

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
 Data File : VX033136.D
 Acq On : 30 Nov 2022 16:51
 Operator : JC/MD
 Sample : N5815-21 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PZ-3R

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: VX033136.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	43	rBV	43427	47782	1.88%	0.188%
2	1.374	43	47	52	rBV	363991	395458	15.58%	1.556%
3	1.752	103	109	124	rVB	1890211	2433366	95.87%	9.575%
4	1.959	137	143	154	rVB	481801	729979	28.76%	2.872%
5	2.069	156	161	168	rVV	76396	107548	4.24%	0.423%
6	2.166	172	177	181	rVV	31172	46448	1.83%	0.183%
7	2.215	181	185	195	rVB	110808	166655	6.57%	0.656%
8	2.343	195	206	211	rBV	30608	61004	2.40%	0.240%
9	2.721	259	268	270	rBV4	11335	26411	1.04%	0.104%
10	2.782	270	278	281	rVV2	104489	232480	9.16%	0.915%
11	2.825	281	285	290	rVV	235651	508489	20.03%	2.001%
12	2.867	290	292	316	rVB2	114740	259771	10.23%	1.022%
13	3.105	320	331	343	rBV	163614	371249	14.63%	1.461%
14	3.319	356	366	378	rVB2	33072	76633	3.02%	0.302%
15	3.447	378	387	399	rBV	62861	139120	5.48%	0.547%
16	3.587	399	410	416	rBV3	19750	51812	2.04%	0.204%
17	3.666	416	423	428	rBV3	16335	40058	1.58%	0.158%
18	3.733	428	434	444	rVB	61490	141905	5.59%	0.558%
19	3.843	444	452	458	rBV	33304	85816	3.38%	0.338%
20	3.953	466	470	484	rVB4	13182	40848	1.61%	0.161%
21	4.105	484	495	504	rVV2	44485	118951	4.69%	0.468%
22	4.215	504	513	518	rVV2	19804	54745	2.16%	0.215%
23	4.306	518	528	540	rVV	279526	791087	31.17%	3.113%
24	4.434	540	549	562	rVB3	13526	42703	1.68%	0.168%
25	4.574	562	572	588	rBV	11679	37790	1.49%	0.149%
26	5.190	664	673	687	rVB3	31983	102211	4.03%	0.402%
27	5.385	691	705	713	rBV	73412	221864	8.74%	0.873%
28	5.483	713	721	725	rBV3	43864	134379	5.29%	0.529%
29	5.556	726	733	740	rVB	123178	327683	12.91%	1.289%
30	5.824	768	777	790	rBV2	41532	122925	4.84%	0.484%
31	5.958	790	799	806	rVV	77725	203577	8.02%	0.801%
32	6.038	806	812	822	rVV	86550	229531	9.04%	0.903%
33	6.160	823	832	839	rVV4	28575	101241	3.99%	0.398%
34	6.257	840	848	857	rVV4	63398	203010	8.00%	0.799%
35	6.361	857	865	877	rVB3	24699	72305	2.85%	0.284%
36	6.623	895	908	922	rBV3	22252	86969	3.43%	0.342%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

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37	6.763	922	931	939	rVV	236063	580771	22.88%	2.285%
38	6.848	941	945	956	rVB3	34371	94503	3.72%	0.372%
39	7.172	990	998	1007	rVB2	22704	51466	2.03%	0.203%
40	7.379	1020	1032	1040	rBV4	68942	189964	7.48%	0.747%
41	7.659	1072	1078	1086	rVB2	22416	46590	1.84%	0.183%
42	7.982	1123	1131	1144	rVB	26981	61677	2.43%	0.243%
43	8.104	1144	1151	1155	rBV	41590	87476	3.45%	0.344%
44	8.141	1155	1157	1162	rVV	32924	51496	2.03%	0.203%
45	8.190	1162	1165	1174	rVB4	16549	31050	1.22%	0.122%
46	8.440	1201	1206	1210	rBV2	16259	27953	1.10%	0.110%
47	8.507	1212	1217	1225	rVB3	30026	53651	2.11%	0.211%
48	8.610	1225	1234	1235	rBV5	12691	25672	1.01%	0.101%
49	8.647	1235	1240	1246	rVV	354665	552609	21.77%	2.174%
50	8.714	1246	1251	1258	rVB2	43016	71008	2.80%	0.279%
51	8.805	1258	1266	1271	rBV	29303	52784	2.08%	0.208%
52	10.055	1465	1471	1476	rBV	485853	636006	25.06%	2.502%
53	10.195	1488	1494	1502	rVV	1638602	2056036	81.01%	8.090%
54	10.305	1503	1512	1518	rVB	1083986	1431685	56.41%	5.633%
55	10.640	1562	1567	1581	rVB	163042	215646	8.50%	0.849%
56	10.964	1614	1620	1627	rBV	156529	202558	7.98%	0.797%
57	11.079	1634	1639	1651	rVB	328806	425125	16.75%	1.673%
58	11.305	1671	1676	1683	rVB	449486	525935	20.72%	2.069%
59	11.403	1683	1692	1696	rVV	509185	712339	28.07%	2.803%
60	11.451	1696	1700	1711	rVB	163442	203133	8.00%	0.799%
61	11.616	1721	1727	1734	rVB	320218	415650	16.38%	1.635%
62	11.750	1744	1749	1756	rVB	2089223	2538124	100.00%	9.987%
63	11.866	1761	1768	1770	rBV	20449	27816	1.10%	0.109%
64	11.890	1770	1772	1777	rVB	26668	29842	1.18%	0.117%
65	12.024	1788	1794	1799	rVB	559086	703779	27.73%	2.769%
66	12.085	1799	1804	1810	rBV	674250	806831	31.79%	3.175%
67	12.244	1824	1830	1837	rBV2	587845	756487	29.80%	2.977%
68	12.311	1837	1841	1852	rVB3	131837	223358	8.80%	0.879%
69	12.408	1852	1857	1862	rBV2	25328	35368	1.39%	0.139%
70	12.463	1862	1866	1872	rVB	90502	108488	4.27%	0.427%
71	12.530	1872	1877	1879	rBV	158177	191015	7.53%	0.752%
72	12.555	1879	1881	1886	rVB	116179	122596	4.83%	0.482%
73	12.616	1886	1891	1894	rBV	295840	361648	14.25%	1.423%
74	12.646	1894	1896	1900	rVB	38698	39721	1.56%	0.156%
75	12.701	1900	1905	1913	rBV2	117084	175763	6.92%	0.692%
76	12.847	1925	1929	1934	rVB	67983	83805	3.30%	0.330%

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ClientSampleId :
PZ-3R

Integration Parameters: RTEINT.P

Integrator: RTE

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Title : SW846 8260

77	12.921	1934	1941	1945	rBV	141315	180967	7.13%	0.712%
78	12.963	1945	1948	1954	rVB	191719	215286	8.48%	0.847%
79	13.170	1977	1982	1986	rVB	123206	147214	5.80%	0.579%
80	13.292	1997	2002	2007	rVB2	250445	321553	12.67%	1.265%
81	13.427	2019	2024	2030	rVB	30340	41467	1.63%	0.163%
82	13.579	2046	2049	2056	rVV3	23098	44590	1.76%	0.175%
83	13.664	2056	2063	2069	rVB2	16777	39017	1.54%	0.154%
84	13.774	2075	2081	2088	rBV	311908	389691	15.35%	1.533%
85	14.640	2218	2223	2234	rVB	102306	128067	5.05%	0.504%
86	14.780	2241	2246	2255	rVB	70821	85828	3.38%	0.338%

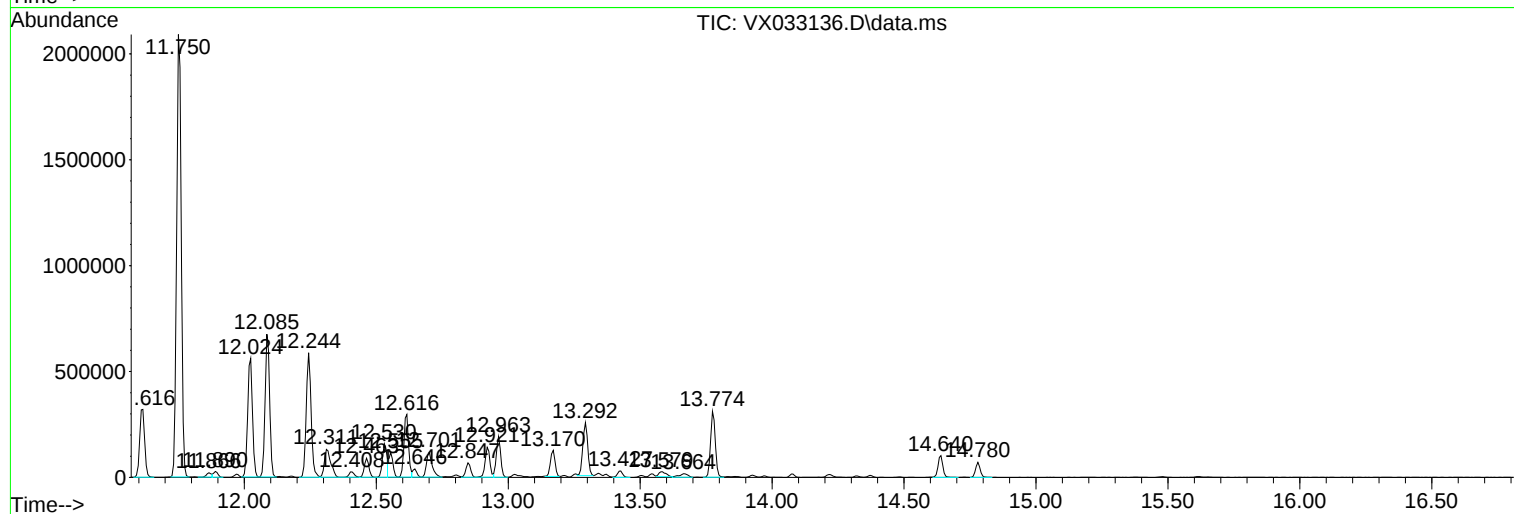
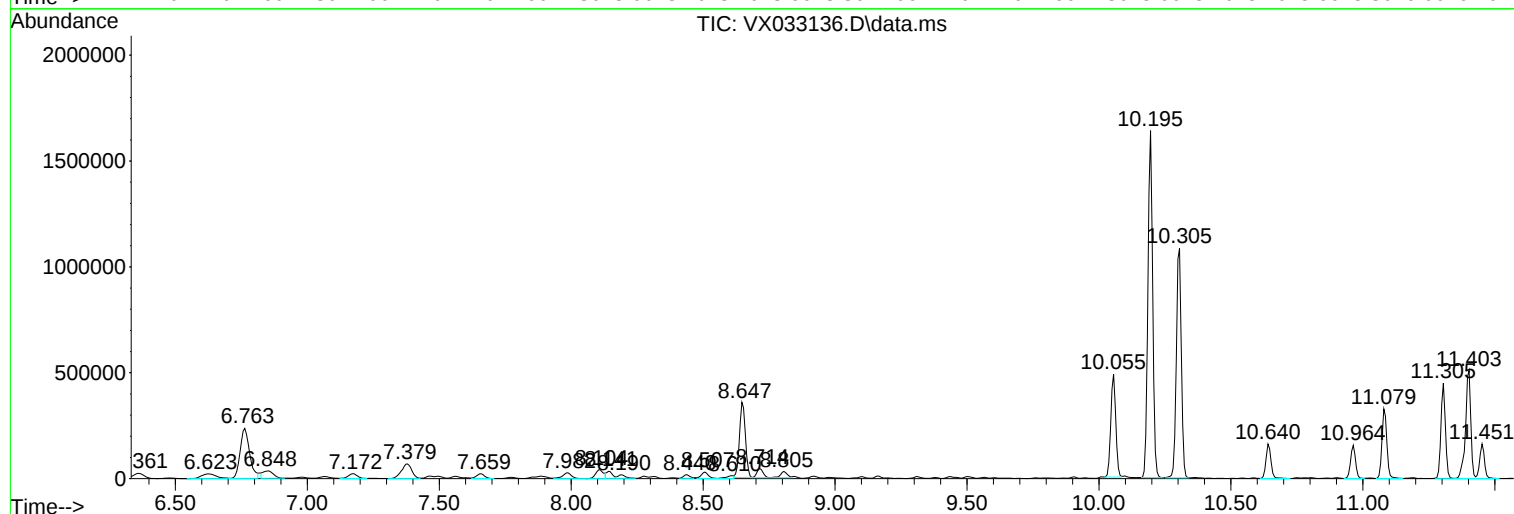
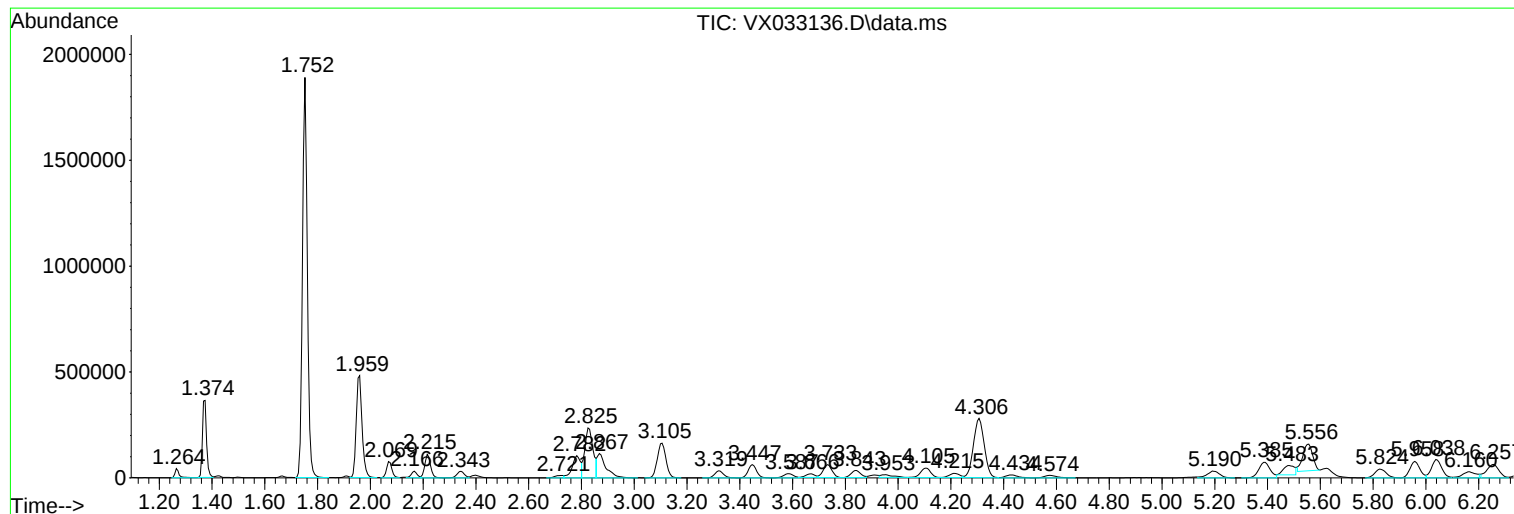
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Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

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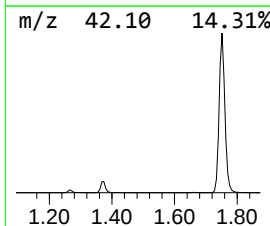
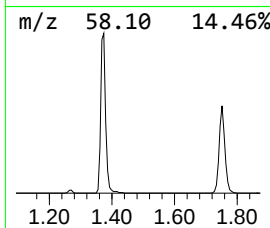
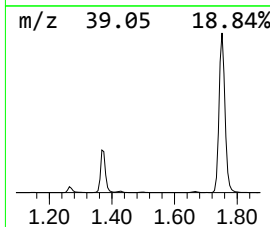
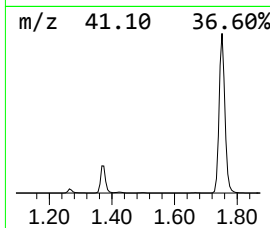
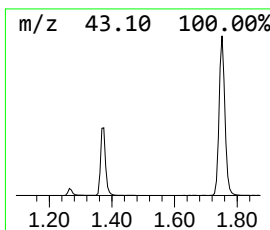
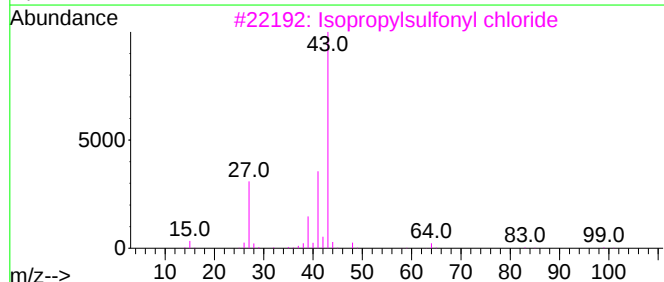
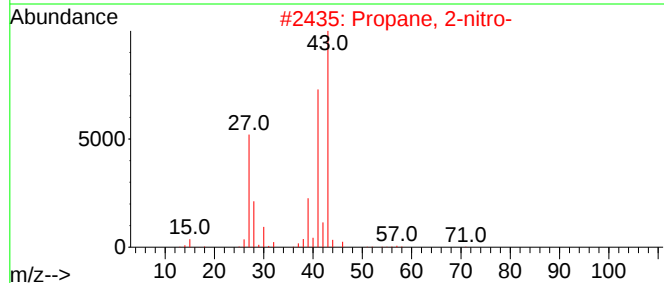
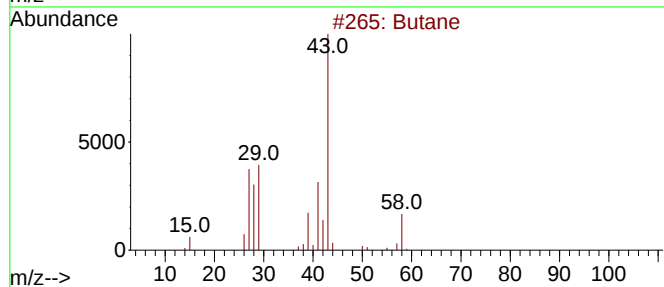
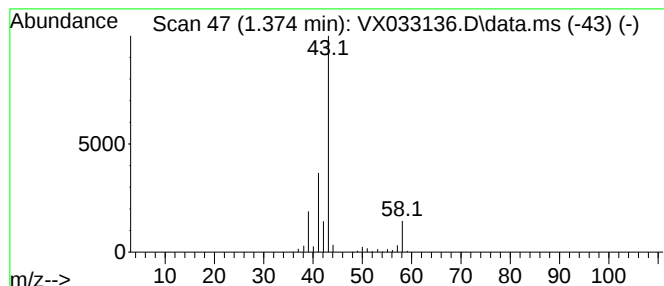
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	60.34 ug/l	395458	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			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Isobutane	58	C4H10	000075-28-5	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

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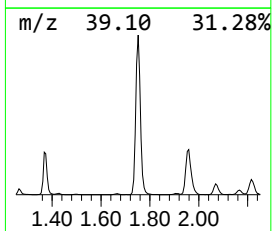
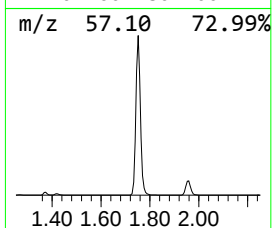
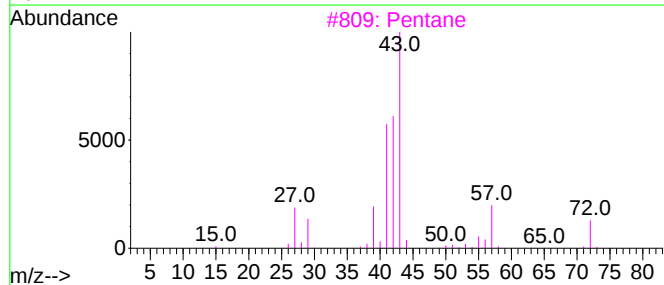
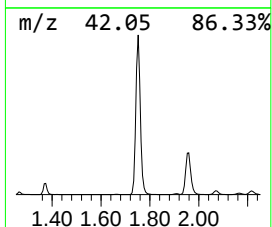
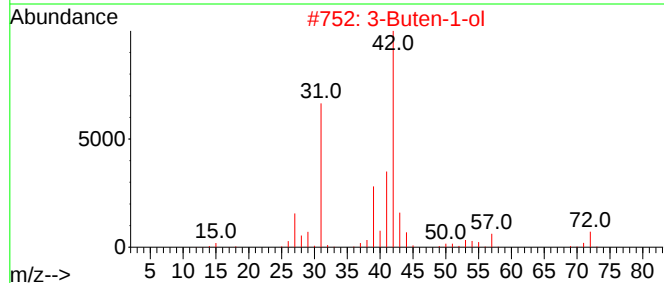
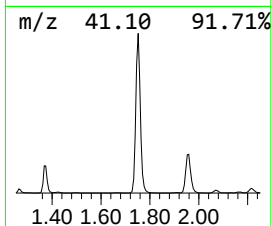
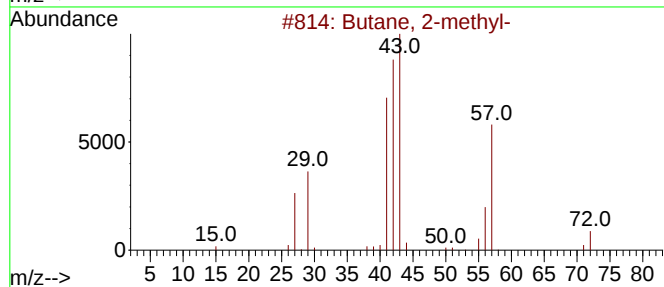
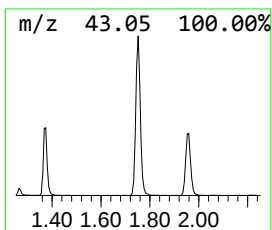
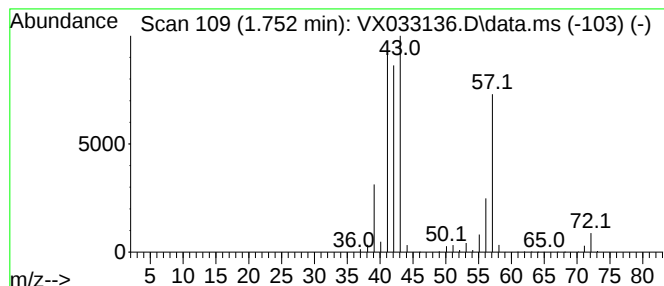
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	371.30 ug/l	2433370	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	91
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	Methane, isocyanato-			57	C2H3NO	000624-83-9	9



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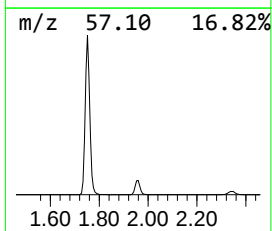
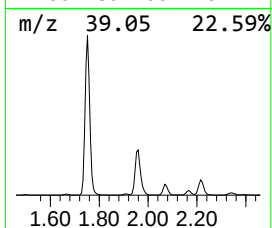
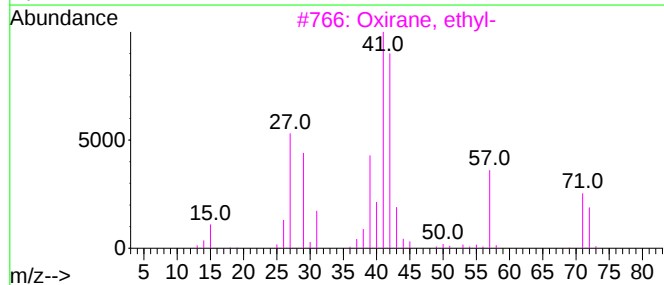
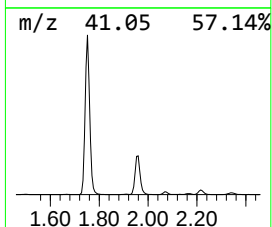
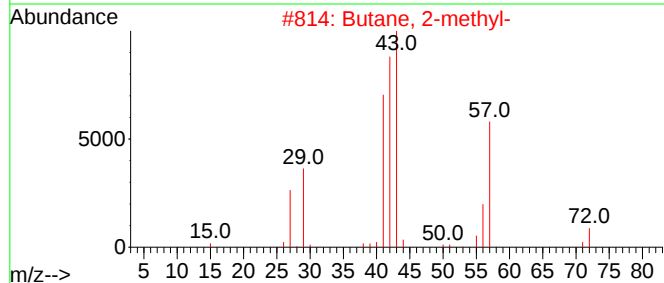
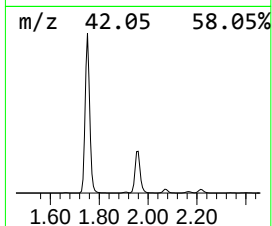
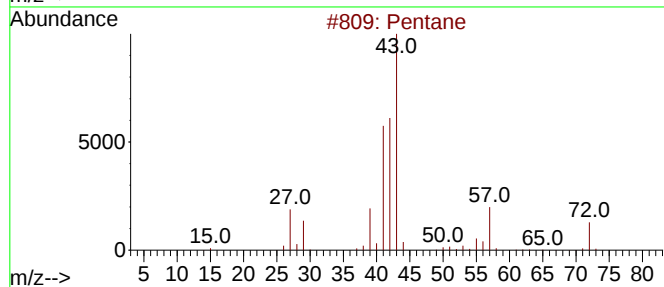
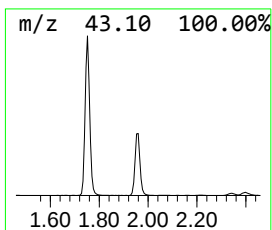
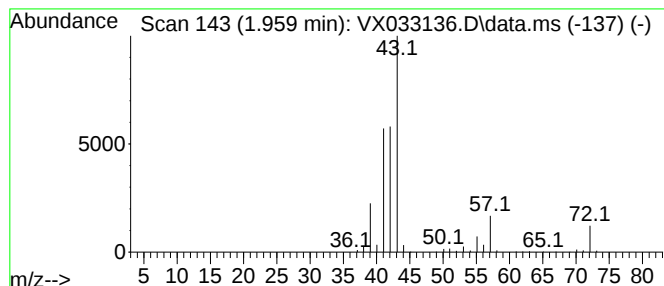
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	111.39 ug/l	729979	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	90
2			Butane, 2-methyl-	72	C5H12	000078-78-4	53
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	9



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PZ-3R

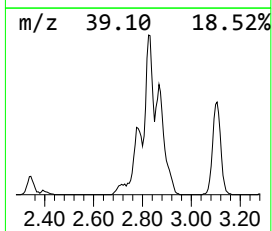
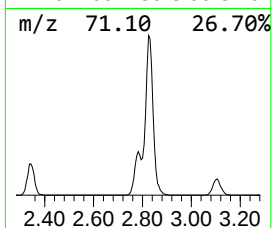
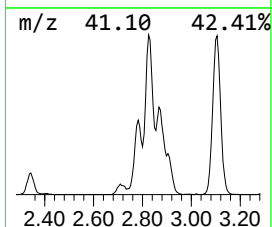
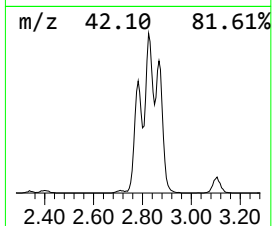
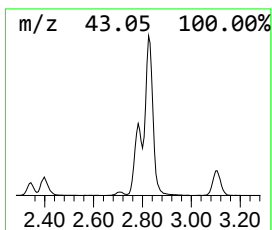
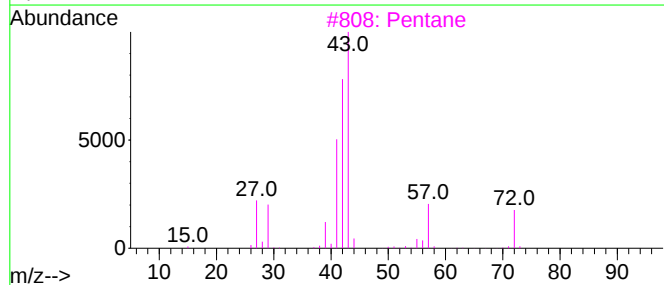
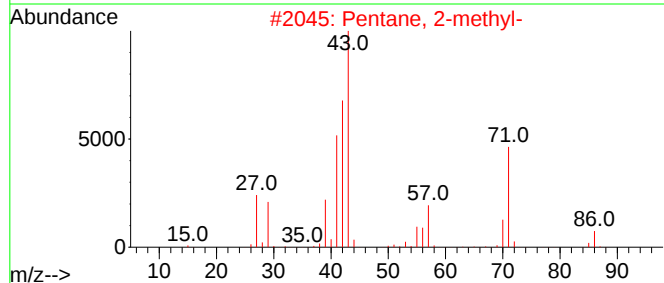
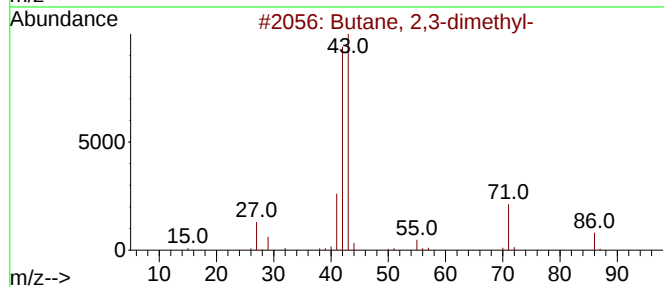
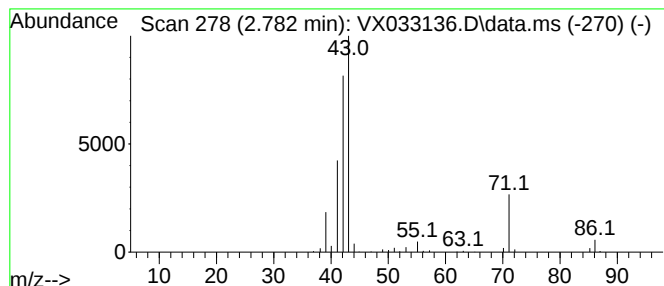
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	35.47 ug/l	232480	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	56
3			Pentane	72	C5H12	000109-66-0	45
4			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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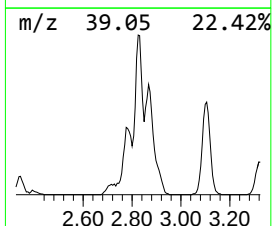
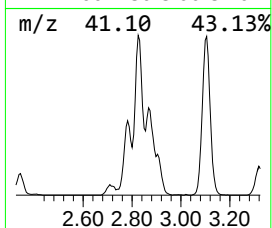
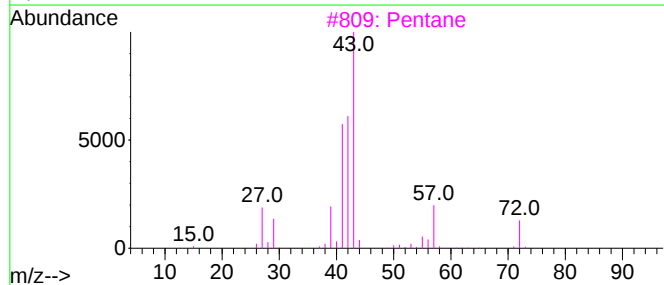
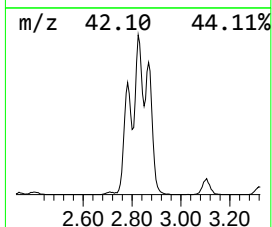
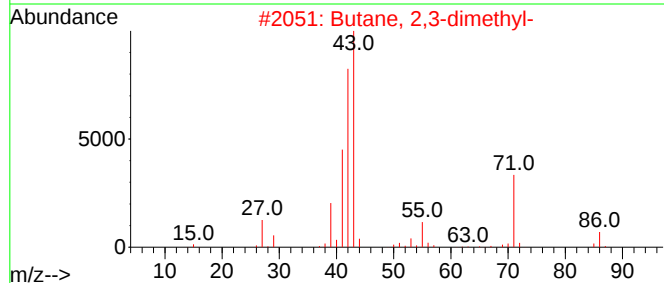
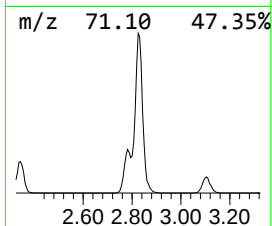
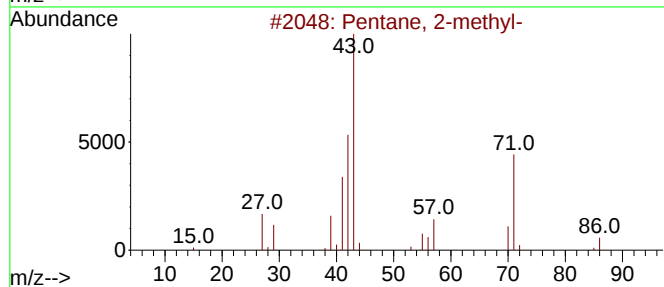
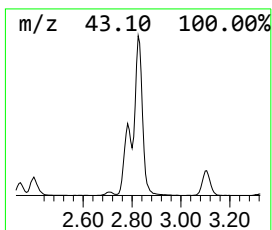
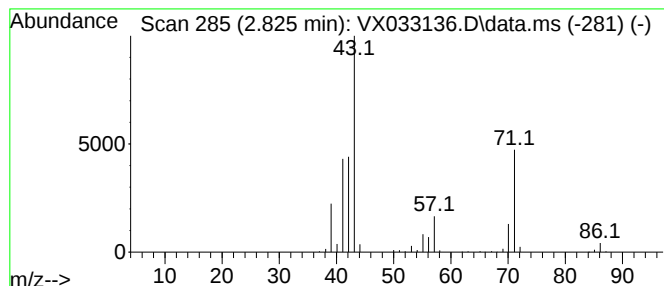
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	77.59 ug/l	508489	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
3			Pentane	72	C5H12	000109-66-0	43
4			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

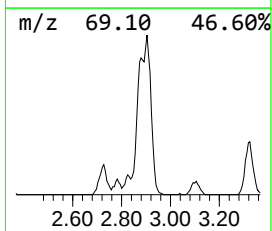
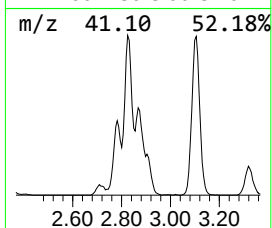
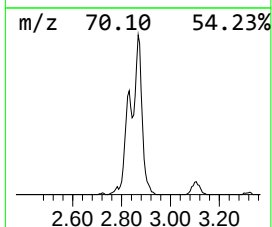
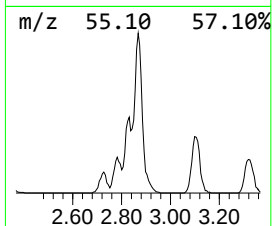
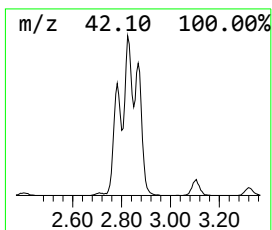
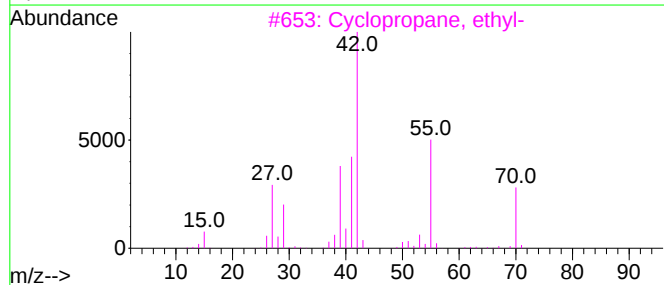
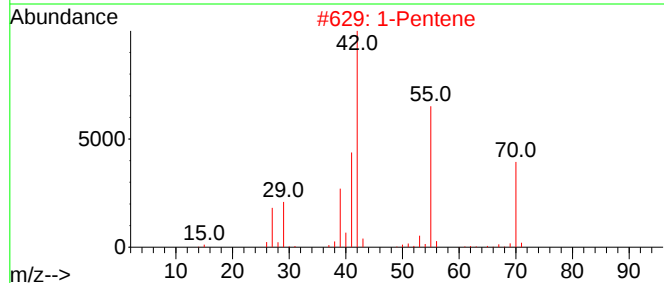
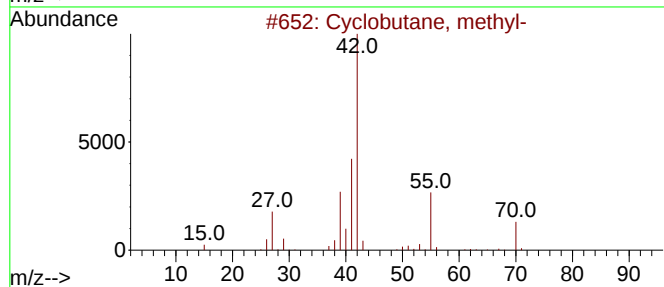
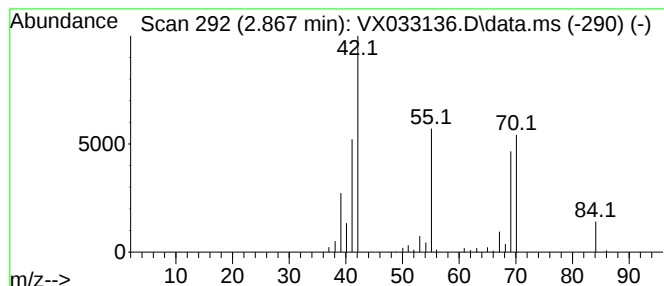
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Quant Title : SW846 8260

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

Peak Number 6 Cyclobutane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	39.64 ug/l	259771	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	64
2			1-Pentene	70	C5H10	000109-67-1	64
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	47
4			2-Pentene	70	C5H10	000109-68-2	38
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

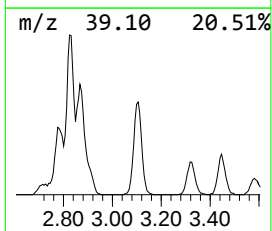
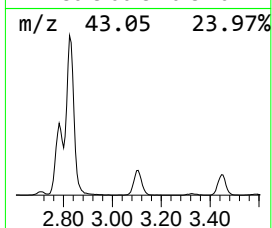
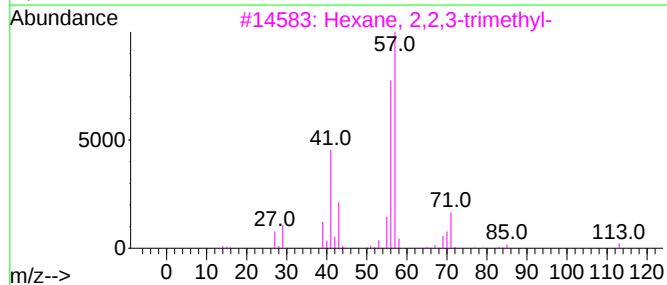
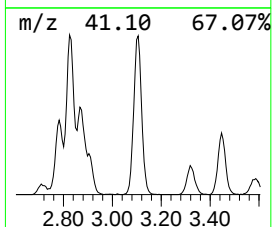
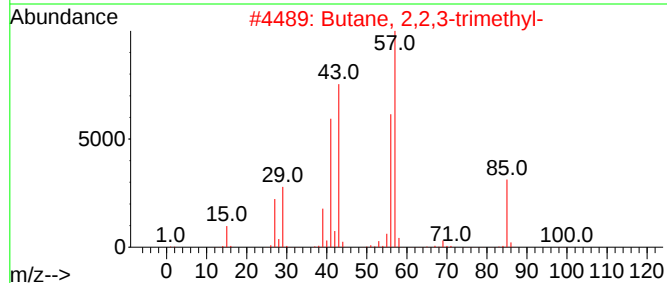
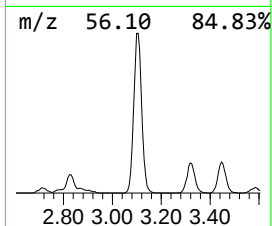
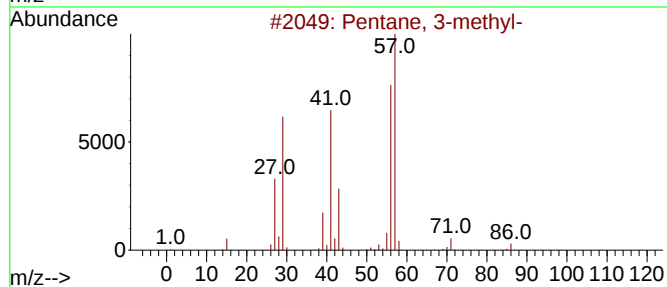
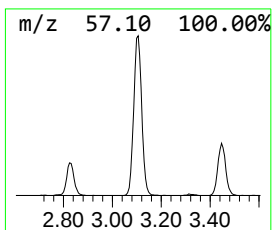
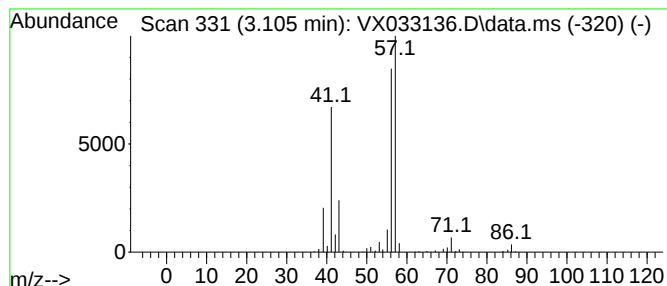
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	56.65 ug/l	371249	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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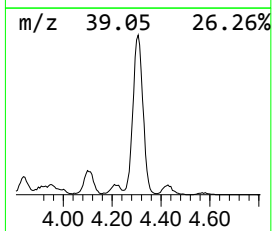
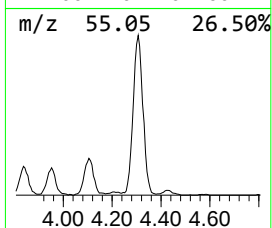
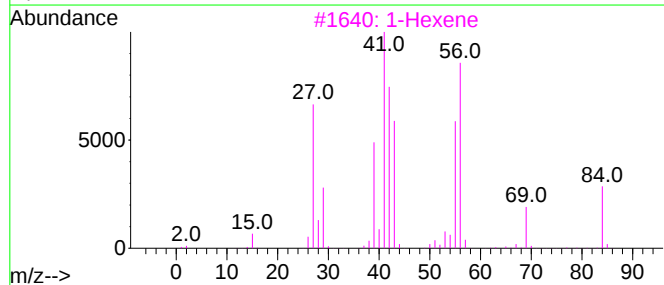
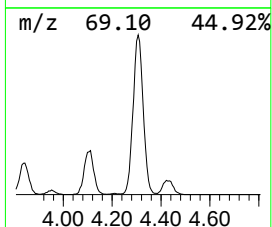
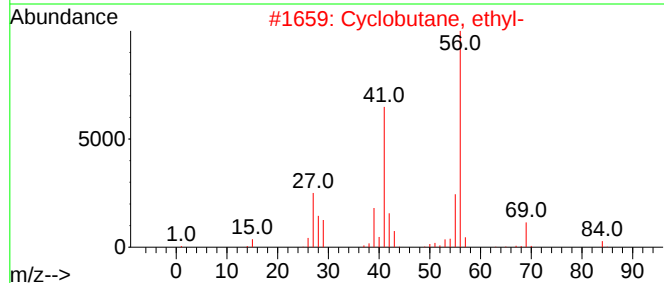
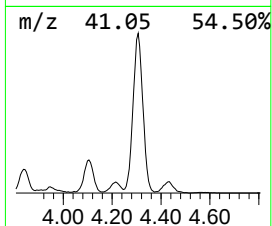
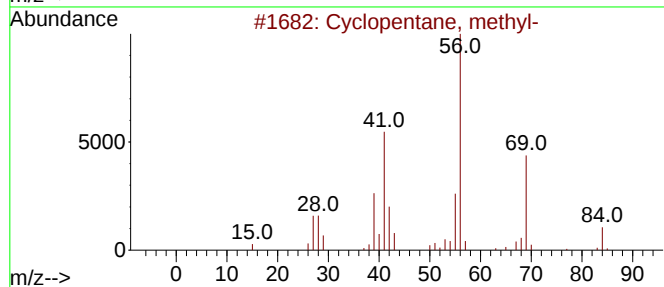
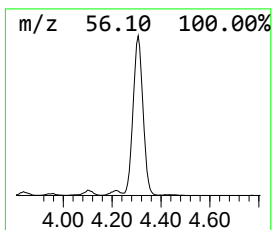
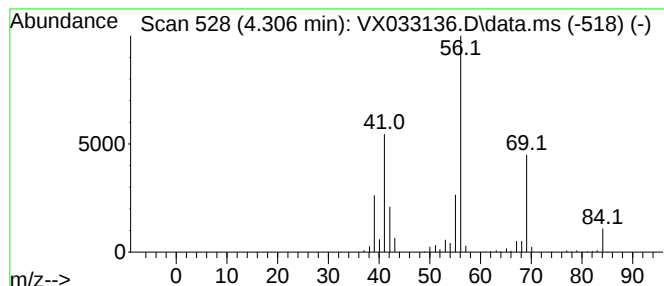
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	120.71 ug/l	791087	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		1-Hexene	84	C6H12	000592-41-6	52
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5		Cyclobutane	56	C4H8	000287-23-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

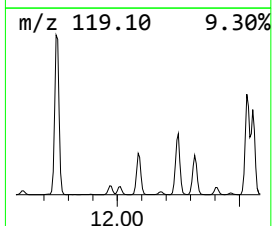
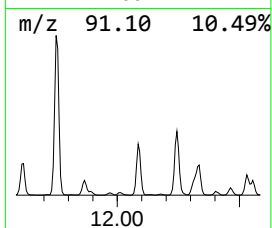
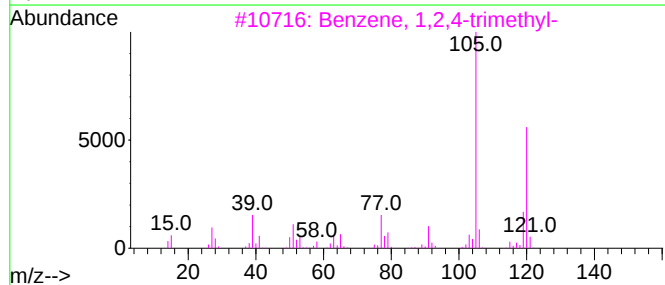
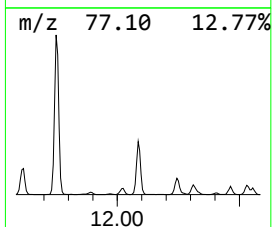
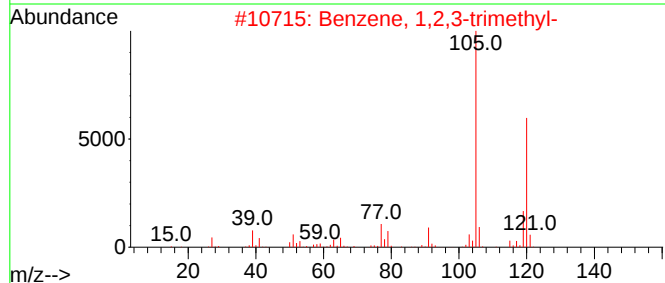
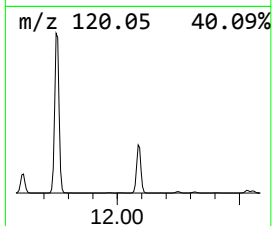
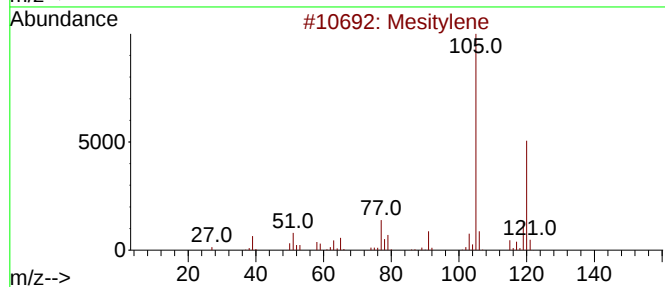
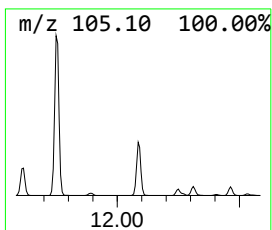
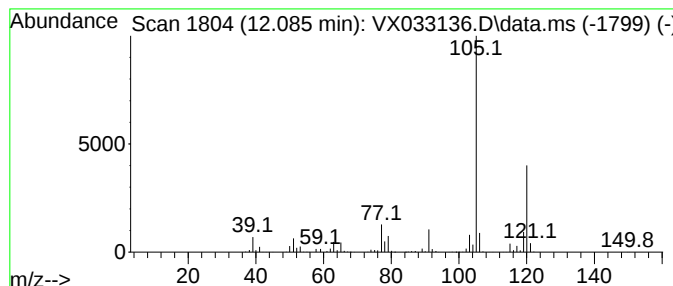
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	57.32 ug/l	806831	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
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ALS Vial : 17 Sample Multiplier: 1

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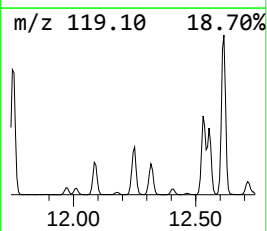
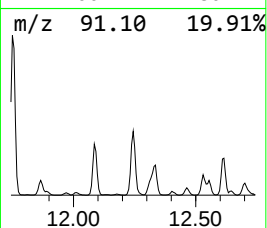
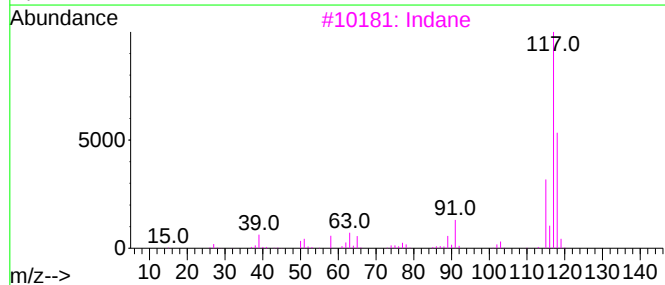
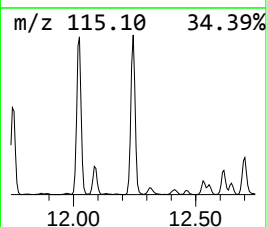
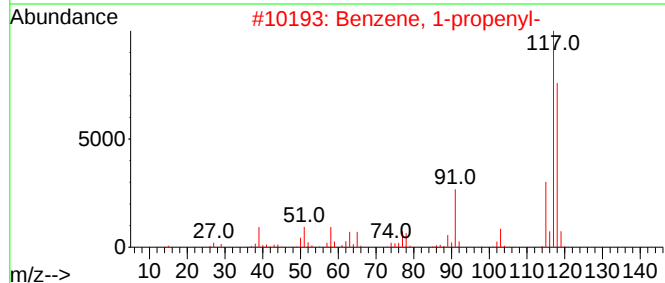
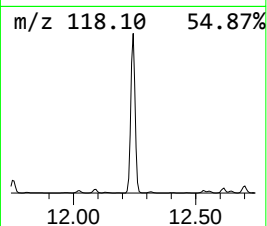
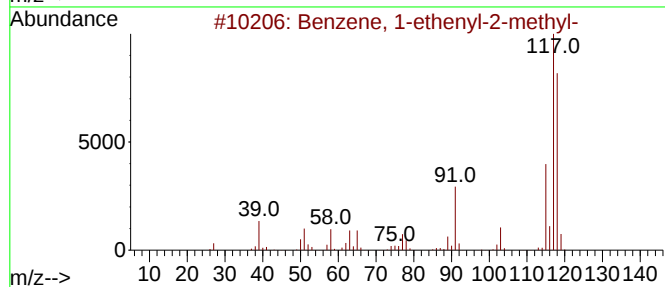
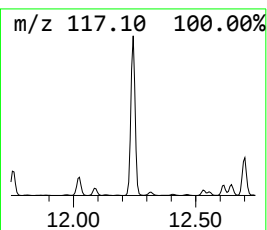
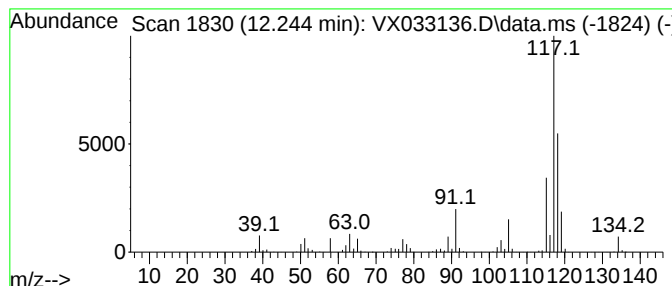
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	53.74 ug/l	756487	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	76
3			Indane	118	C9H10	000496-11-7	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033136.D
Acq On : 30 Nov 2022 16:51
Operator : JC/MD
Sample : N5815-21 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PZ-3R

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
Butane	1.374	60.3	ug/l	395458	1	5.556	327683	50.0
Butane, 2-methyl-	1.752	371.3	ug/l	2433370	1	5.556	327683	50.0
Pentane	1.959	111.4	ug/l	729979	1	5.556	327683	50.0
Butane, 2,3-dim...	2.782	35.5	ug/l	232480	1	5.556	327683	50.0
Pentane, 2-methyl-	2.825	77.6	ug/l	508489	1	5.556	327683	50.0
Cyclobutane, me...	2.867	39.6	ug/l	259771	1	5.556	327683	50.0
Pentane, 3-methyl-	3.105	56.6	ug/l	371249	1	5.556	327683	50.0
Cyclopentane, m...	4.306	120.7	ug/l	791087	1	5.556	327683	50.0
Benzene, 1,2,3-...	12.085	57.3	ug/l	806831	4	12.024	703779	50.0
Benzene, 1-ethe...	12.244	53.7	ug/l	756487	4	12.024	703779	50.0