

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
 Data File : VX033144.D
 Acq On : 30 Nov 2022 19:56
 Operator : JC/MD
 Sample : N5815-23
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 RW-1

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: VX033144.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	294796	354119	4.52%	0.708%
2	1.374	43	47	53	rBV	1840939	2018794	25.77%	4.035%
3	1.752	104	109	125	rVB	6079005	7834713	100.00%	15.659%
4	1.959	137	143	156	rVB2	822053	1304506	16.65%	2.607%
5	2.069	156	161	168	rBV	173412	249314	3.18%	0.498%
6	2.166	173	177	181	rVV	77472	117485	1.50%	0.235%
7	2.215	181	185	198	rVB	525709	805084	10.28%	1.609%
8	2.343	198	206	223	rVB	112366	221950	2.83%	0.444%
9	2.782	259	278	281	rBV2	320666	765748	9.77%	1.530%
10	2.831	281	286	289	rVV	467470	1028003	13.12%	2.055%
11	2.867	289	292	305	rVB2	656737	1356487	17.31%	2.711%
12	3.105	322	331	352	rVB2	559834	1288785	16.45%	2.576%
13	3.319	355	366	377	rBV	51903	116301	1.48%	0.232%
14	3.447	377	387	399	rVB	56824	126703	1.62%	0.253%
15	3.581	399	409	416	rBV2	30166	79883	1.02%	0.160%
16	3.733	427	434	443	rVB	157282	376551	4.81%	0.753%
17	3.837	443	451	458	rBV	101895	257673	3.29%	0.515%
18	3.904	458	462	472	rVB2	32038	78617	1.00%	0.157%
19	4.105	485	495	504	rVV	103972	271421	3.46%	0.542%
20	4.306	518	528	540	rVV	936442	2647963	33.80%	5.292%
21	4.428	540	548	564	rVB2	51029	154963	1.98%	0.310%
22	5.196	646	674	690	rBV	125718	416841	5.32%	0.833%
23	5.385	693	705	711	rBV2	70005	204899	2.62%	0.410%
24	5.477	711	720	727	rVV2	172181	511408	6.53%	1.022%
25	5.550	727	732	740	rVV	118976	320210	4.09%	0.640%
26	5.623	740	744	763	rVB4	68896	210300	2.68%	0.420%
27	5.830	766	778	790	rBV5	39795	128683	1.64%	0.257%
28	5.958	790	799	804	rBV	69151	175732	2.24%	0.351%
29	6.038	804	812	824	rVB	699784	1812603	23.14%	3.623%
30	6.166	824	833	834	rBV2	51946	107667	1.37%	0.215%
31	6.257	843	848	857	rVB3	87876	238159	3.04%	0.476%
32	6.361	857	865	878	rVB2	52294	151668	1.94%	0.303%
33	6.763	922	931	939	rBV	215736	564852	7.21%	1.129%
34	6.848	941	945	958	rVB4	64970	175273	2.24%	0.350%
35	7.172	990	998	1008	rVB	54079	119707	1.53%	0.239%
36	7.379	1020	1032	1044	rVB3	148836	414466	5.29%	0.828%

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37	7.885	1103	1115	1122	rBV2	28711	96678	1.23%	0.193%
38	8.104	1143	1151	1154	rBV	46424	92773	1.18%	0.185%
39	8.141	1154	1157	1162	rVB	68945	116051	1.48%	0.232%
40	8.507	1211	1217	1222	rBV	94873	157283	2.01%	0.314%
41	8.647	1235	1240	1247	rVB	327508	507092	6.47%	1.014%
42	8.720	1247	1252	1258	rVB	56791	89630	1.14%	0.179%
43	10.055	1460	1471	1476	rBV	449745	626472	8.00%	1.252%
44	10.195	1488	1494	1500	rVB	5886030	7363862	93.99%	14.718%
45	10.305	1505	1512	1518	rVB	1042261	1320523	16.85%	2.639%
46	10.964	1614	1620	1626	rBV	398420	497386	6.35%	0.994%
47	11.079	1634	1639	1645	rBV	304291	390860	4.99%	0.781%
48	11.305	1671	1676	1683	rVB	842414	1010016	12.89%	2.019%
49	11.403	1685	1692	1696	rVV	330893	416517	5.32%	0.832%
50	11.451	1696	1700	1708	rVB	157745	188337	2.40%	0.376%
51	11.616	1721	1727	1736	rVB	1022402	1324307	16.90%	2.647%
52	11.750	1744	1749	1755	rVB	710603	842460	10.75%	1.684%
53	12.024	1788	1794	1799	rVB	506634	663416	8.47%	1.326%
54	12.085	1799	1804	1809	rBV	263954	326801	4.17%	0.653%
55	12.244	1824	1830	1837	rBV	2330489	2824387	36.05%	5.645%
56	12.311	1837	1841	1850	rVV3	160308	247114	3.15%	0.494%
57	12.408	1852	1857	1861	rBV2	65405	90834	1.16%	0.182%
58	12.463	1861	1866	1872	rVB	156922	186070	2.37%	0.372%
59	12.530	1872	1877	1885	rBV	139858	192471	2.46%	0.385%
60	12.610	1885	1890	1894	rBV	401295	516100	6.59%	1.032%
61	12.646	1894	1896	1900	rVV	90545	91376	1.17%	0.183%
62	12.701	1900	1905	1912	rVB2	310539	463718	5.92%	0.927%
63	12.847	1924	1929	1934	rVB	78355	98389	1.26%	0.197%
64	12.921	1934	1941	1945	rBV	268247	322186	4.11%	0.644%
65	12.963	1945	1948	1954	rVB	162588	185819	2.37%	0.371%
66	13.170	1977	1982	1987	rVB	265207	310608	3.96%	0.621%
67	13.292	1997	2002	2007	rVB2	558161	714971	9.13%	1.429%
68	13.420	2019	2023	2032	rVB	74636	96578	1.23%	0.193%
69	13.774	2076	2081	2090	rBV	439630	545641	6.96%	1.091%
70	14.780	2241	2246	2258	rVB	84924	109179	1.39%	0.218%

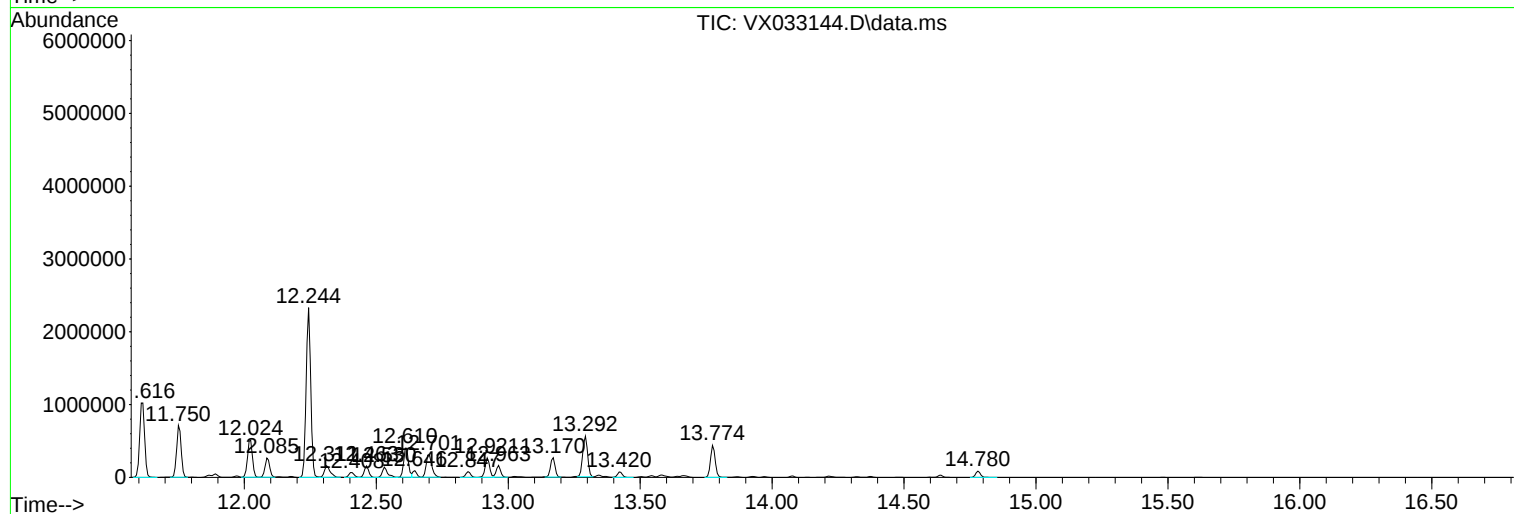
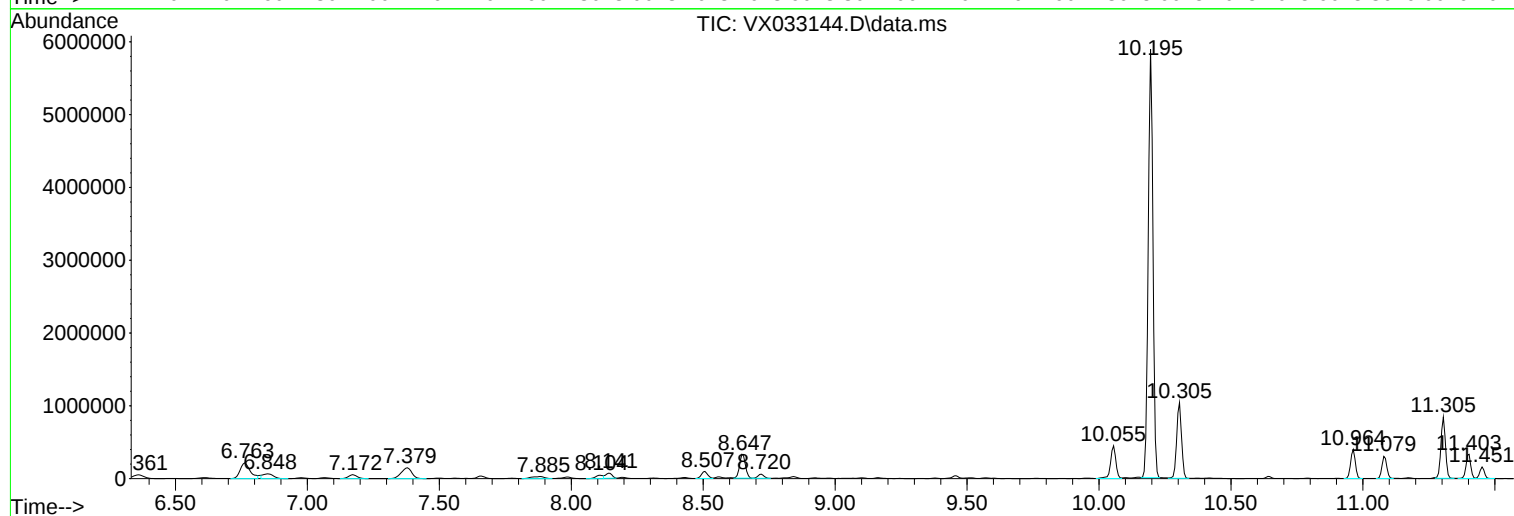
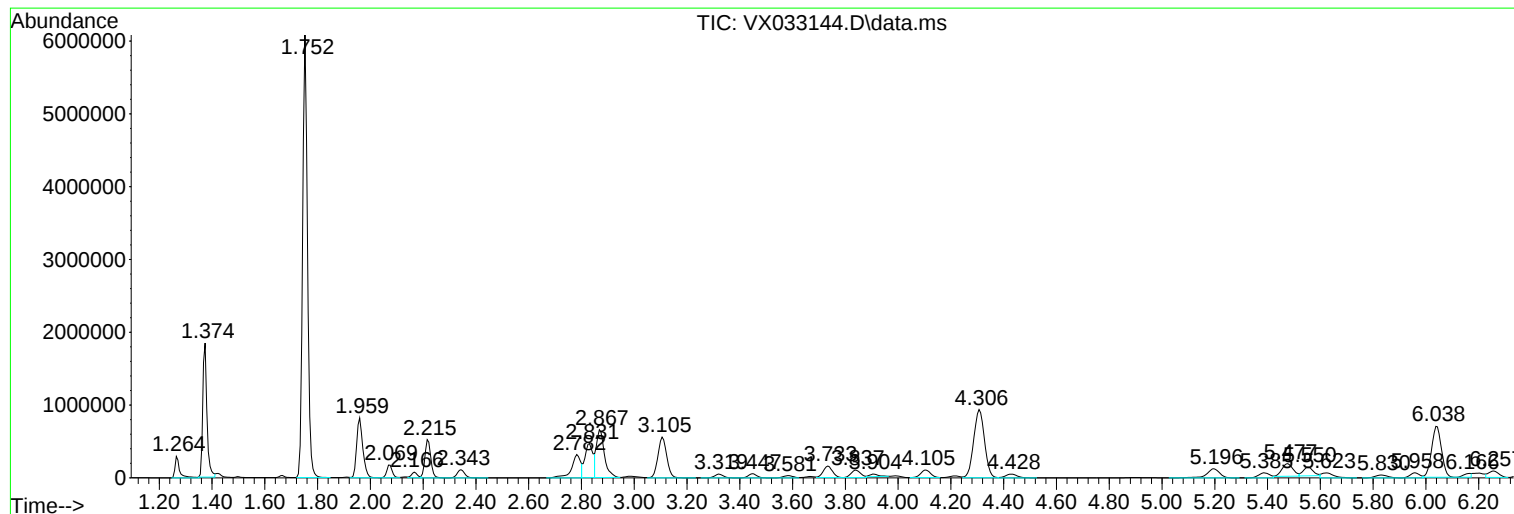
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Instrument :
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ClientSampleId :
RW-1

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
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

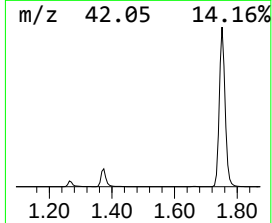
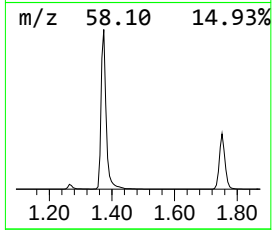
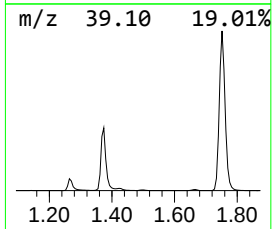
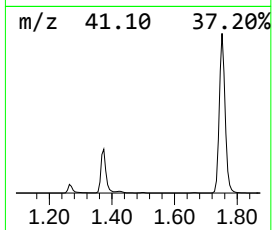
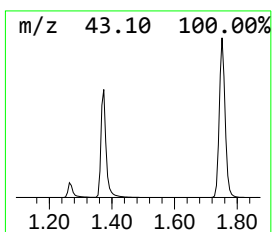
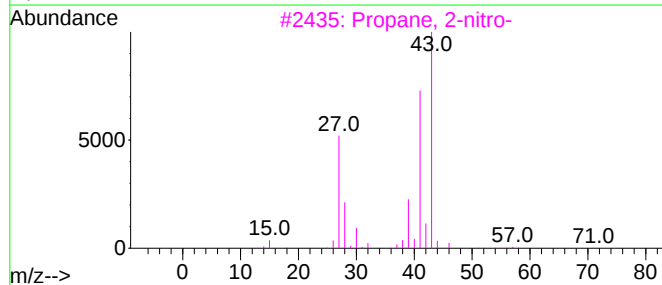
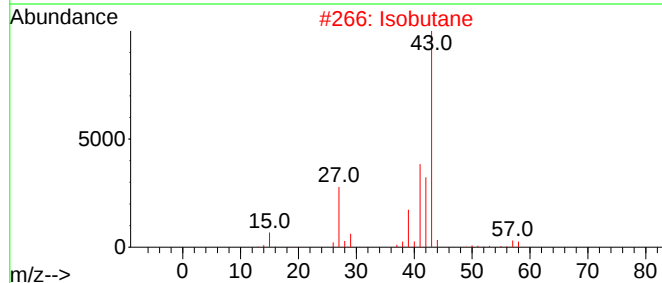
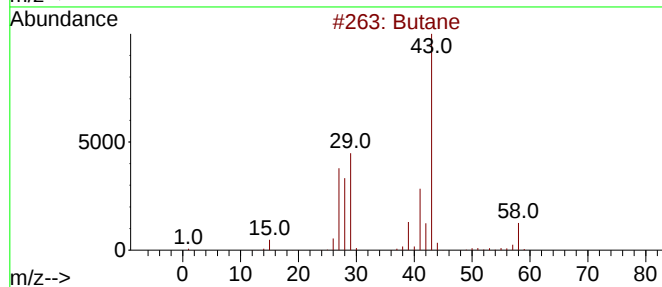
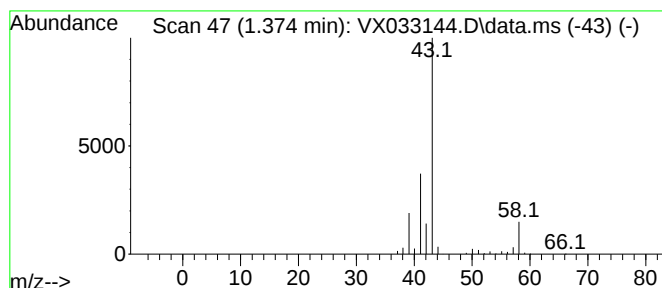
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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	315.23 ug/l	2018790	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	72
2			Isobutane	58	C4H10	000075-28-5	9
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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MSVOA_X
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RW-1

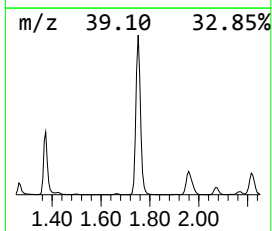
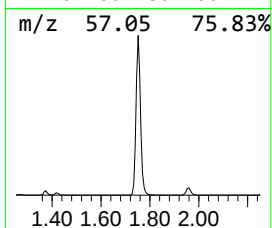
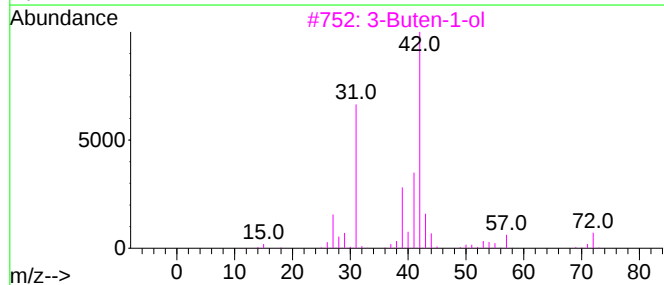
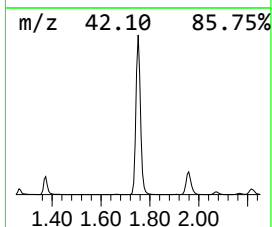
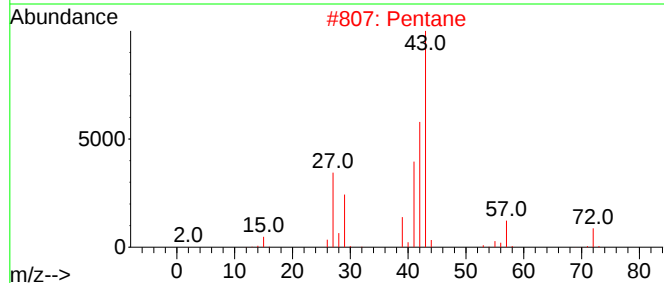
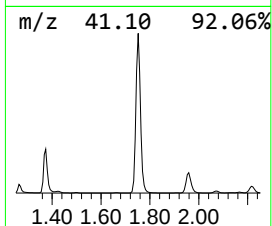
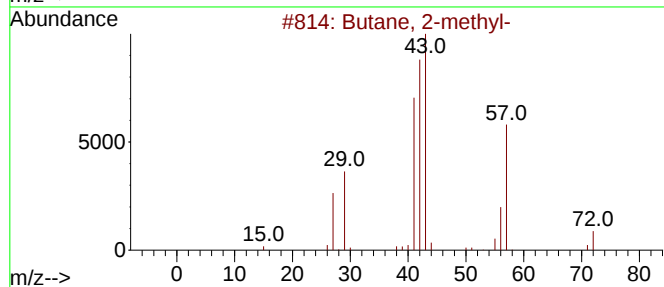
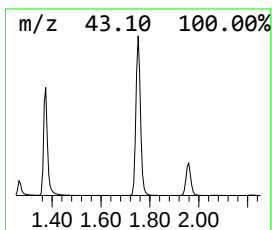
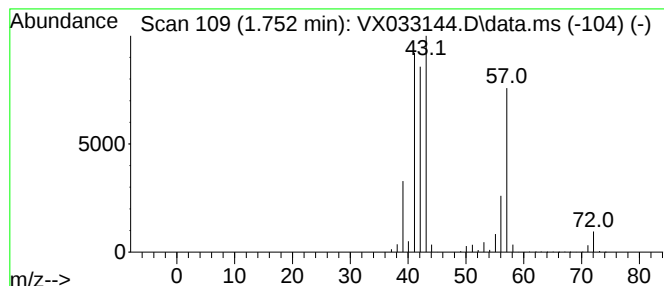
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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	1223.37 ug/l	7834710	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	42
3			3-Buten-1-ol	72	C4H8O	000627-27-0	25
4			1-Butene	56	C4H8	000106-98-9	10
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10



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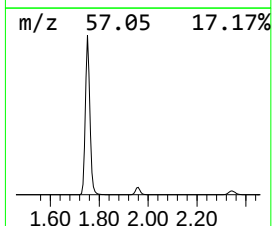
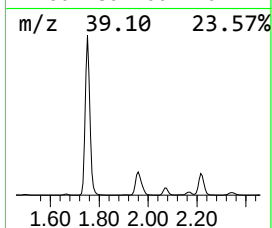
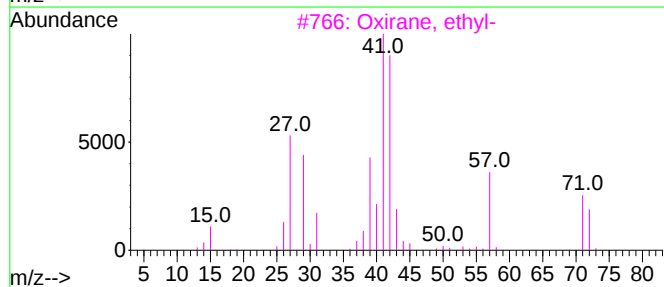
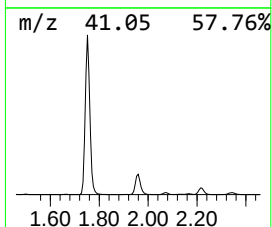
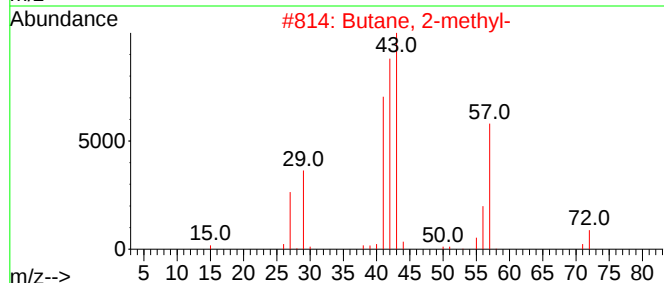
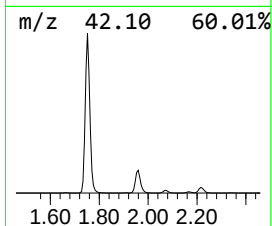
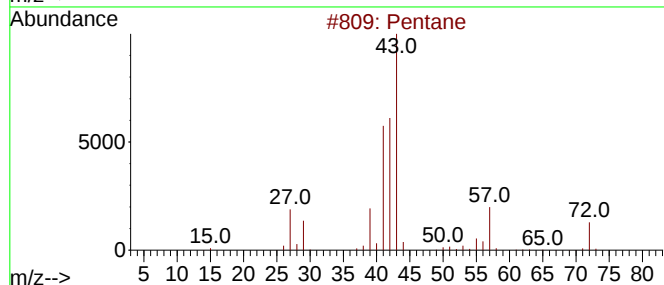
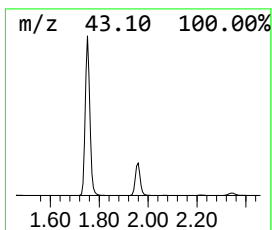
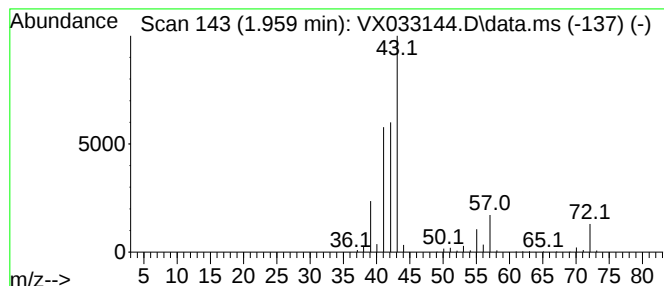
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Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	203.69 ug/l	1304510	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	59
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5			Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	10



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Instrument :
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ClientSampleId :
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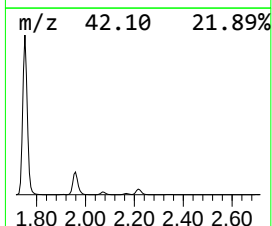
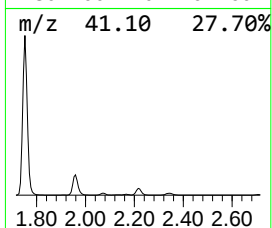
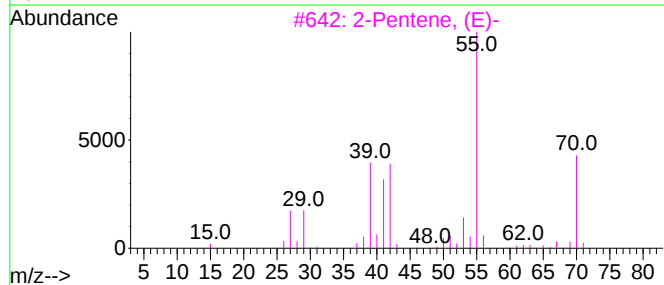
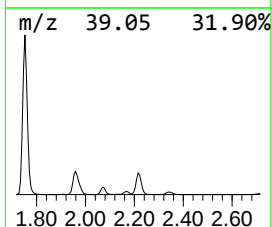
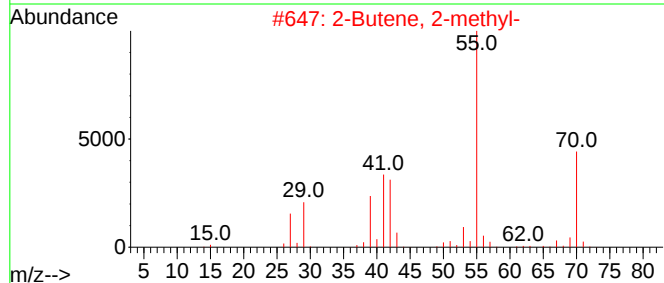
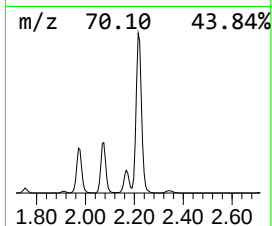
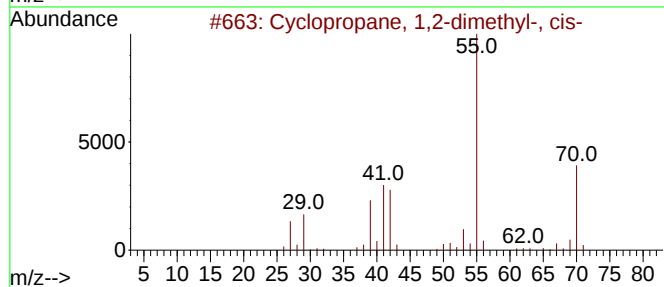
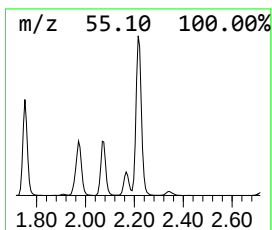
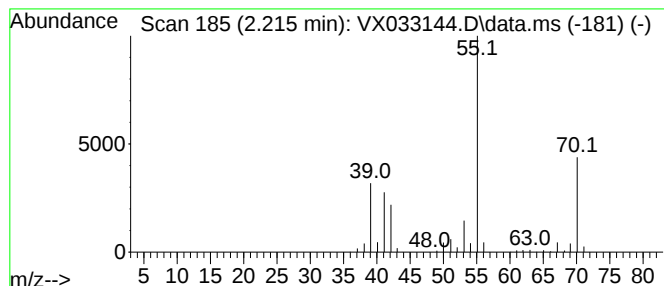
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	125.71 ug/l	805084	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3			2-Pentene, (E)-	70	C5H10	000646-04-8	86
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

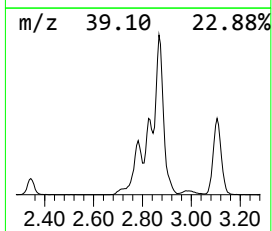
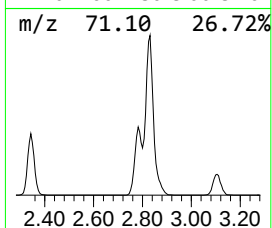
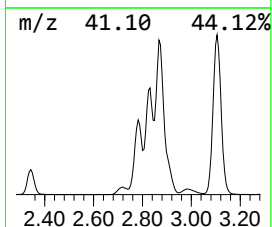
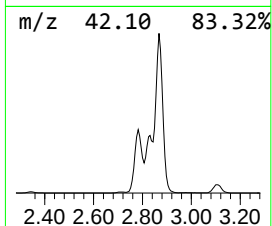
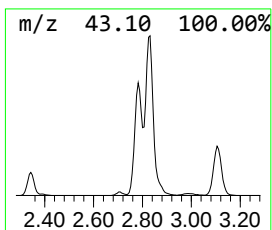
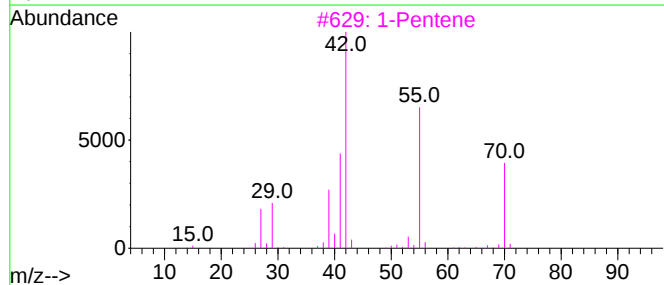
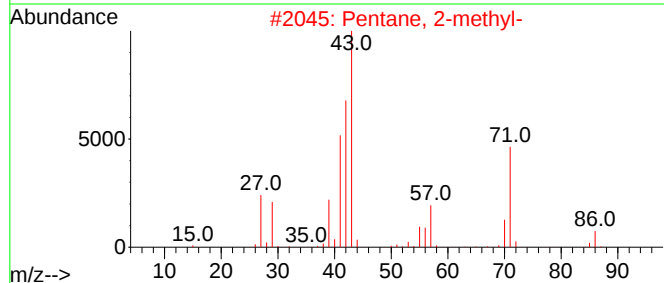
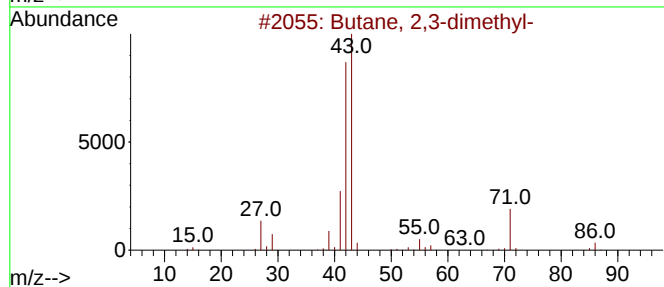
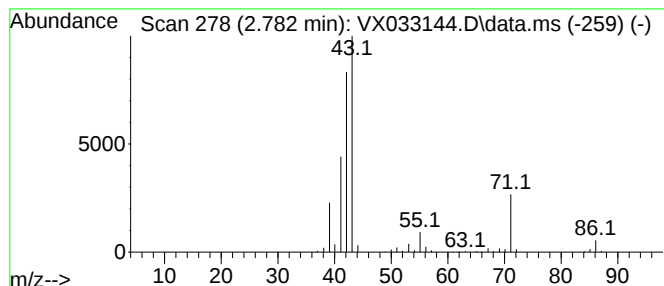
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Quant Title : SW846 8260

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

Peak Number 5 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	119.57 ug/l	765748	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	78
3			1-Pentene	70	C5H10	000109-67-1	28
4			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	10
5			Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

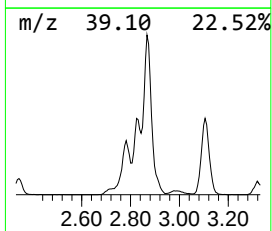
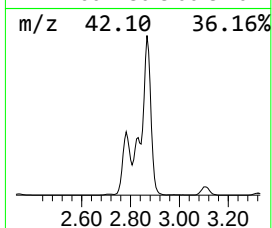
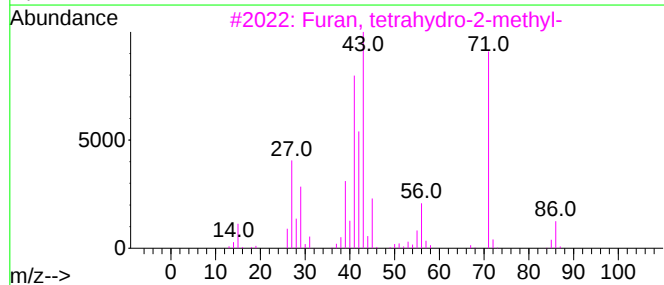
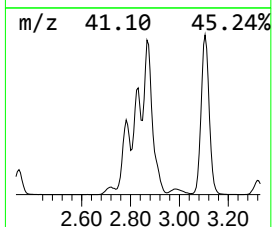
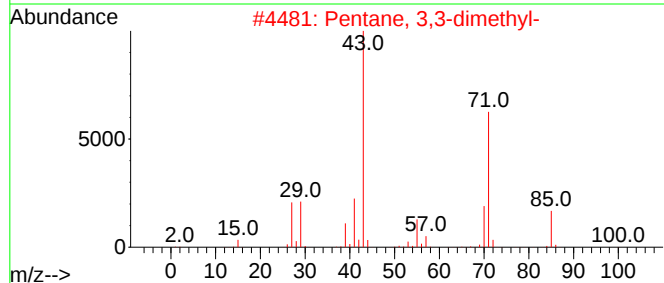
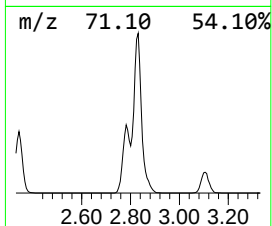
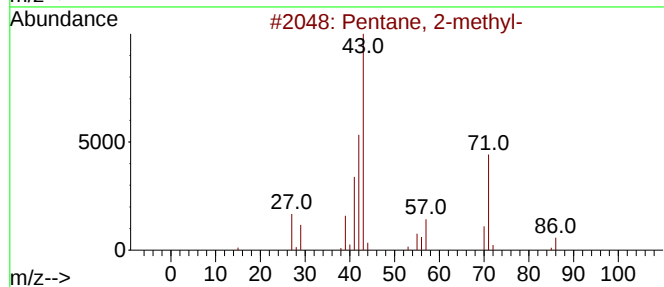
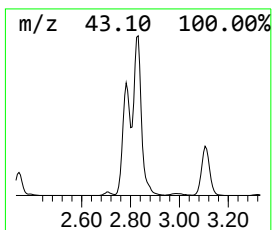
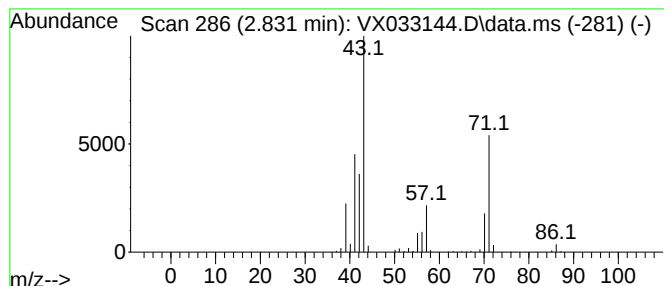
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.831	160.52 ug/l	1028000	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	42
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	36
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	33
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

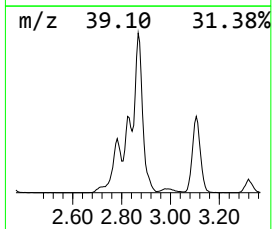
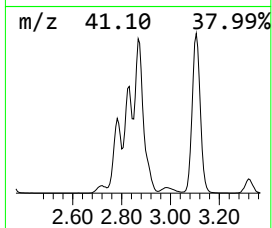
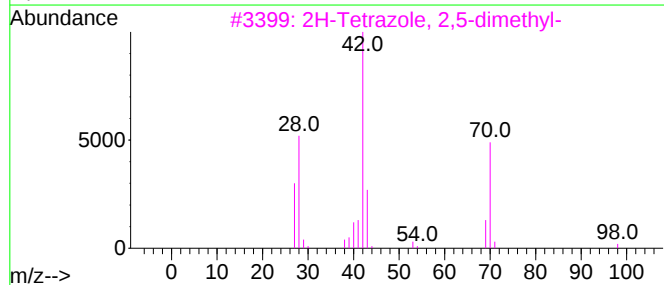
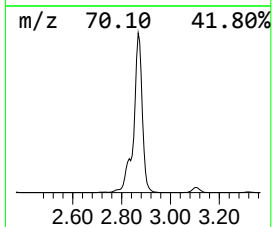
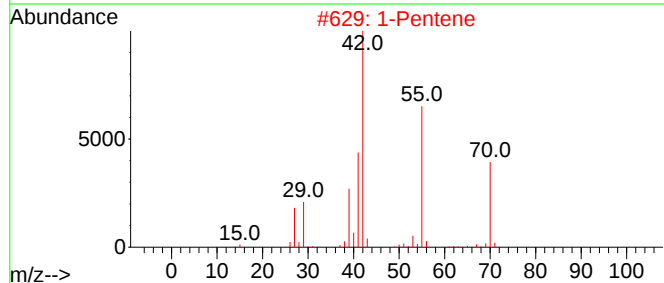
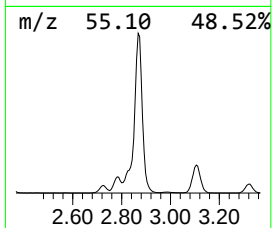
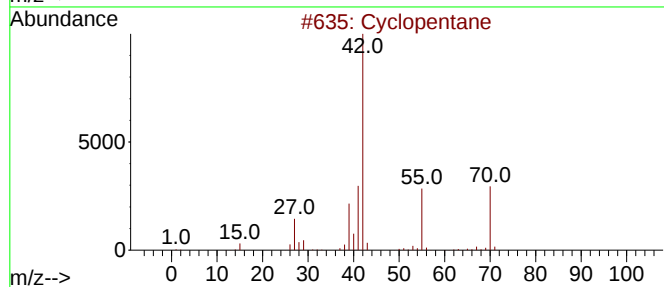
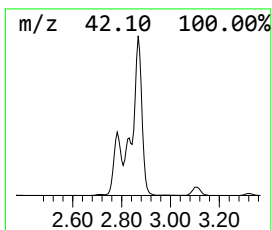
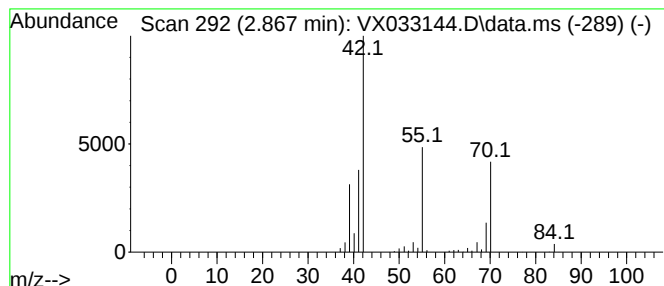
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	211.81 ug/l	1356490	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	72
2			1-Pentene	70	C5H10	000109-67-1	72
3			2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	40
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	16
5			n-Propyl chloride	78	C3H7Cl	000540-54-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

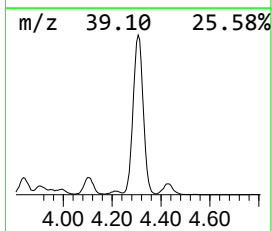
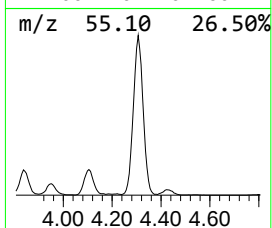
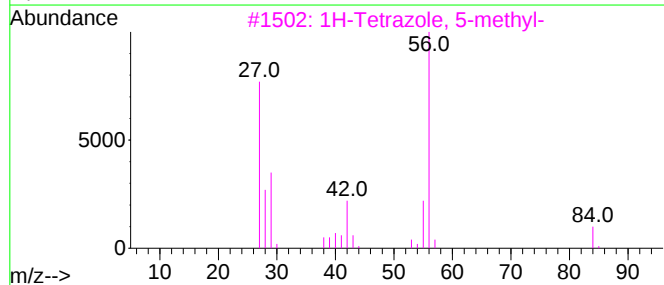
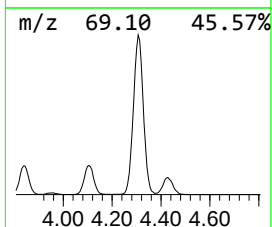
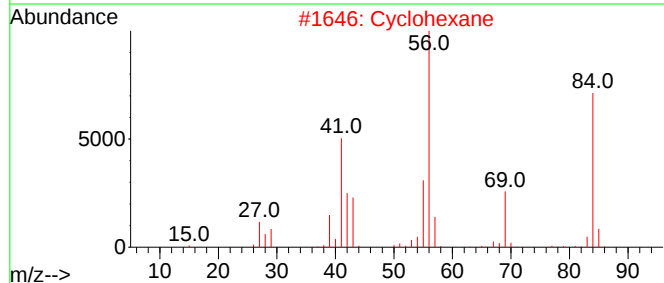
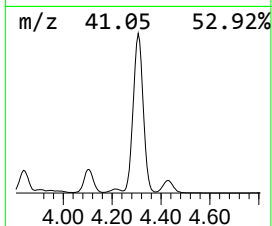
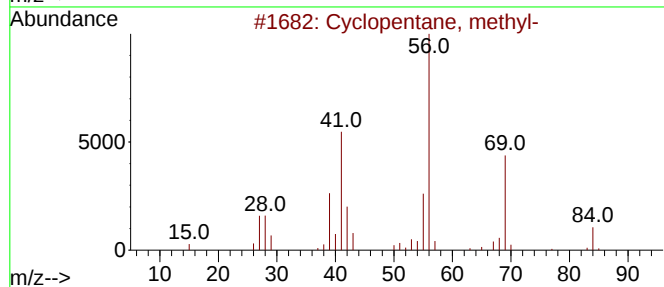
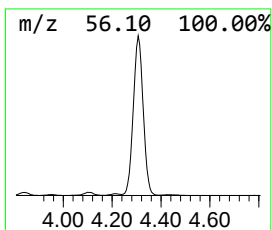
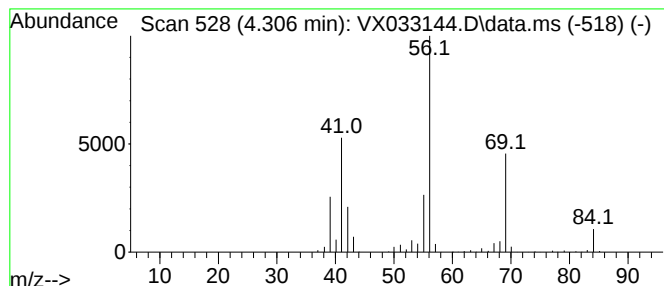
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Quant Title : SW846 8260

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	413.47 ug/l	2647960	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

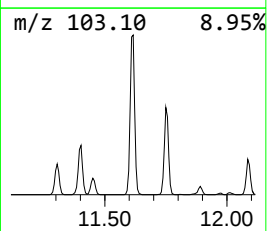
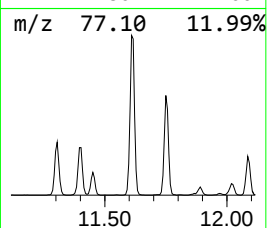
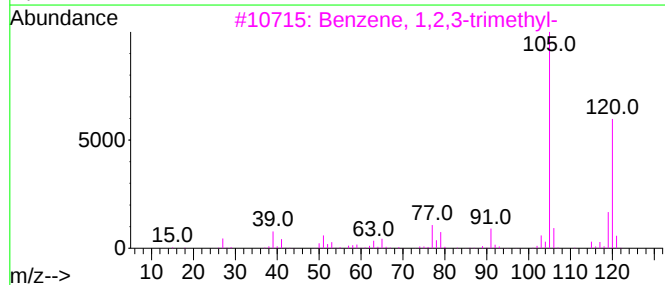
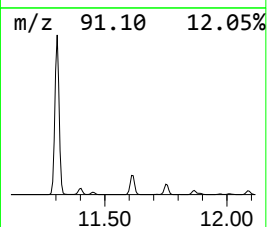
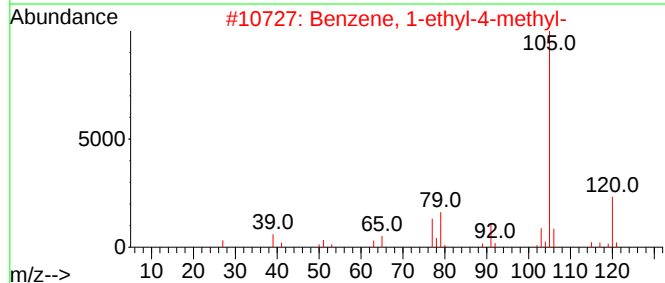
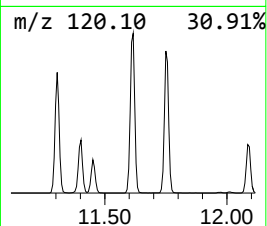
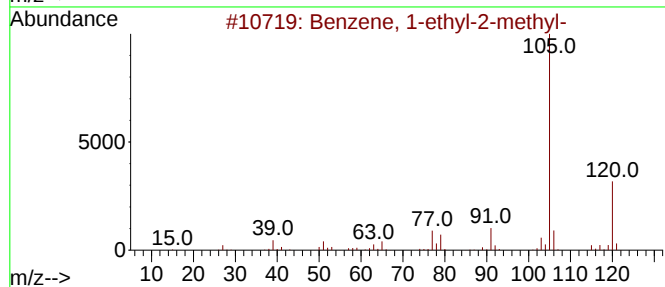
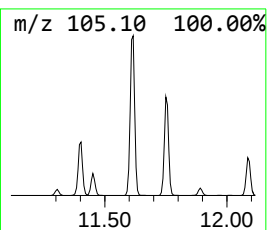
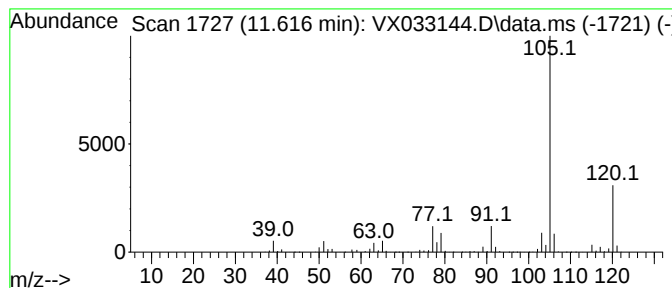
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	99.81 ug/l	1324310	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

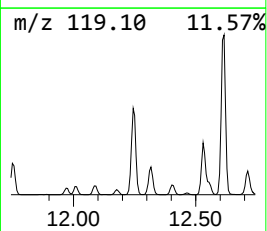
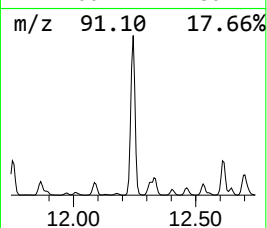
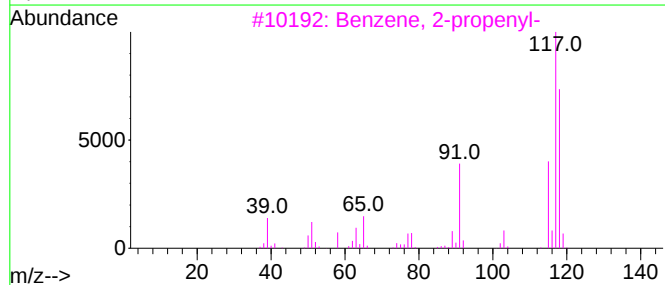
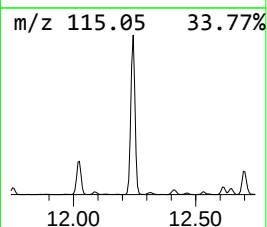
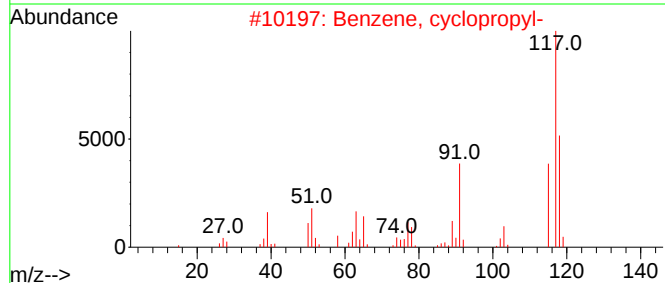
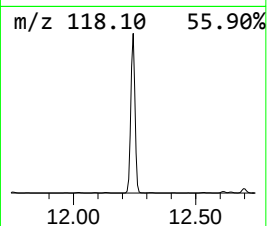
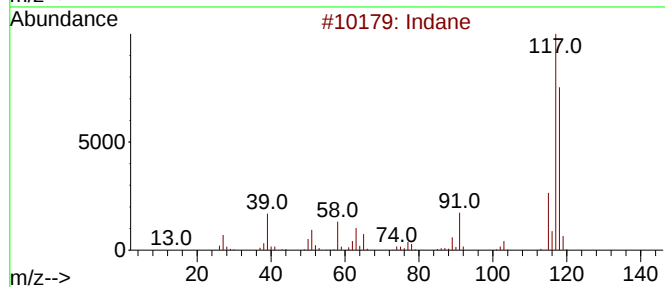
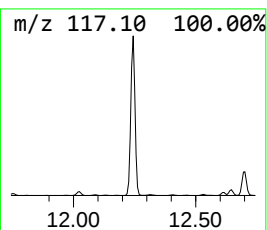
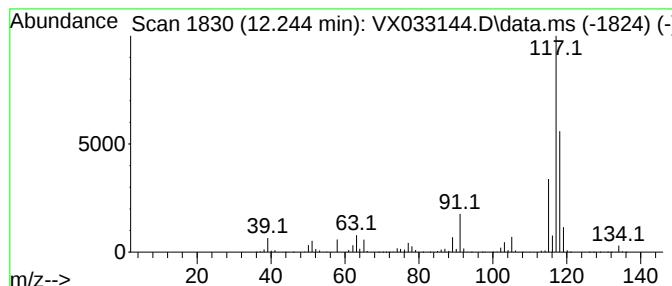
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Quant Title : SW846 8260

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.
12.244	212.87 ug/l	2824390	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indane	118	C9H10	000496-11-7	81
2		Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3		Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
4		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5		Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033144.D
Acq On : 30 Nov 2022 19:56
Operator : JC/MD
Sample : N5815-23
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
RW-1

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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Pentane	1.959	203.7	ug/l	1304510	1	5.556	320210	50.0
Cyclopropane, 1...	2.215	125.7	ug/l	805084	1	5.556	320210	50.0
Butane, 2,3-dim...	2.782	119.6	ug/l	765748	1	5.556	320210	50.0
Pentane, 2-methyl-	2.831	160.5	ug/l	1028000	1	5.556	320210	50.0
Cyclopentane	2.867	211.8	ug/l	1356490	1	5.556	320210	50.0
Cyclopentane, m...	4.306	413.5	ug/l	2647960	1	5.556	320210	50.0
Benzene, 1-ethy...	11.616	99.8	ug/l	1324310	4	12.024	663416	50.0
Indane	12.244	212.9	ug/l	2824390	4	12.024	663416	50.0