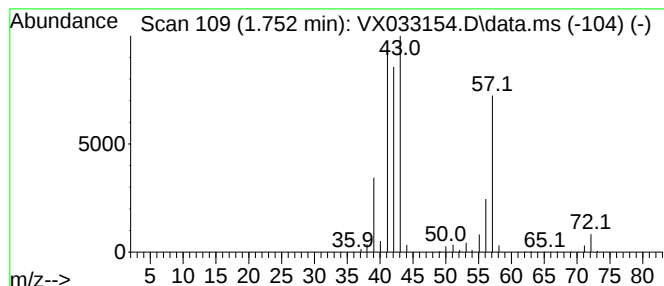
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	158.03 ug/l	1023600	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	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Butene	56	C4H8	000106-98-9	10
5			Azetidine	57	C3H7N	000503-29-7	9



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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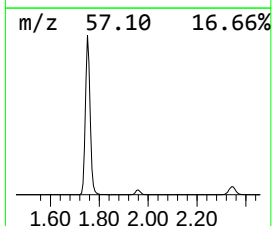
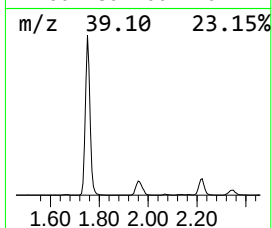
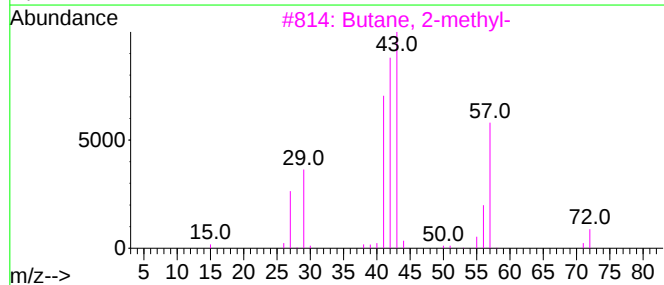
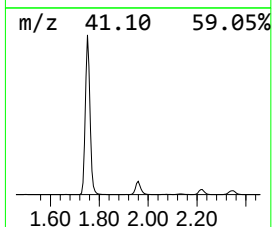
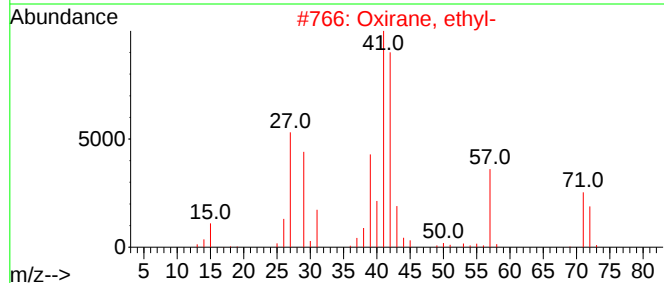
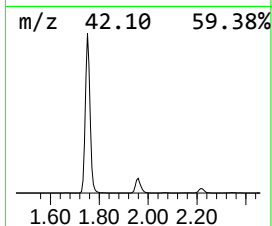
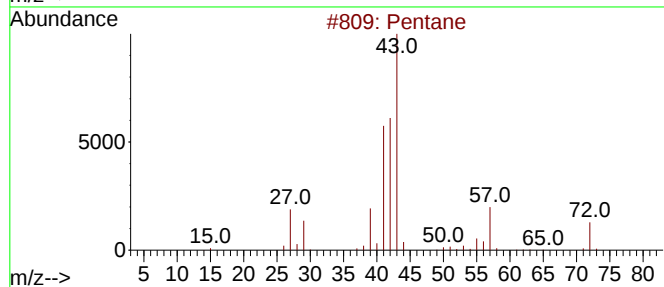
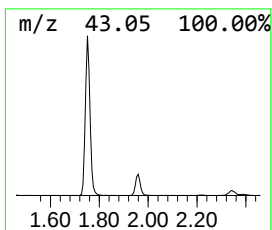
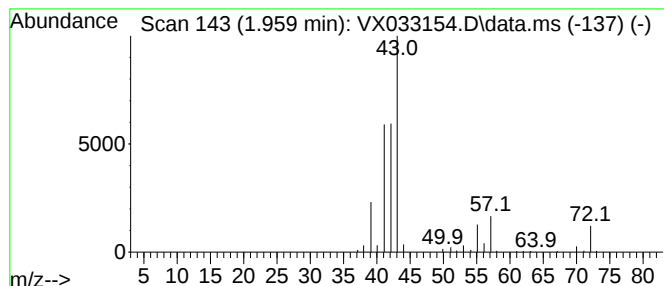
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	17.61 ug/l	114045	Pentafluorobenzene	5.556

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	53
3			Butane, 2-methyl-	72	C5H12	000078-78-4	39
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	16



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Instrument :
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ClientSampleId :
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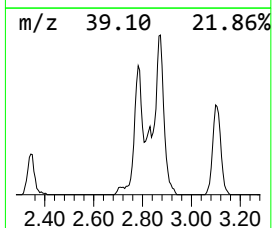
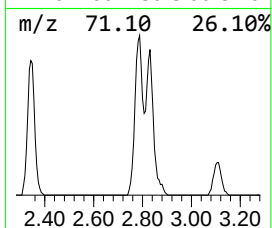
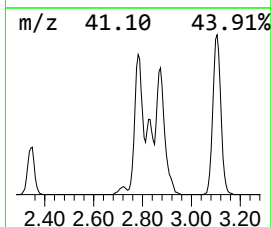
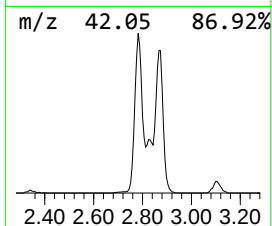
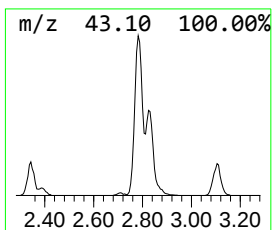
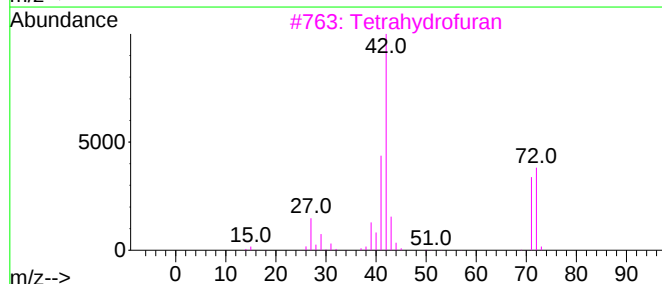
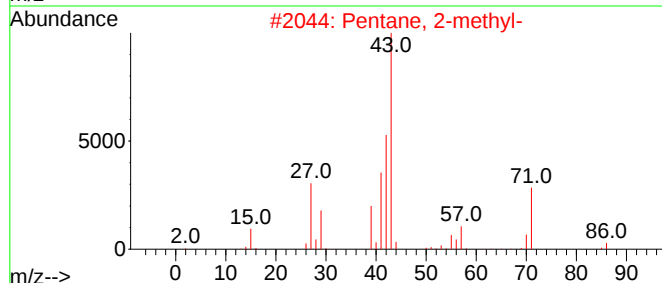
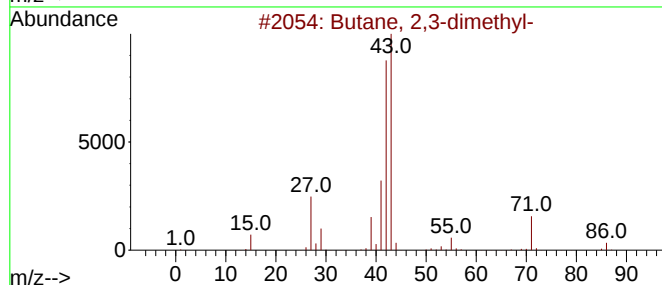
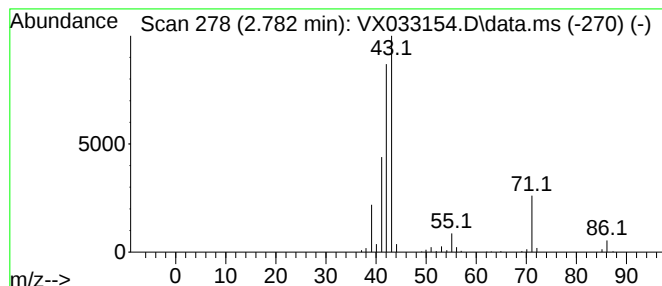
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	27.68 ug/l	179294	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Tetrahydrofuran	72	C4H8O	000109-99-9	38
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	28
5			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	27



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MW-04

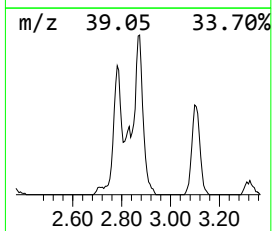
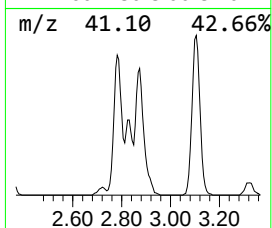
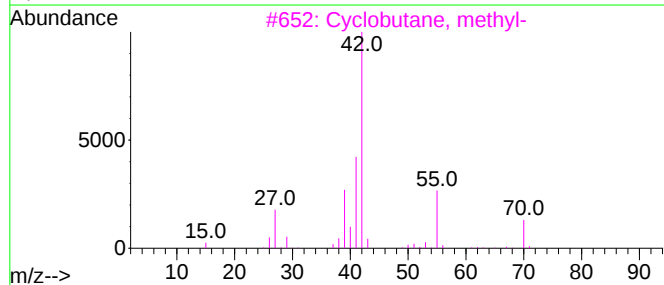
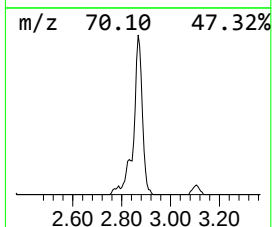
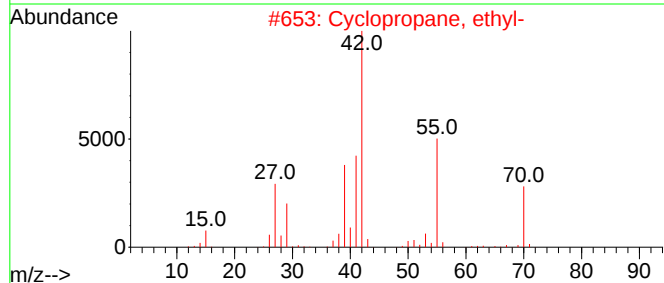
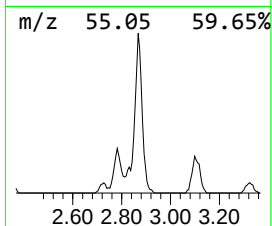
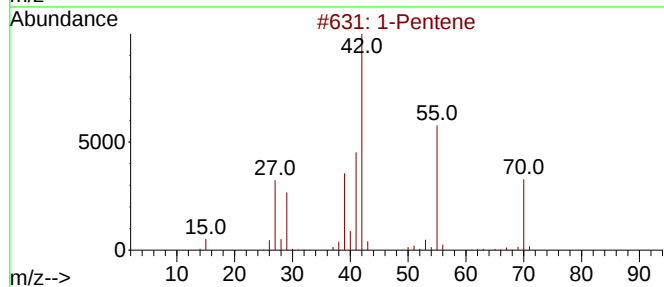
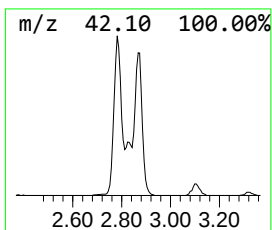
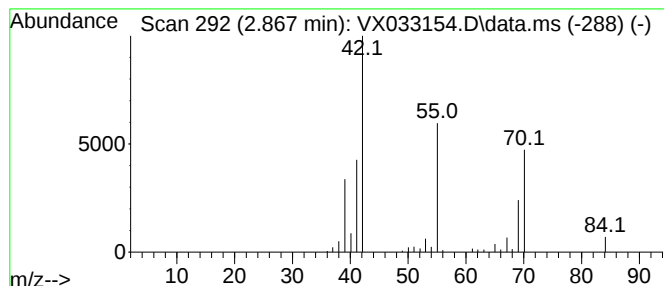
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Quant Title : SW846 8260

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

Peak Number 5 1-Pentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	25.11 ug/l	162636	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene			70	C5H10	000109-67-1	80
2	Cyclopropane, ethyl-			70	C5H10	001191-96-4	72
3	Cyclobutane, methyl-			70	C5H10	000598-61-8	72
4	Cyclopropane, 1,1-dimethyl-			70	C5H10	001630-94-0	38
5	2-Pentene, (E)-			70	C5H10	000646-04-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

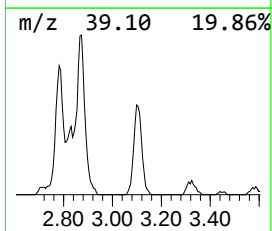
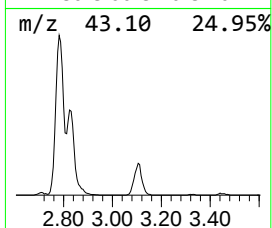
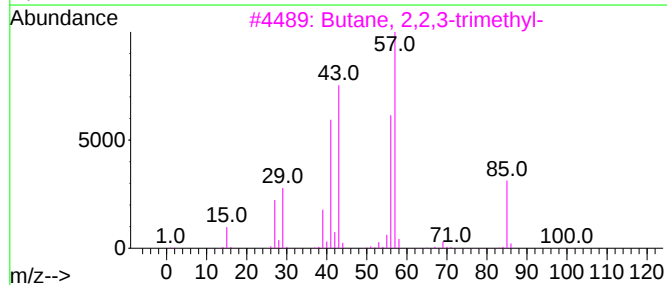
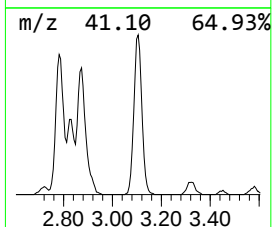
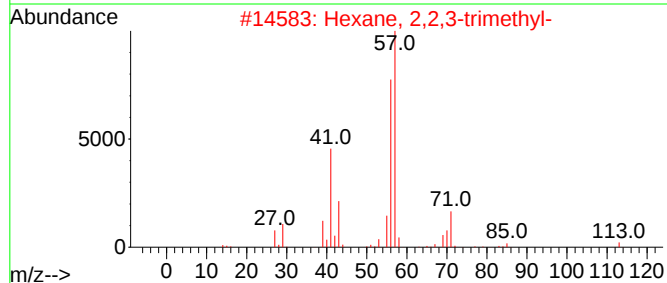
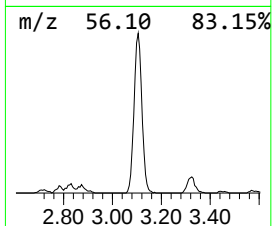
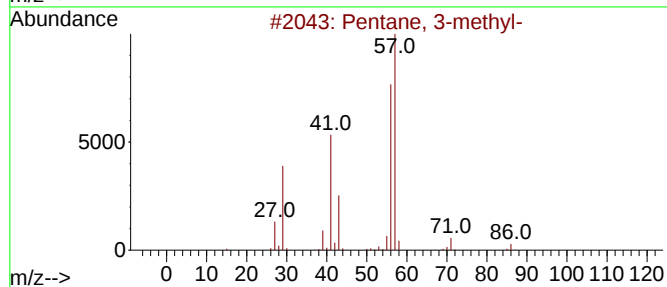
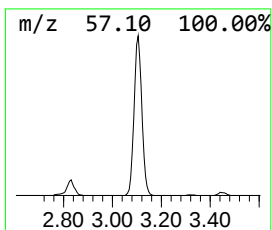
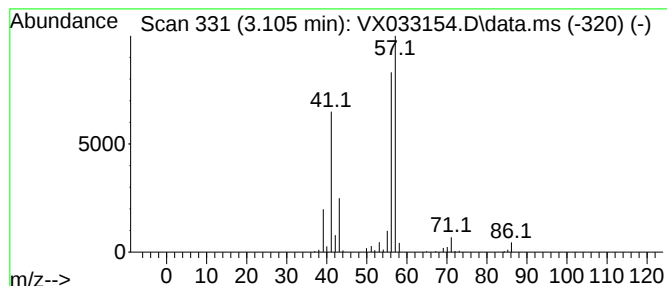
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	24.07 ug/l	155885	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

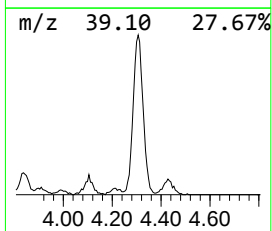
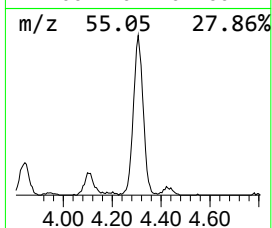
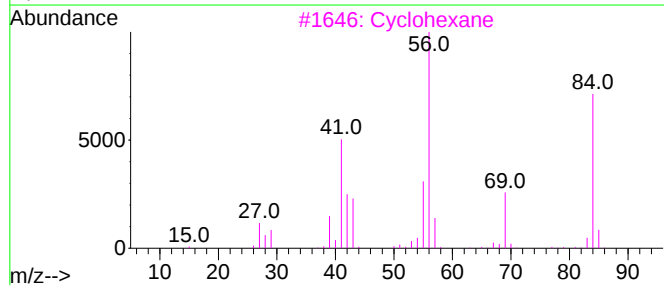
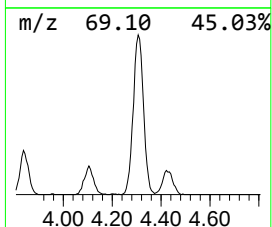
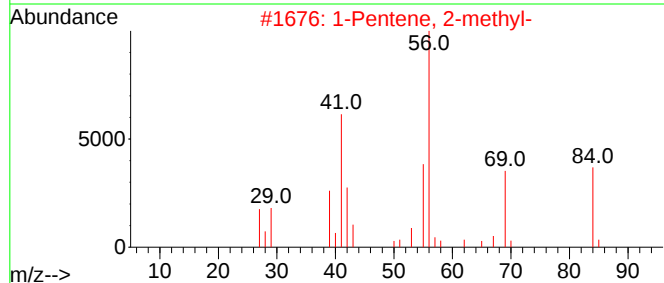
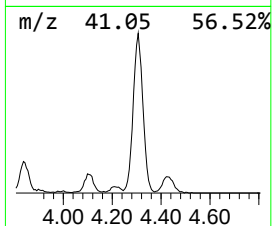
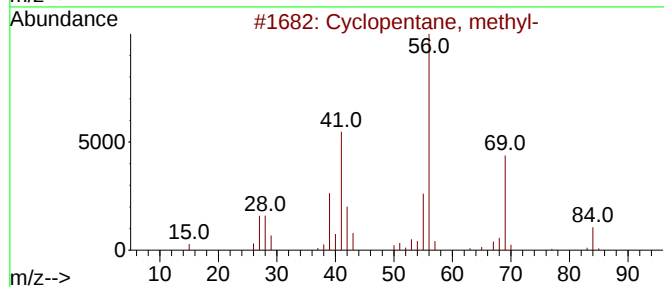
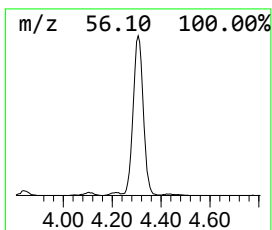
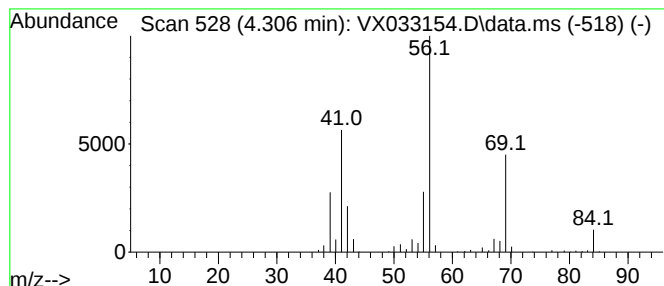
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	56.21 ug/l	364078	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	78
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

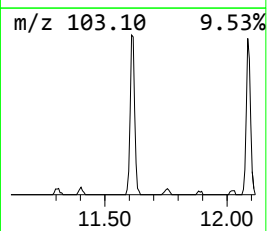
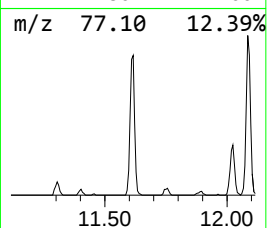
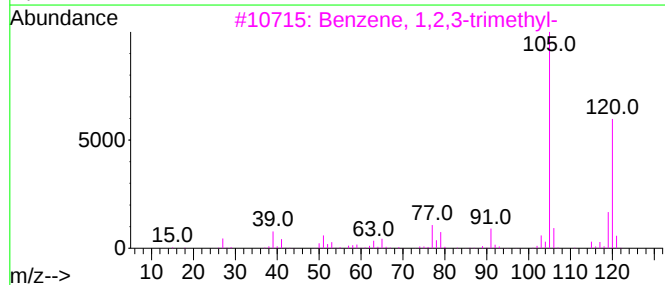
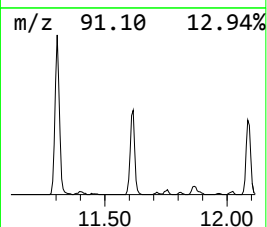
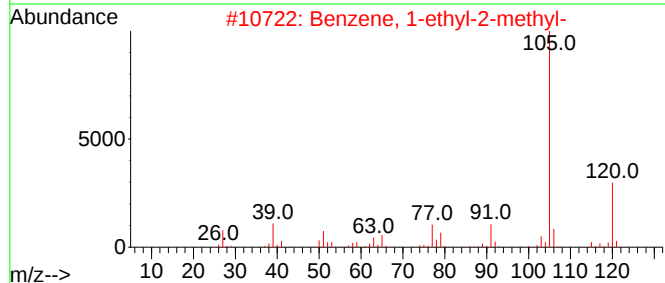
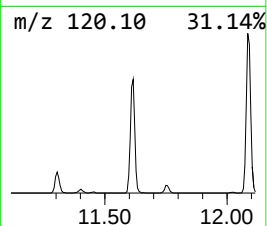
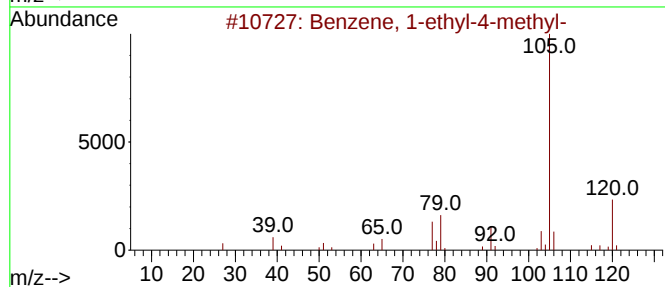
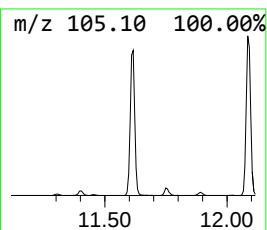
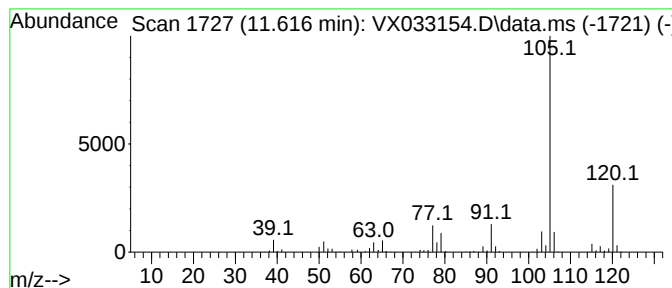
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	18.91 ug/l	200777	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Mesitylene	120	C9H12	000108-67-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

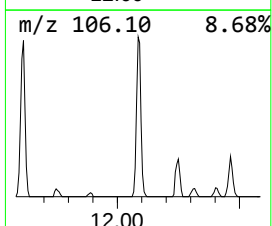
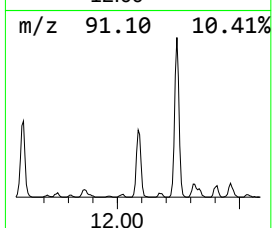
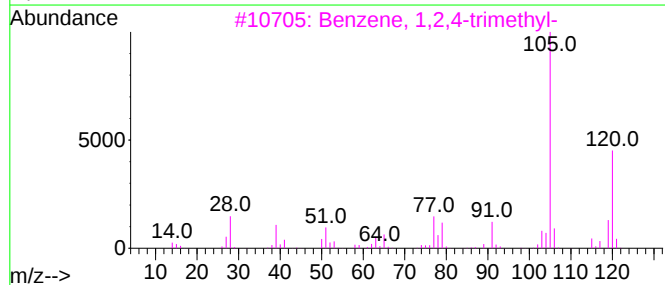
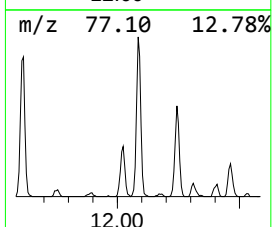
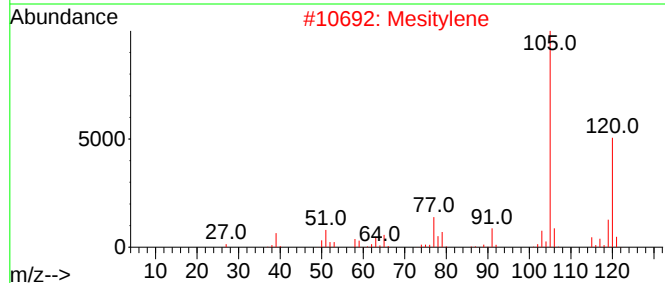
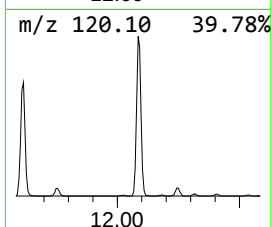
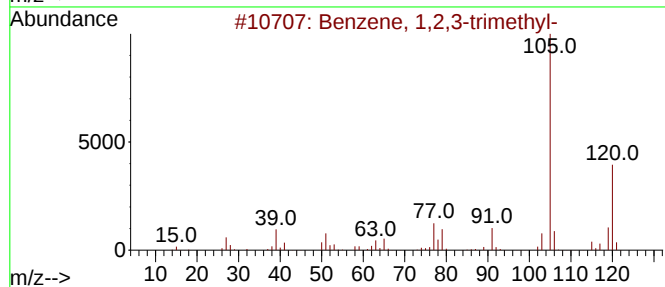
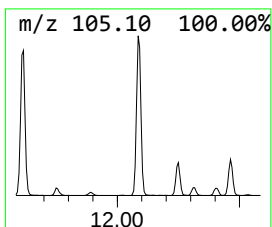
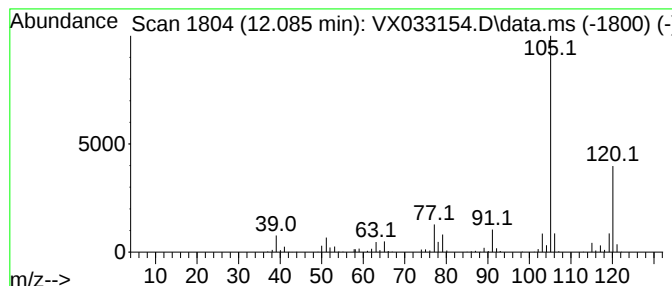
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	21.85 ug/l	231934	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

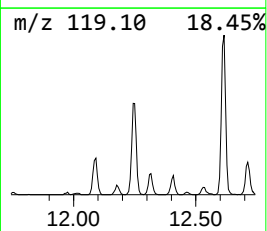
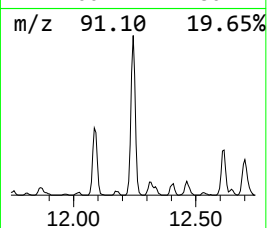
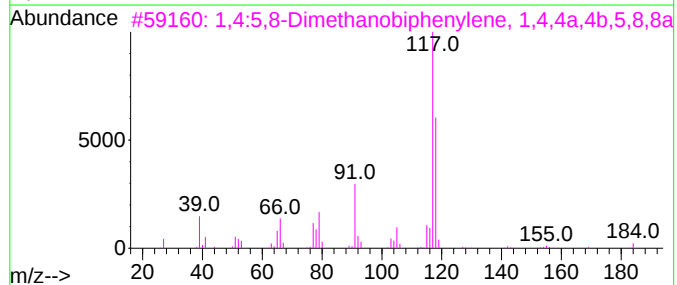
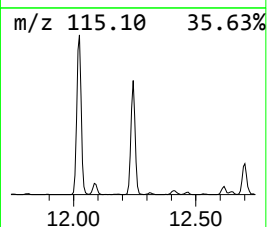
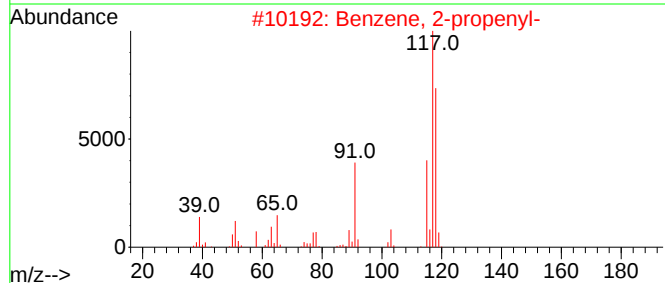
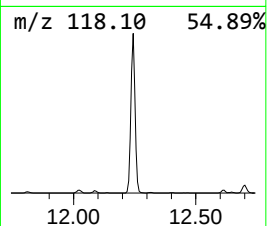
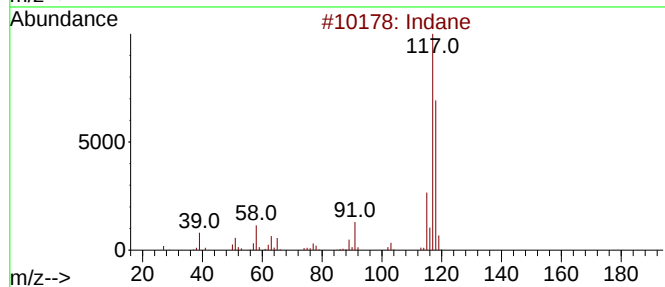
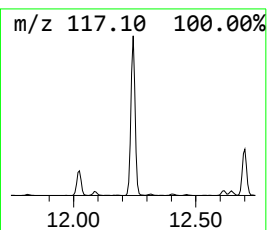
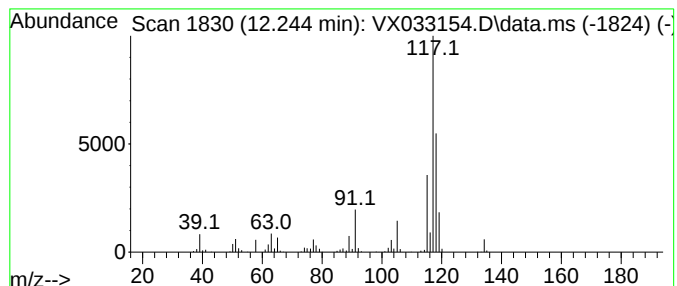
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	35.02 ug/l	371706	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, 2-propenyl-	118	C9H10	000300-57-2	76
3			1,4:5,8-Dimethanobiphenylene, 1,...	184	C14H16	001624-13-1	72
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120122\
Data File : VX033154.D
Acq On : 01 Dec 2022 11:42
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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-	1.752	158.0	ug/l	1023600	1	5.556	323869	50.0
Pentane	1.959	17.6	ug/l	114045	1	5.556	323869	50.0
Butane, 2,3-dim...	2.782	27.7	ug/l	179294	1	5.556	323869	50.0
1-Pentene	2.867	25.1	ug/l	162636	1	5.556	323869	50.0
Pentane, 3-methyl-	3.105	24.1	ug/l	155885	1	5.556	323869	50.0
Cyclopentane, m...	4.306	56.2	ug/l	364078	1	5.556	323869	50.0
Benzene, 1-ethy...	11.616	18.9	ug/l	200777	4	12.024	530765	50.0
Benzene, 1,2,3-...	12.085	21.9	ug/l	231934	4	12.024	530765	50.0
Indane	12.243	35.0	ug/l	371706	4	12.024	530765	50.0