

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
 Data File : VX032689.D
 Acq On : 09 Nov 2022 18:57
 Operator : JC/MD
 Sample : N5551-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-14

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\82X102622W.M
 Title : SW846 8260

Signal : TIC: VX032689.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	808396	904159	6.06%	1.282%
2	1.368	43	46	53	rBV	1380836	1504282	10.08%	2.133%
3	1.752	103	109	123	rVB	4180644	5681764	38.08%	8.057%
4	1.959	137	143	156	rVB3	551643	1008422	6.76%	1.430%
5	2.069	156	161	167	rBV	191715	262285	1.76%	0.372%
6	2.215	180	185	197	rVB	652843	978264	6.56%	1.387%
7	2.343	198	206	217	rVB	78587	156467	1.05%	0.222%
8	2.782	258	278	281	rBV2	298648	762495	5.11%	1.081%
9	2.825	281	285	289	rVV	484493	1044163	7.00%	1.481%
10	2.867	289	292	305	rVB2	514078	1056467	7.08%	1.498%
11	3.105	321	331	348	rVB2	592673	1378220	9.24%	1.954%
12	3.447	378	387	399	rBV	69881	154362	1.03%	0.219%
13	3.733	426	434	444	rBV2	172156	451437	3.03%	0.640%
14	3.837	444	451	458	rBV	128877	321787	2.16%	0.456%
15	4.105	485	495	505	rBV	114966	297794	2.00%	0.422%
16	4.306	518	528	539	rVV	560392	1600073	10.72%	2.269%
17	4.428	539	548	562	rVB	70590	211268	1.42%	0.300%
18	5.196	650	674	690	rBV	150400	512658	3.44%	0.727%
19	5.385	692	705	712	rBV2	82055	250147	1.68%	0.355%
20	5.477	712	720	727	rBV3	124653	380722	2.55%	0.540%
21	5.556	727	733	738	rVV	89208	223191	1.50%	0.316%
22	5.623	739	744	764	rVB3	116677	383032	2.57%	0.543%
23	5.830	764	778	790	rBV2	62963	193578	1.30%	0.275%
24	5.958	790	799	804	rBV	79326	202543	1.36%	0.287%
25	6.044	804	813	825	rVB	696435	1802045	12.08%	2.555%
26	6.166	825	833	835	rBV2	71242	168511	1.13%	0.239%
27	6.251	842	847	857	rVB2	159665	455481	3.05%	0.646%
28	6.361	857	865	876	rVB2	61685	180098	1.21%	0.255%
29	6.763	921	931	937	rBV	194764	515641	3.46%	0.731%
30	6.854	942	946	958	rVB4	97723	240273	1.61%	0.341%
31	7.171	988	998	1008	rVB2	83883	194106	1.30%	0.275%
32	7.379	1020	1032	1045	rBV4	156633	459794	3.08%	0.652%
33	7.988	1122	1132	1143	rVB2	70642	169320	1.13%	0.240%
34	8.110	1143	1152	1155	rBV	135916	292369	1.96%	0.415%
35	8.141	1155	1157	1162	rVB	106551	153985	1.03%	0.218%
36	8.507	1209	1217	1227	rVB	111421	197948	1.33%	0.281%

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37	8.647	1235	1240	1246	rVB	393652	626710	4.20%	0.889%
38	8.720	1246	1252	1258	rVB	499794	753740	5.05%	1.069%
39	8.958	1280	1291	1299	rBV	285251	477567	3.20%	0.677%
40	9.049	1299	1306	1311	rBV	299557	462153	3.10%	0.655%
41	10.055	1461	1471	1476	rBV	403097	543329	3.64%	0.770%
42	10.201	1488	1495	1500	rBV	11202575	14921100	100.00%	21.159%
43	10.305	1505	1512	1519	rVB	1867909	2500856	16.76%	3.546%
44	10.640	1562	1567	1574	rVB	616673	789705	5.29%	1.120%
45	10.963	1614	1620	1627	rBV	580209	713411	4.78%	1.012%
46	11.079	1634	1639	1645	rBV	382822	495568	3.32%	0.703%
47	11.305	1667	1676	1683	rBV	1404855	1709593	11.46%	2.424%
48	11.402	1686	1692	1696	rVV	407069	513928	3.44%	0.729%
49	11.451	1696	1700	1707	rVB	400840	481699	3.23%	0.683%
50	11.616	1721	1727	1734	rBV	1881949	2387763	16.00%	3.386%
51	11.756	1744	1750	1755	rBV	5254765	6521353	43.71%	9.248%
52	12.024	1788	1794	1799	rVB	473473	602887	4.04%	0.855%
53	12.085	1799	1804	1809	rBV	1070201	1289748	8.64%	1.829%
54	12.244	1824	1830	1836	rBV	2463479	3020042	20.24%	4.283%
55	12.311	1836	1841	1852	rVB3	252631	420290	2.82%	0.596%
56	12.408	1852	1857	1862	rBV2	160442	217931	1.46%	0.309%
57	12.463	1862	1866	1871	rVB	131092	153170	1.03%	0.217%
58	12.530	1872	1877	1879	rBV	318807	391521	2.62%	0.555%
59	12.555	1879	1881	1886	rVV	215143	230407	1.54%	0.327%
60	12.616	1886	1891	1894	rVV	558953	694665	4.66%	0.985%
61	12.646	1894	1896	1900	rVV	158368	162603	1.09%	0.231%
62	12.701	1900	1905	1912	rVB	542898	715755	4.80%	1.015%
63	12.920	1934	1941	1944	rBV	337996	410931	2.75%	0.583%
64	12.963	1944	1948	1954	rVB	388969	450411	3.02%	0.639%
65	13.170	1978	1982	1987	rVB	391223	451092	3.02%	0.640%
66	13.292	1997	2002	2007	rVB2	735847	940411	6.30%	1.334%
67	13.420	2019	2023	2030	rVB	129693	176395	1.18%	0.250%
68	13.774	2074	2081	2090	rBV	1103029	1337084	8.96%	1.896%
69	14.780	2241	2246	2260	rVB	165049	205940	1.38%	0.292%

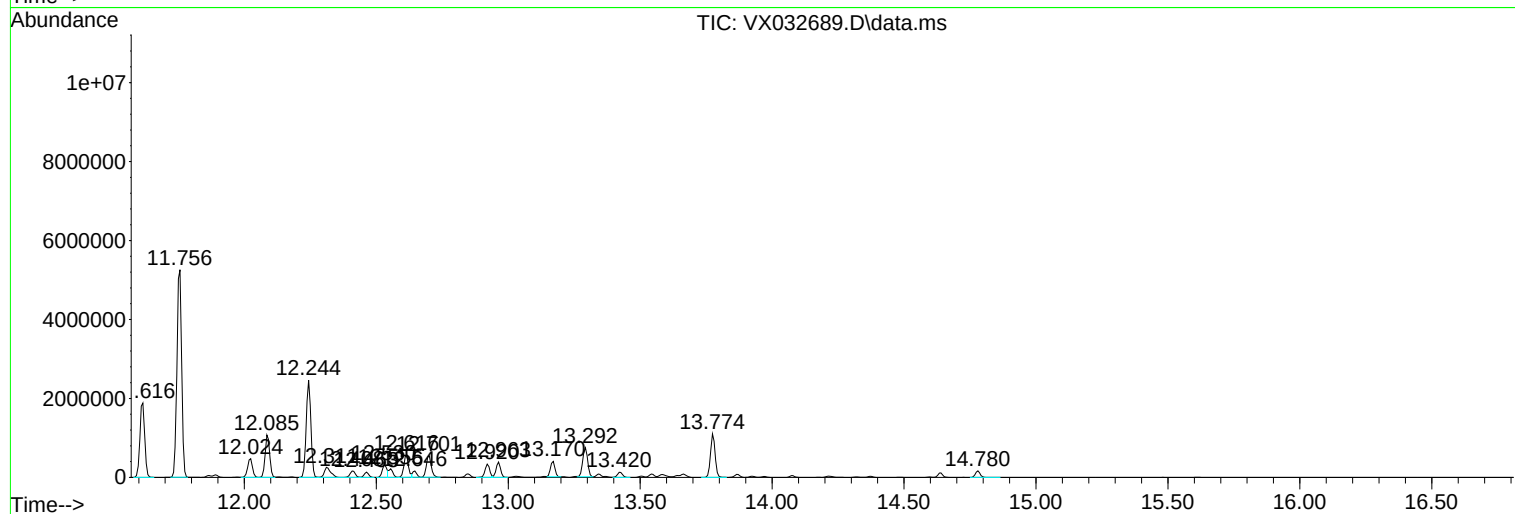
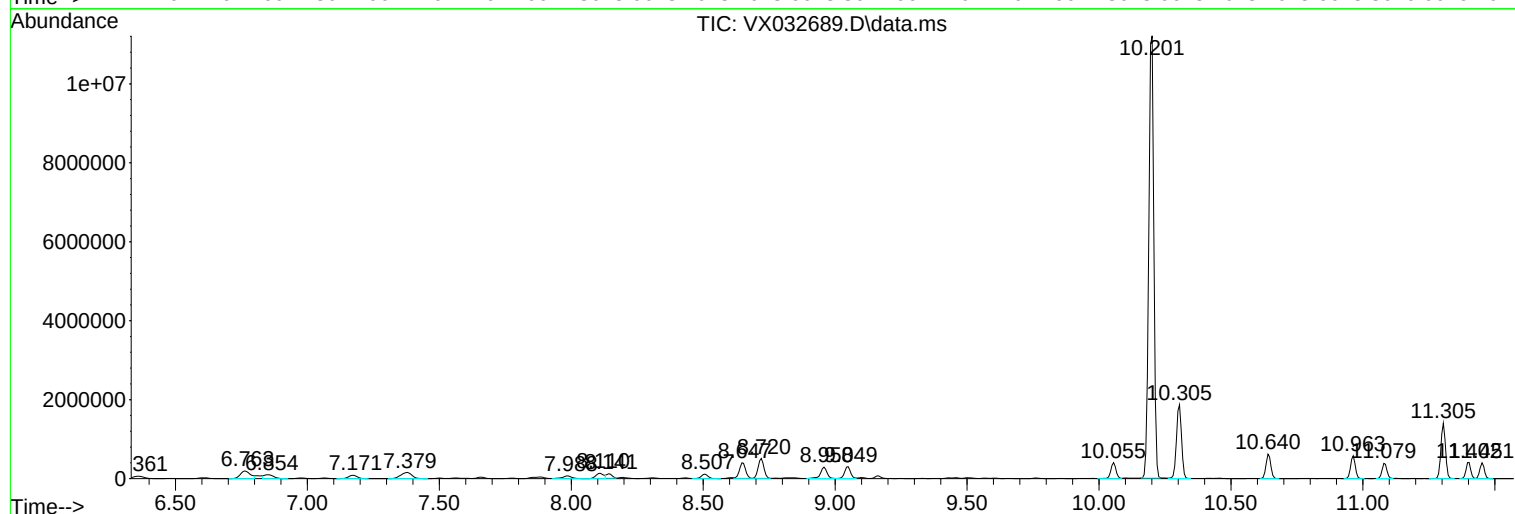
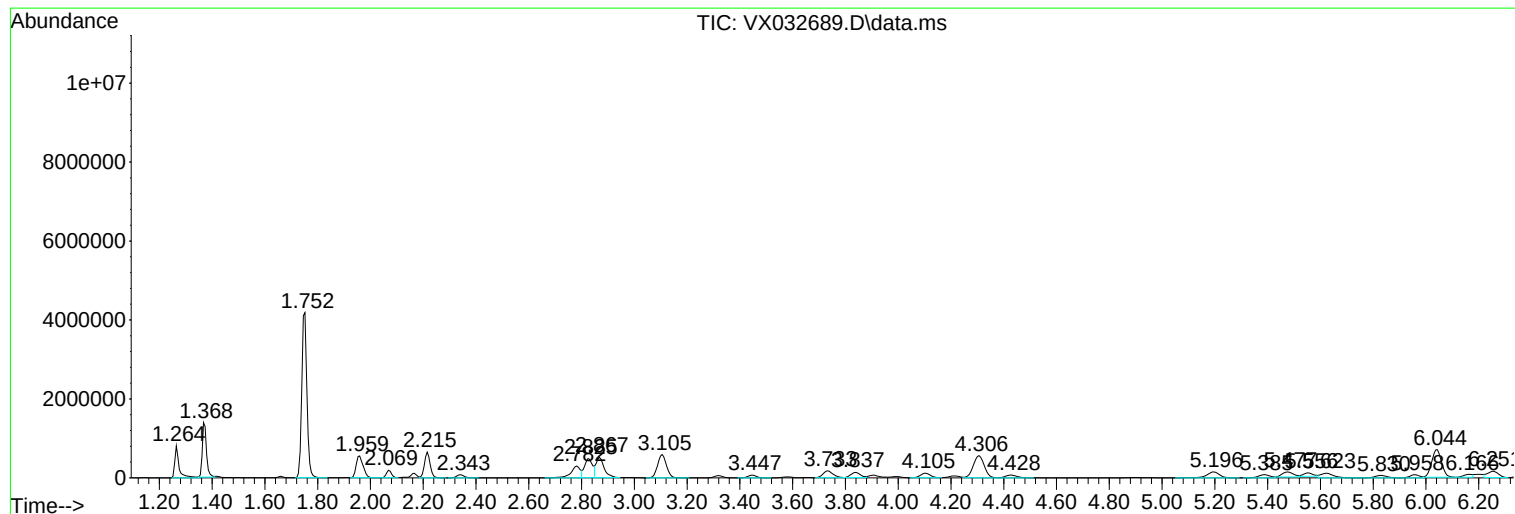
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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-14

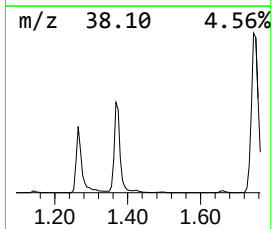
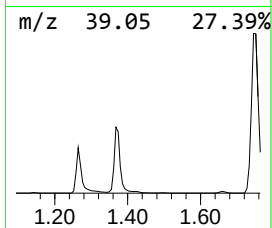
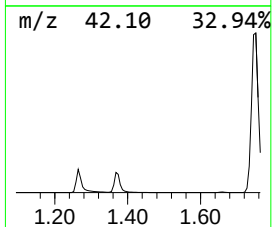
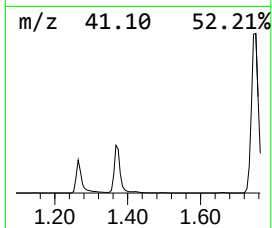
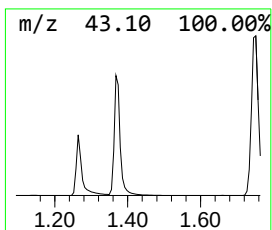
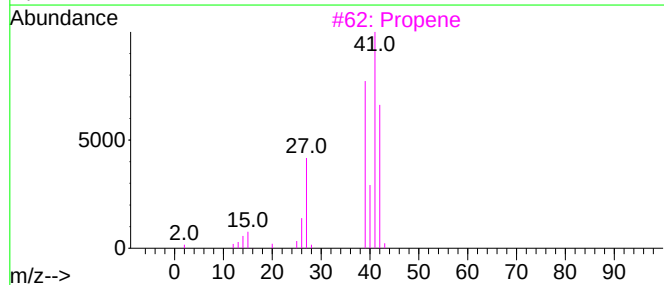
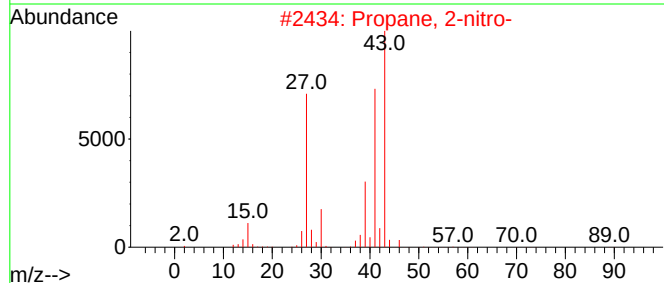
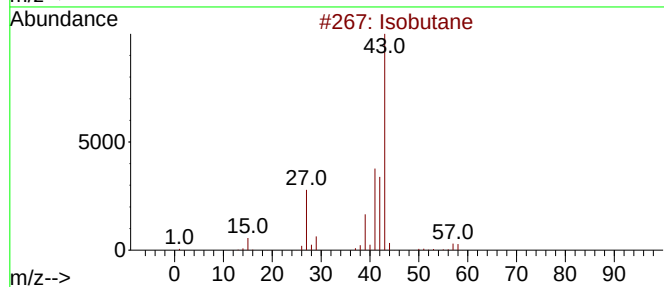
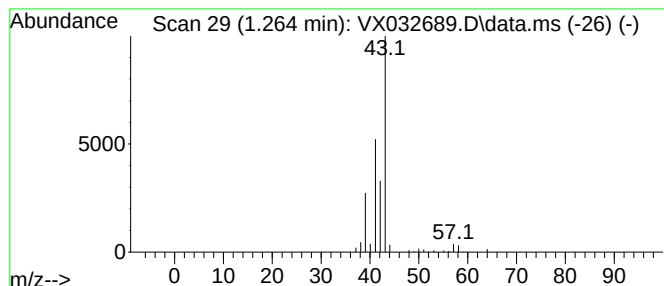
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	202.55 ug/l	904159	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	64
2		Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3		Propene	42	C3H6	000115-07-1	7
4		Hydrogen isocyanate	43	CHNO	000075-13-8	4
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	4



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Instrument :
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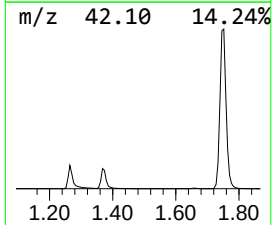
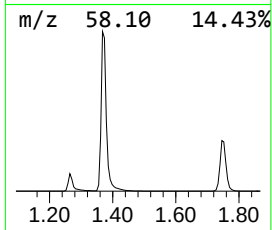
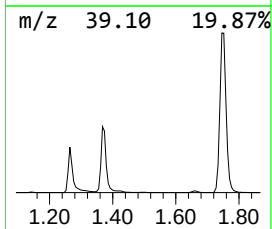
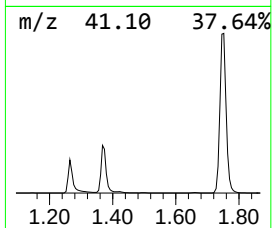
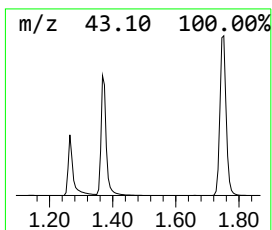
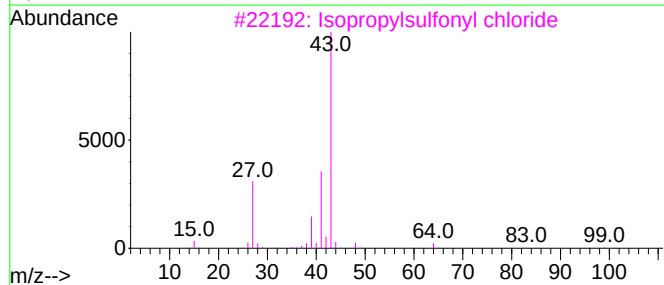
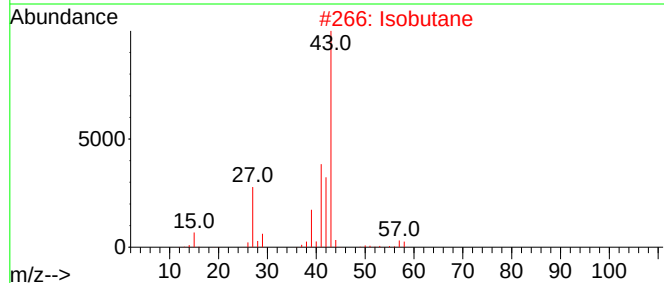
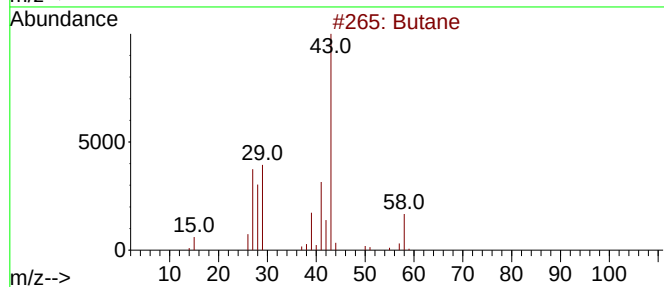
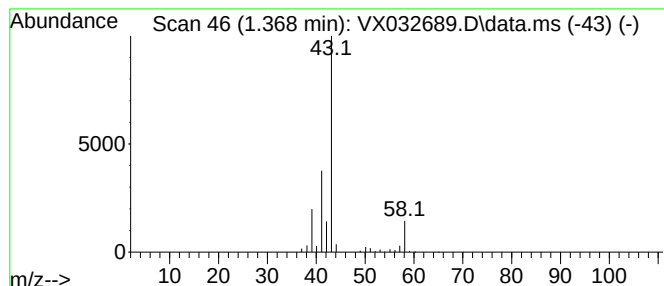
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	336.99 ug/l	1504280	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isobutane	58	C4H10	000075-28-5	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Diazene, dimethyl-	58	C2H6N2	000503-28-6	4



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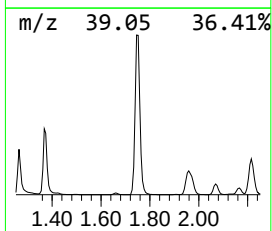
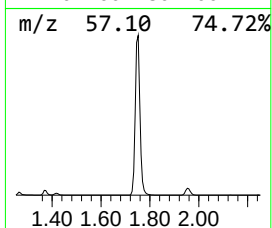
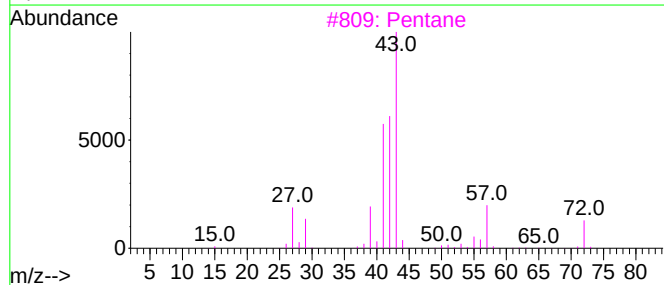
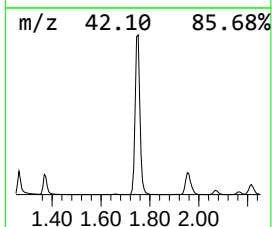
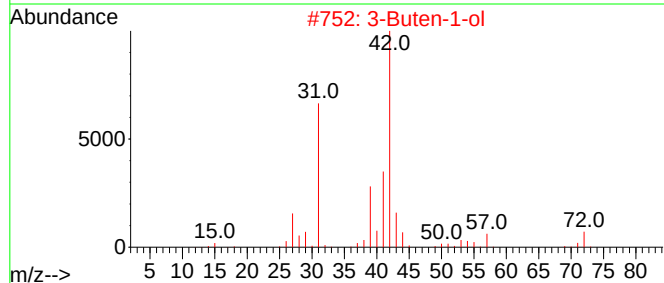
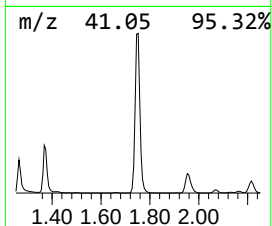
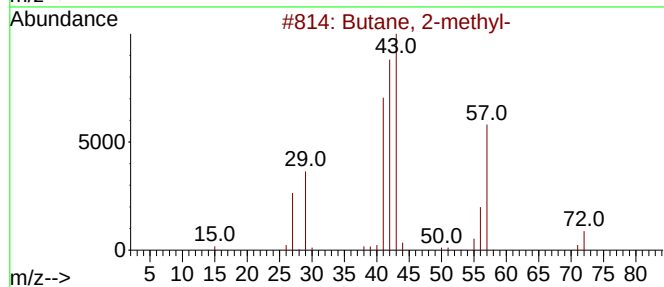
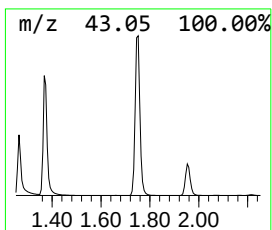
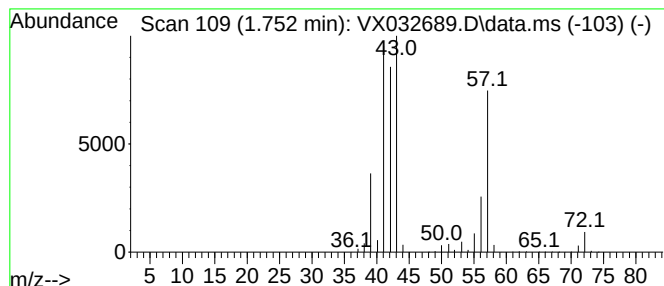
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	1272.85 ug/l	5681760	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	86
2	3-Buten-1-ol			72	C4H8O	000627-27-0	43
3	Pentane			72	C5H12	000109-66-0	28
4	Butane, 1-chloro-2-methyl-			106	C5H11Cl	000616-13-7	16
5	Propane, 2-methyl-2-nitro-			103	C4H9NO2	000594-70-7	10



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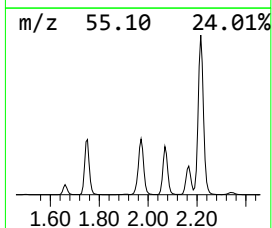
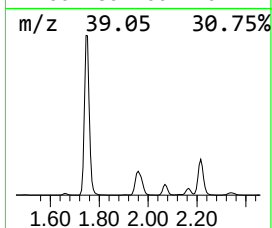
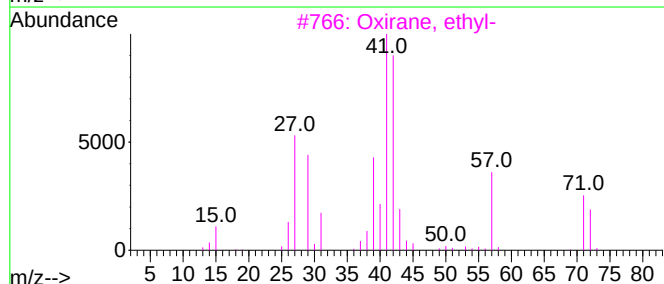
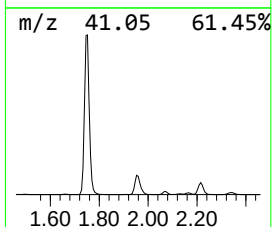
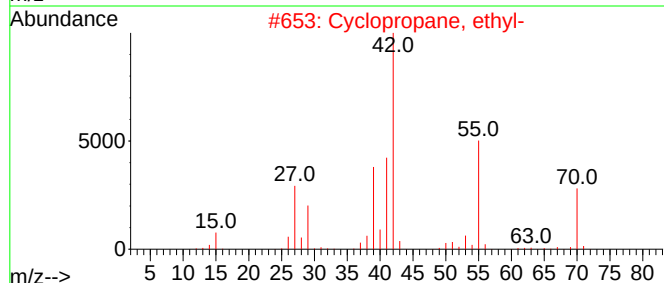
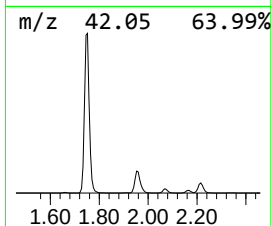
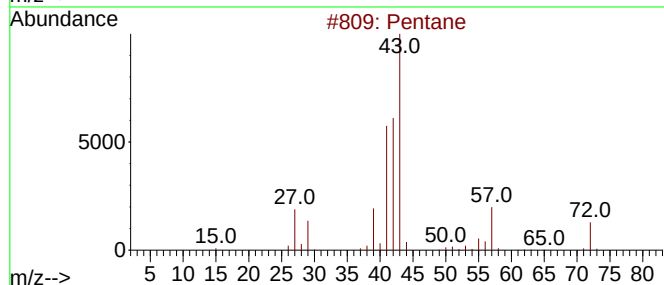
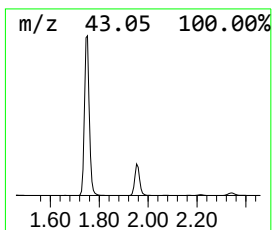
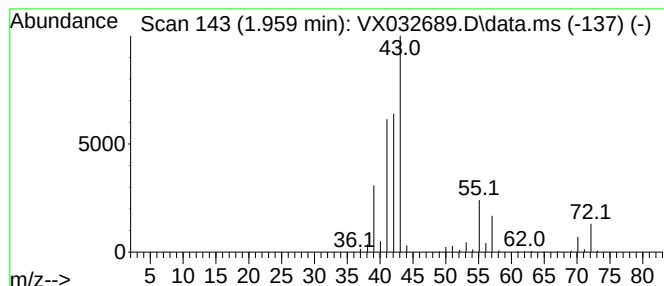
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	225.91 ug/l	1008420	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	86
2	Cyclopropane, ethyl-			70	C5H10	001191-96-4	43
3	Oxirane, ethyl-			72	C4H8O	000106-88-7	38
4	Cyclobutane, methyl-			70	C5H10	000598-61-8	38
5	Tetrahydrofuran			72	C4H8O	000109-99-9	25



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Data File : VX032689.D
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Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

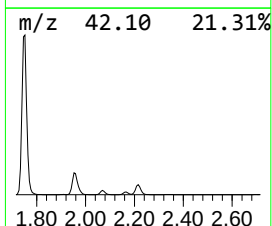
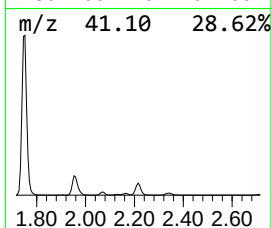
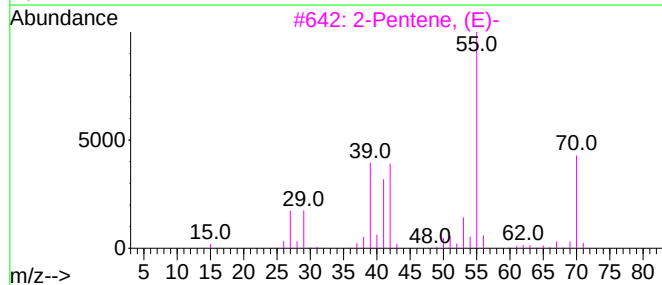
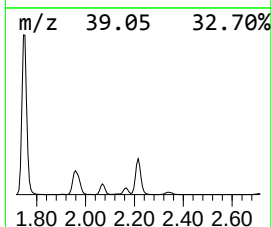
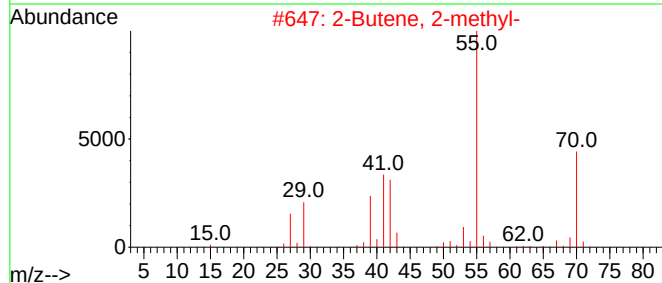
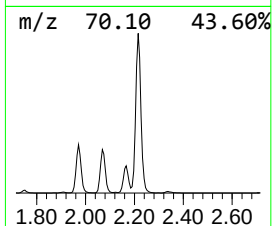
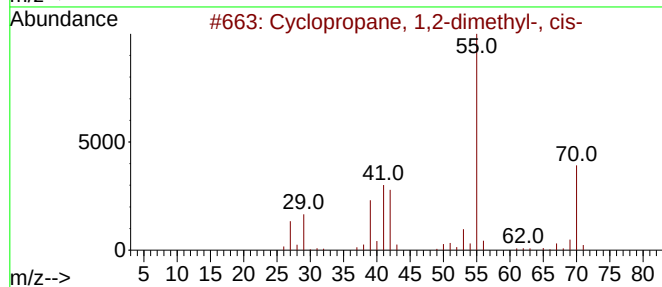
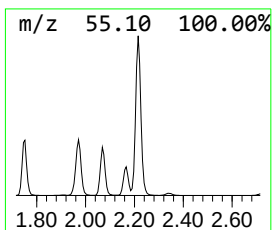
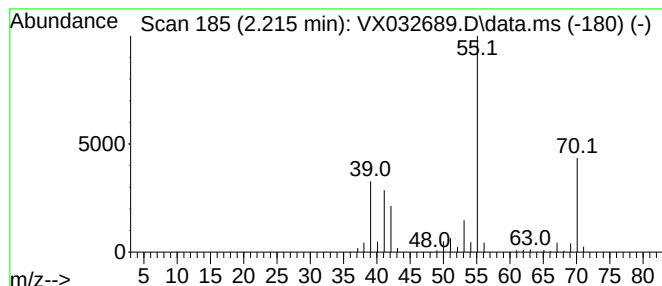
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	219.15 ug/l	978264	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			2-Pentene, (E)-	70	C5H10	000646-04-8	87
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

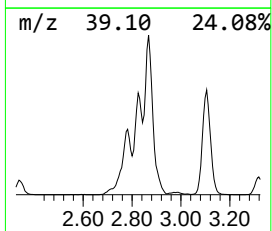
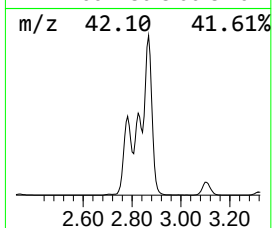
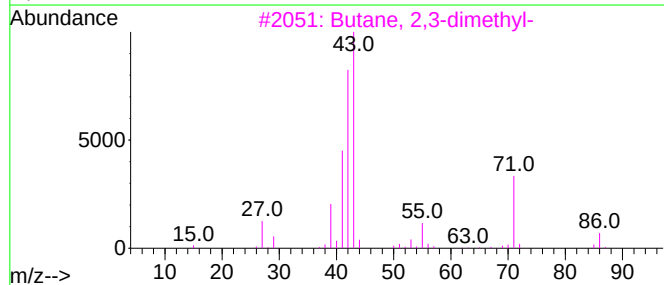
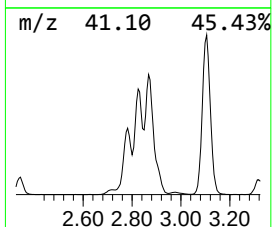
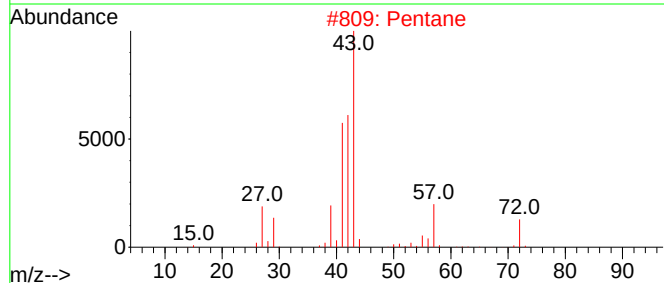
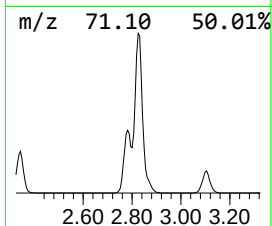
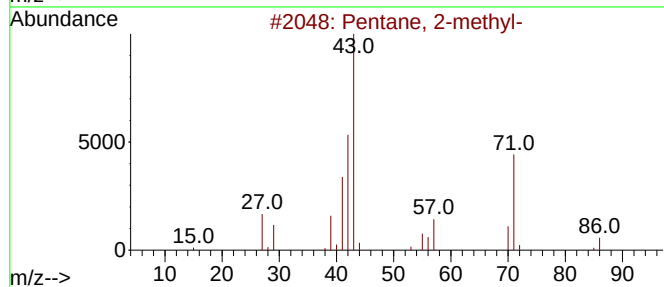
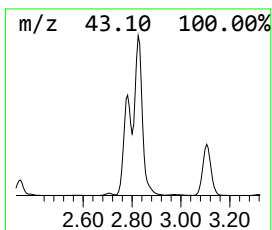
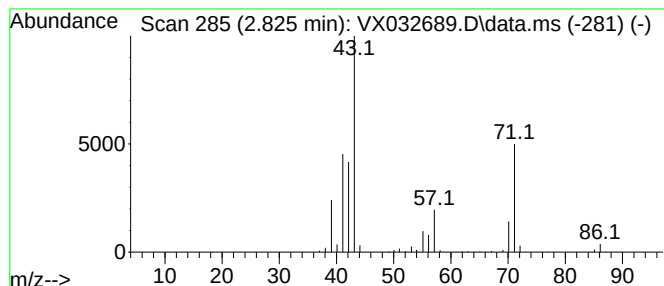
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	233.92 ug/l	1044160	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane	72	C5H12	000109-66-0	43
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	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\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

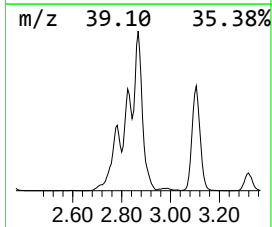
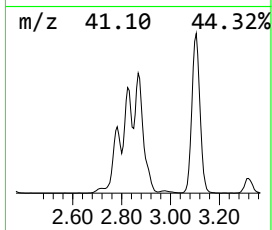
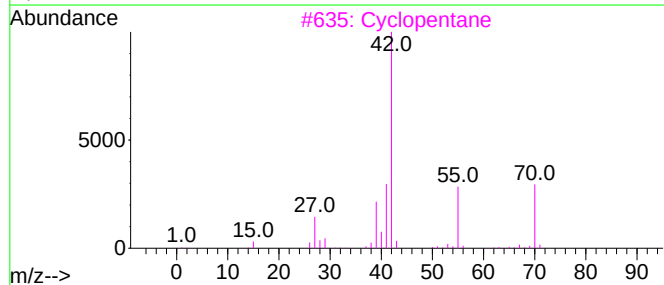
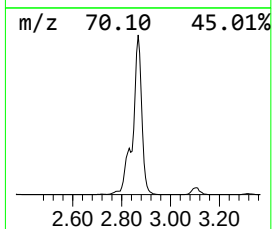
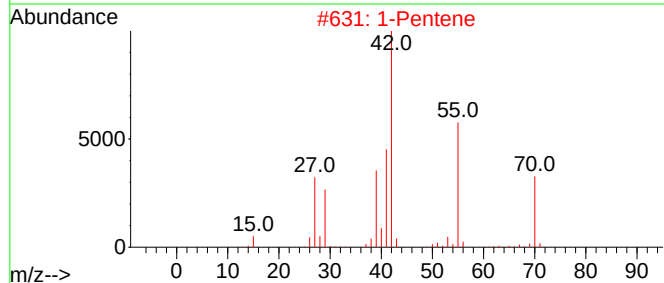
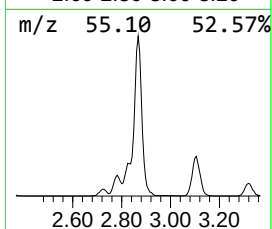
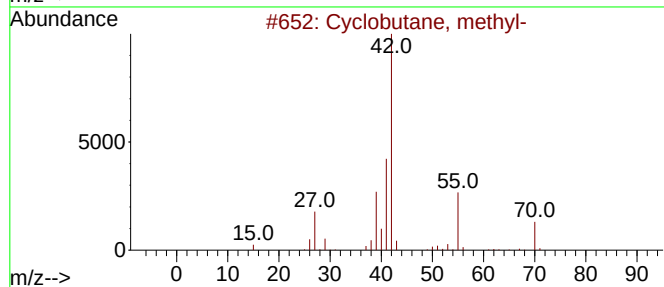
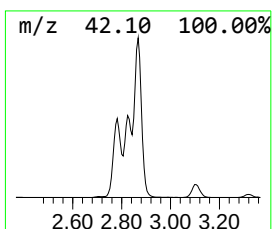
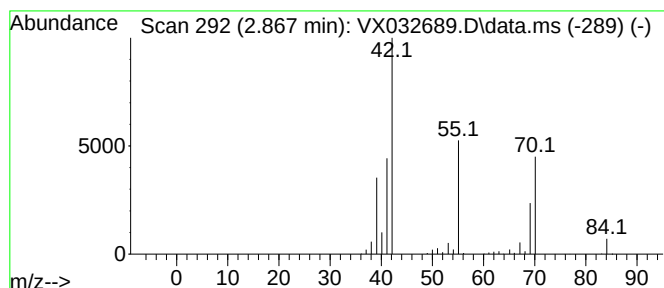
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Quant Title : SW846 8260

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

Peak Number 7 Cyclobutane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	236.67 ug/l	1056470	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2			1-Pentene	70	C5H10	000109-67-1	72
3			Cyclopentane	70	C5H10	000287-92-3	56
4			2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	40
5			2-Pentene, (E)-	70	C5H10	000646-04-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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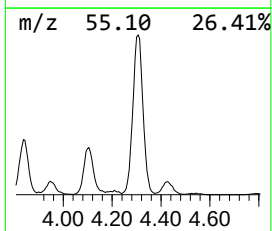
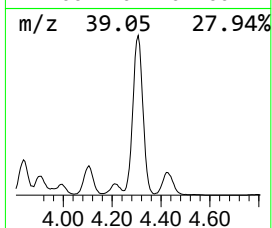
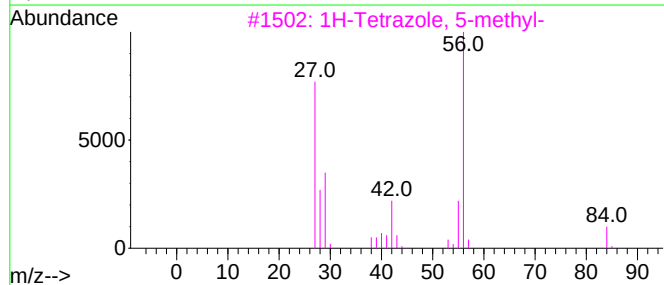
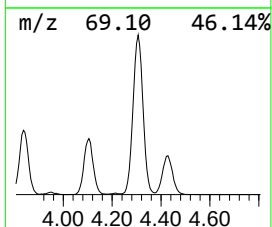
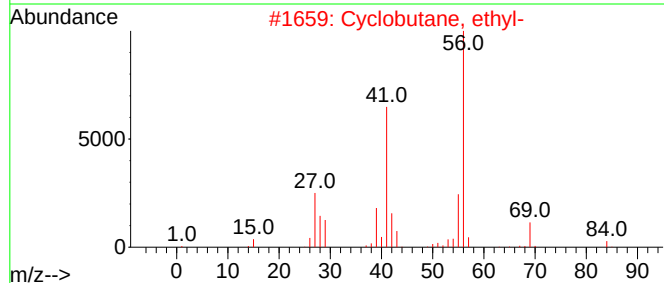
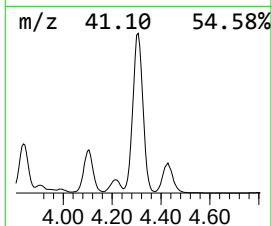
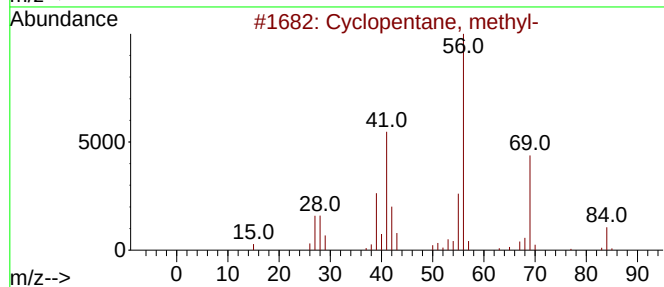
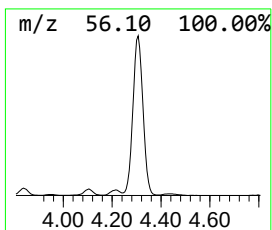
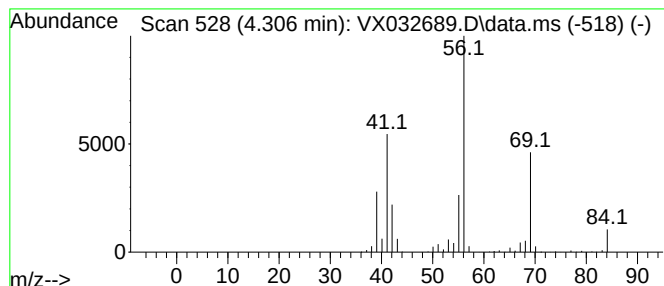
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Quant Title : SW846 8260

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	358.45 ug/l	1600070	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46
5			Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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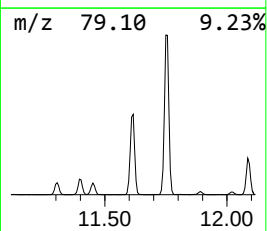
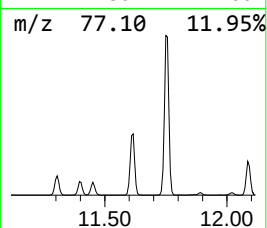
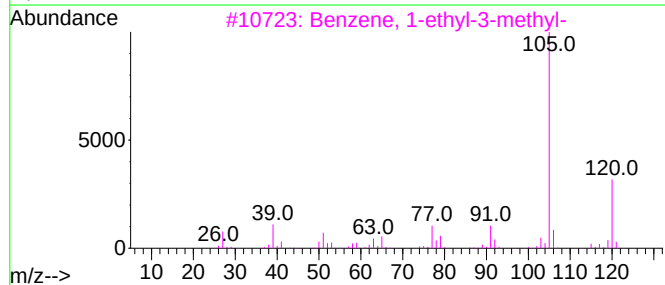
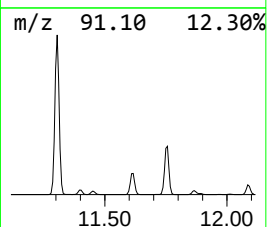
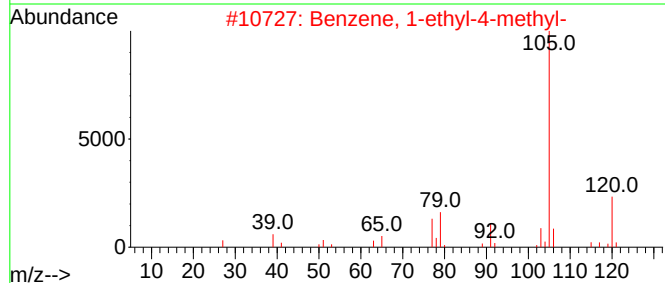
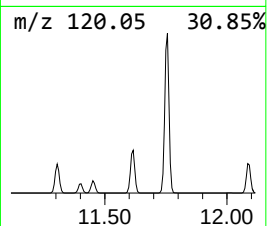
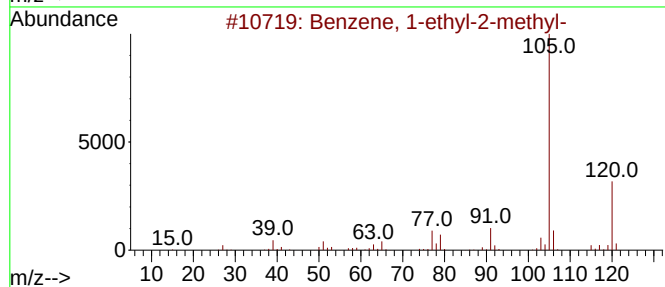
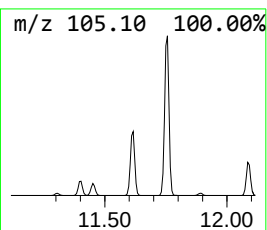
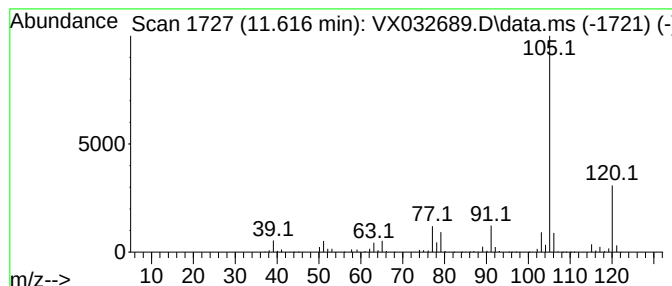
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	198.03 ug/l	2387760	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	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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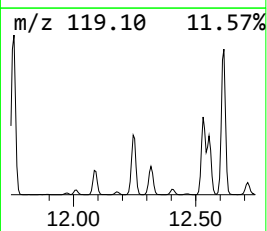
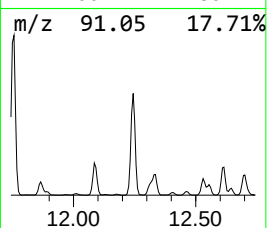
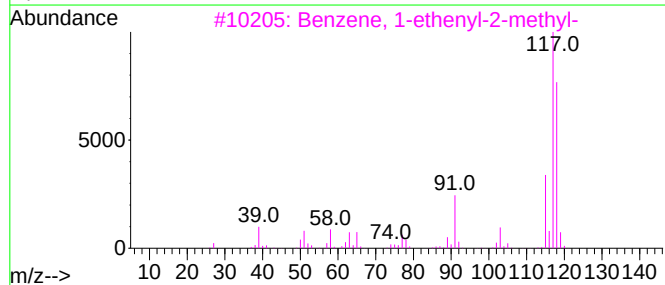
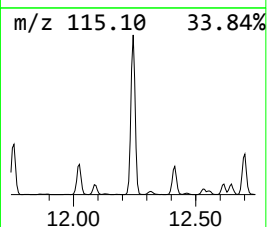
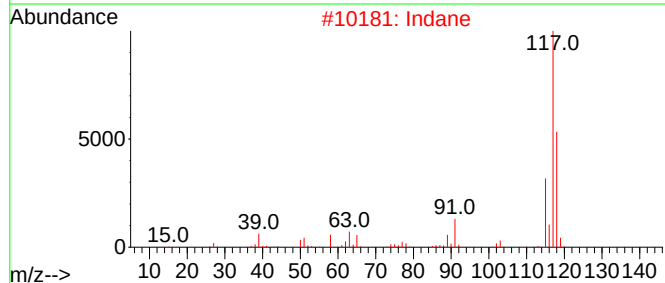
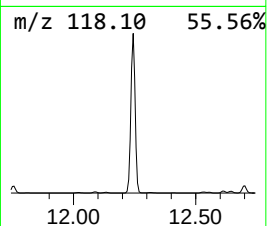
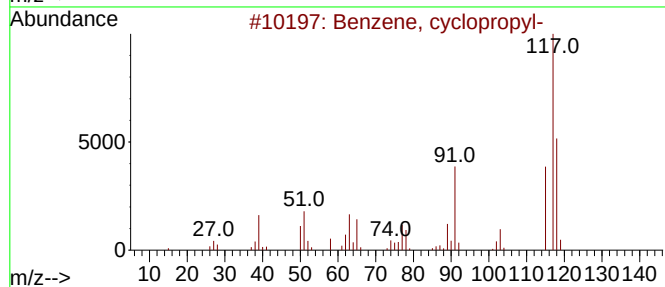
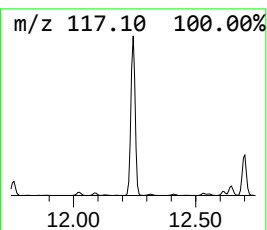
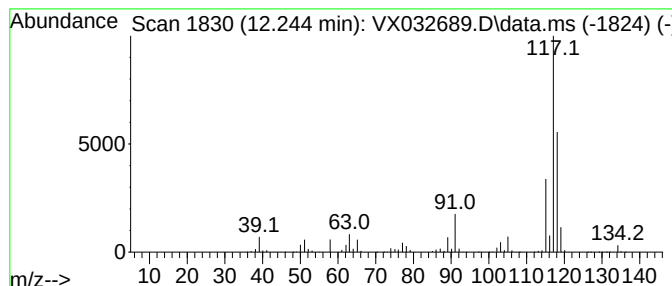
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	250.47 ug/l	3020040	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110922\
Data File : VX032689.D
Acq On : 09 Nov 2022 18:57
Operator : JC/MD
Sample : N5551-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.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	1.368	337.0	ug/l	1504280	1	5.556	223191	50.0
Butane, 2-methyl-	1.752	1272.8	ug/l	5681760	1	5.556	223191	50.0
Pentane	1.959	225.9	ug/l	1008420	1	5.556	223191	50.0
Cyclopropane, 1...	2.215	219.2	ug/l	978264	1	5.556	223191	50.0
Pentane, 2-methyl-	2.825	233.9	ug/l	1044160	1	5.556	223191	50.0
Cyclobutane, me...	2.867	236.7	ug/l	1056470	1	5.556	223191	50.0
Cyclopentane, m...	4.306	358.4	ug/l	1600070	1	5.556	223191	50.0
Benzene, 1-ethy...	11.616	198.0	ug/l	2387760	4	12.024	602887	50.0
Benzene, cyclop...	12.244	250.5	ug/l	3020040	4	12.024	602887	50.0