

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
 Data File : VX032728.D
 Acq On : 10 Nov 2022 15:10
 Operator : JC/MD
 Sample : N5551-15 40X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-21

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: VX032728.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	34	rBV	23023	21443	2.79%	0.287%
2	1.368	41	46	53	rVB	63002	64292	8.37%	0.859%
3	1.660	88	94	101	rVB2	5851	10425	1.36%	0.139%
4	1.746	103	108	120	rVB	89868	120750	15.72%	1.614%
5	1.965	137	144	154	rVB3	72958	139375	18.15%	1.863%
6	2.069	156	161	168	rVV	40319	55430	7.22%	0.741%
7	2.166	171	177	180	rVV	24364	37614	4.90%	0.503%
8	2.215	180	185	195	rVB	186112	279333	36.37%	3.733%
9	2.751	261	273	281	rBV2	25022	61854	8.05%	0.827%
10	2.825	281	285	287	rVV2	8709	15273	1.99%	0.204%
11	2.867	287	292	301	rVB3	36495	79943	10.41%	1.068%
12	3.099	323	330	339	rVB	8984	20202	2.63%	0.270%
13	3.318	358	366	377	rBV2	7795	17355	2.26%	0.232%
14	3.446	380	387	395	rVV2	4284	9204	1.20%	0.123%
15	3.581	401	409	417	rBV3	3902	9347	1.22%	0.125%
16	3.727	426	433	443	rVB2	23232	55234	7.19%	0.738%
17	3.837	443	451	458	rVV2	13070	33632	4.38%	0.449%
18	3.904	458	462	471	rVV3	8131	20725	2.70%	0.277%
19	3.989	471	476	486	rVV3	3876	9558	1.24%	0.128%
20	4.099	486	494	508	rVB2	18047	47622	6.20%	0.636%
21	4.306	517	528	539	rBV2	37011	106893	13.92%	1.429%
22	4.428	539	548	560	rVB2	6569	17616	2.29%	0.235%
23	5.196	662	674	692	rVB3	27329	85777	11.17%	1.146%
24	5.385	692	705	714	rBV2	70434	208717	27.18%	2.789%
25	5.470	715	719	724	rVV3	11042	28679	3.73%	0.383%
26	5.556	724	733	748	rVB	117616	337127	43.90%	4.506%
27	5.958	789	799	806	rBV2	79940	206610	26.90%	2.761%
28	6.037	806	812	825	rVB2	33982	93170	12.13%	1.245%
29	6.202	825	839	845	rBV4	8322	26867	3.50%	0.359%
30	6.763	921	931	943	rBV	184173	456301	59.42%	6.098%
31	6.854	943	946	956	rVB4	9015	19989	2.60%	0.267%
32	7.171	987	998	1008	rVB4	8011	16747	2.18%	0.224%
33	7.379	1022	1032	1041	rBV6	9717	25309	3.30%	0.338%
34	7.885	1103	1115	1124	rVB6	2639	8355	1.09%	0.112%
35	8.147	1153	1158	1162	rVV	11600	19655	2.56%	0.263%
36	8.507	1210	1217	1226	rVB	8727	14166	1.84%	0.189%

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37	8.653	1234	1241	1247	rBV	380240	601560	78.34%	8.040%
38	8.720	1247	1252	1261	rVB	79410	119335	15.54%	1.595%
39	8.958	1280	1291	1299	rBV2	15548	25944	3.38%	0.347%
40	9.049	1299	1306	1312	rBV	16649	26401	3.44%	0.353%
41	10.055	1465	1471	1486	rVB	387122	509906	66.40%	6.815%
42	10.195	1488	1494	1503	rVV	602587	767926	100.00%	10.263%
43	10.299	1505	1511	1521	rVB	328024	445934	58.07%	5.960%
44	10.640	1562	1567	1575	rBV	79853	104966	13.67%	1.403%
45	10.963	1615	1620	1626	rBV	31593	38362	5.00%	0.513%
46	11.079	1634	1639	1652	rBV	353606	452646	58.94%	6.049%
47	11.305	1671	1676	1682	rBV	79440	95251	12.40%	1.273%
48	11.402	1684	1692	1696	rVV	17912	31101	4.05%	0.416%
49	11.451	1696	1700	1709	rVB	17555	21547	2.81%	0.288%
50	11.616	1721	1727	1736	rBV	74994	94069	12.25%	1.257%
51	11.756	1744	1750	1757	rBV	81814	103004	13.41%	1.377%
52	12.024	1788	1794	1800	rBV	392750	485639	63.24%	6.490%
53	12.085	1800	1804	1810	rVB	138234	172400	22.45%	2.304%
54	12.244	1824	1830	1837	rBV	149971	186256	24.25%	2.489%
55	12.317	1837	1842	1850	rVB3	7951	14883	1.94%	0.199%
56	12.414	1852	1858	1862	rBV3	6970	9769	1.27%	0.131%
57	12.463	1862	1866	1870	rVB	7705	8199	1.07%	0.110%
58	12.616	1886	1891	1894	rBV	29754	35927	4.68%	0.480%
59	12.701	1900	1905	1911	rVB2	23307	31355	4.08%	0.419%
60	12.847	1925	1929	1934	rVB	6259	7859	1.02%	0.105%
61	12.920	1936	1941	1945	rVV	16408	19946	2.60%	0.267%
62	13.170	1978	1982	1988	rVB	22145	26608	3.46%	0.356%
63	13.292	1997	2002	2007	rBV2	44647	57018	7.42%	0.762%
64	13.426	2020	2024	2028	rVB2	6139	7860	1.02%	0.105%
65	13.774	2076	2081	2090	rBV	139175	174937	22.78%	2.338%
66	14.640	2219	2223	2228	rBV	12628	15621	2.03%	0.209%
67	14.780	2241	2246	2251	rVB2	7841	9700	1.26%	0.130%

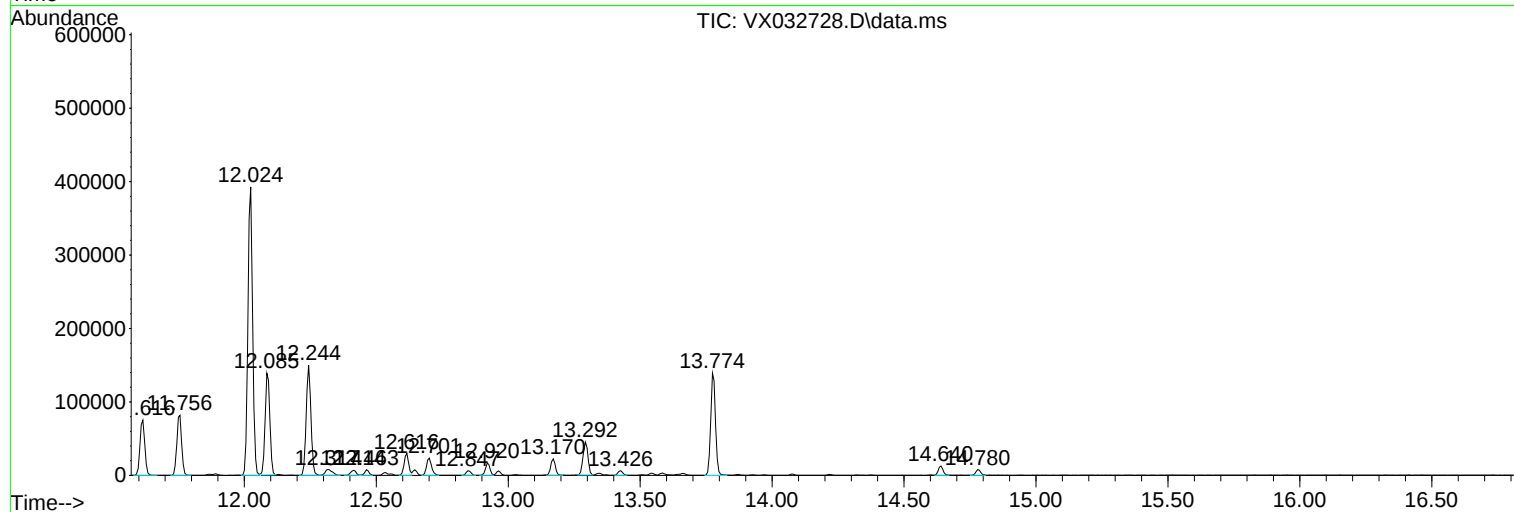
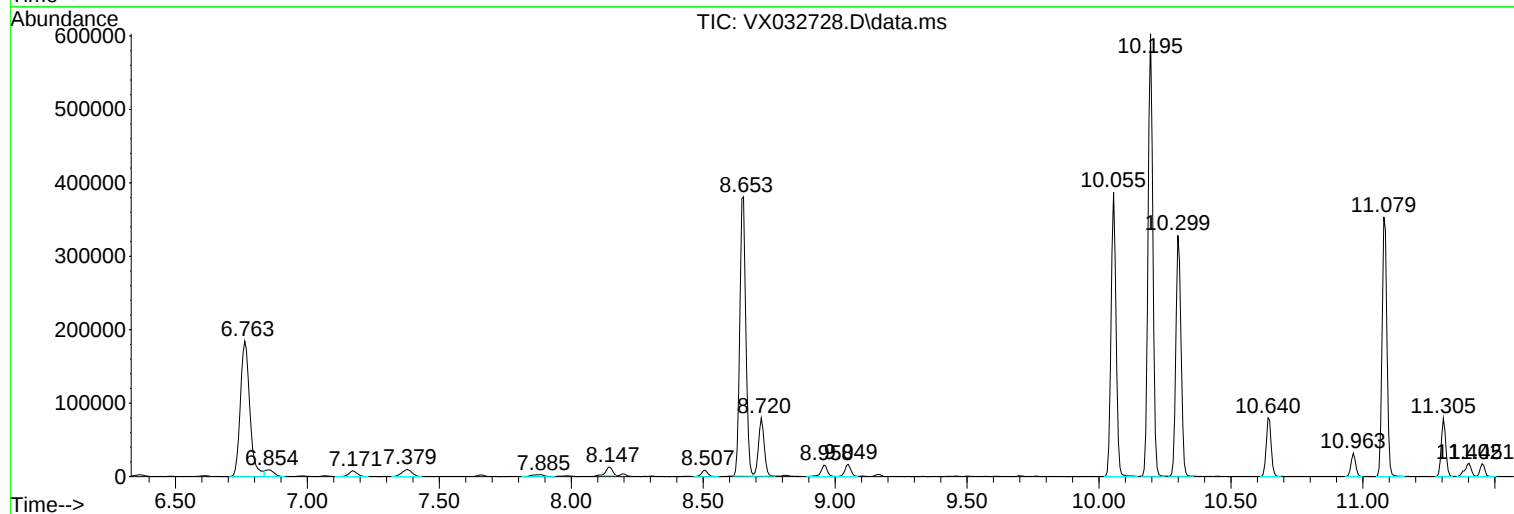
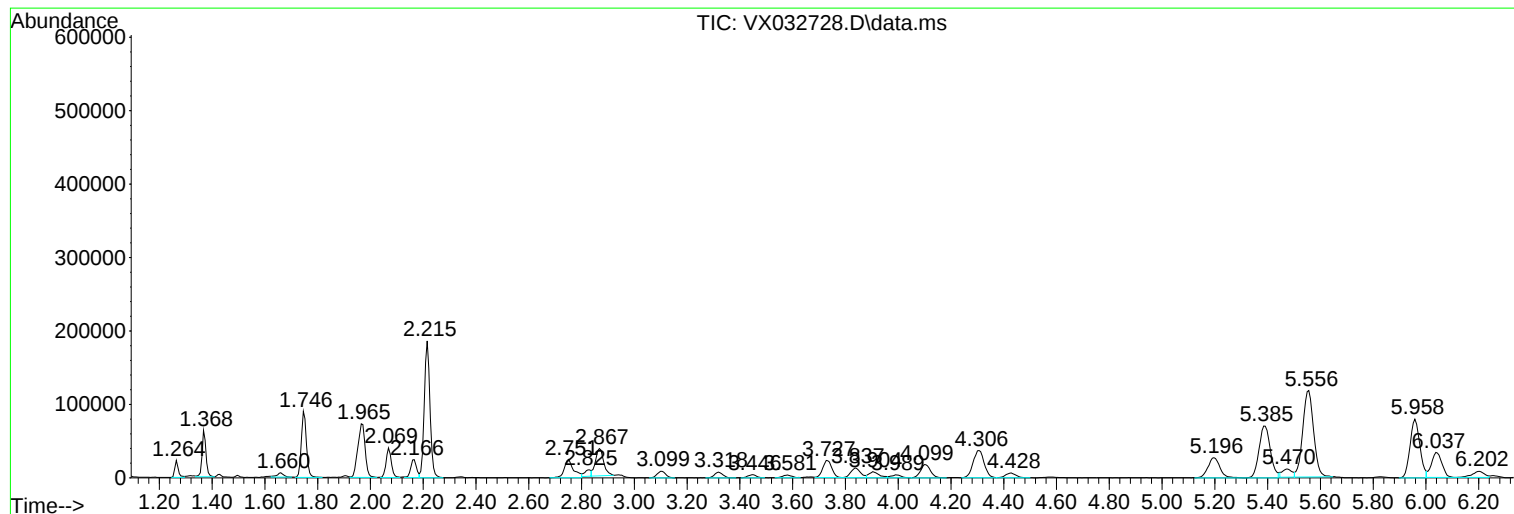
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ClientSampleId :
MW-21

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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Instrument :
MSVOA_X
ClientSampleId :
MW-21

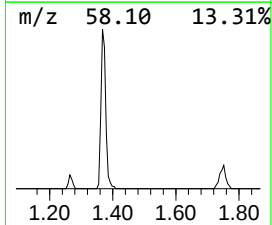
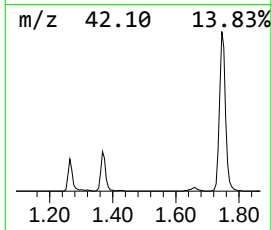
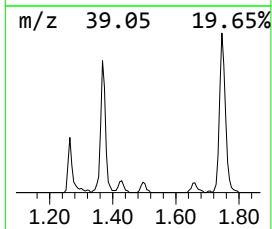
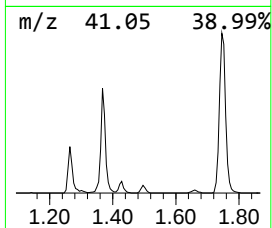
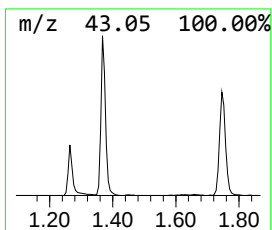
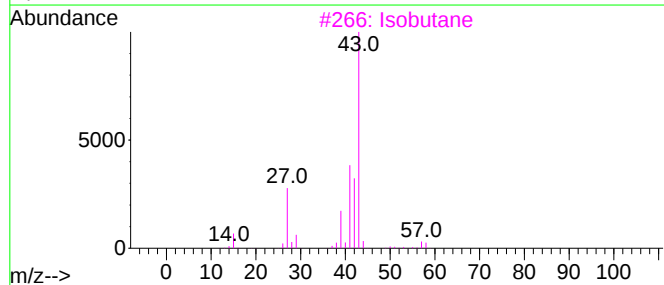
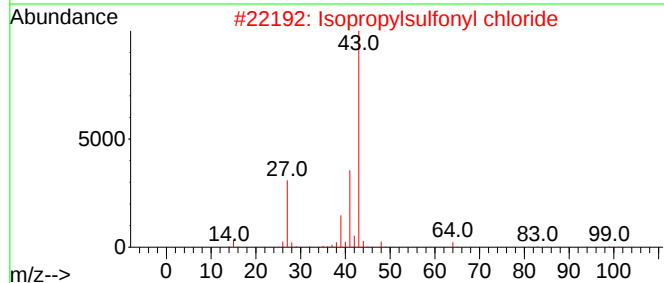
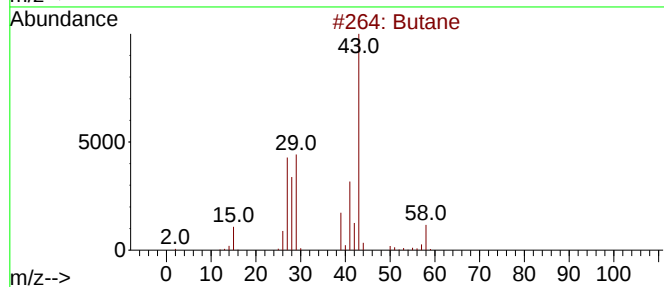
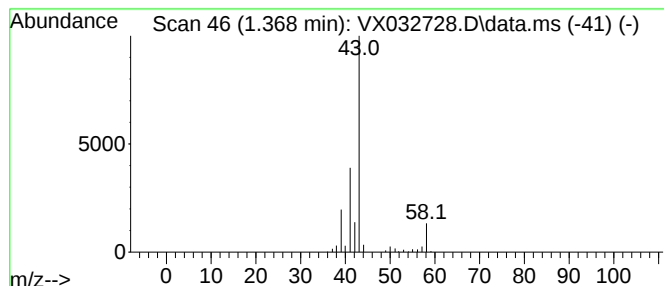
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	9.54 ug/l	64292	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane	58	C4H10	000106-97-8	72
2		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3		Isobutane	58	C4H10	000075-28-5	9
4		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5		Diazene, dimethyl-	58	C2H6N2	000503-28-6	5



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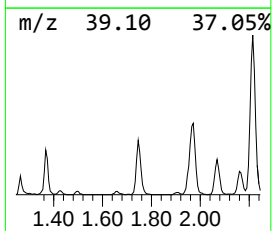
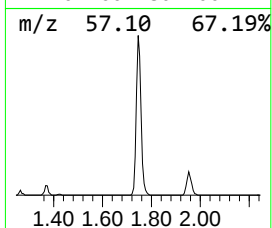
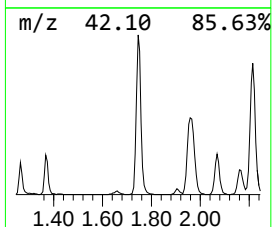
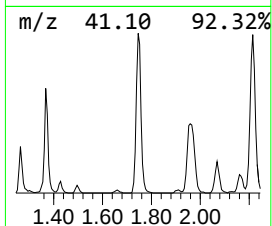
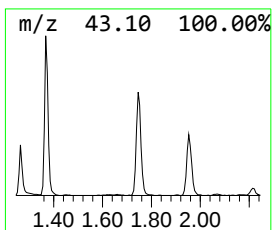
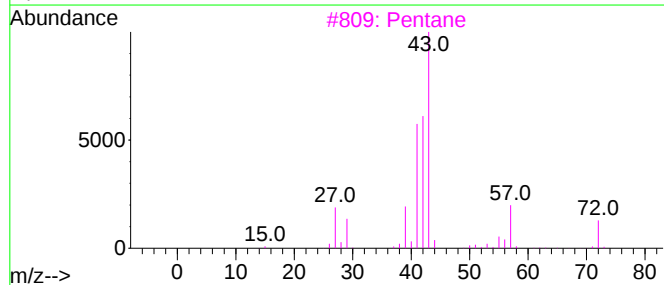
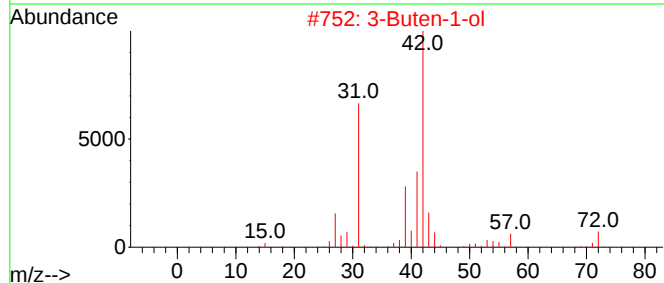
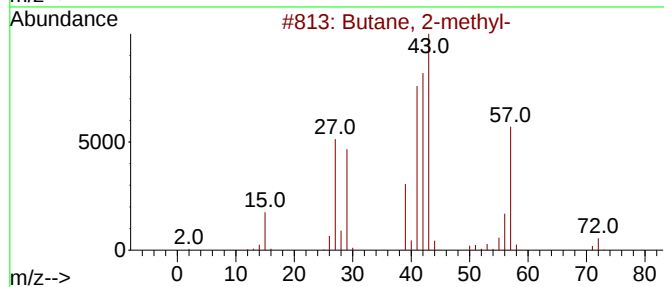
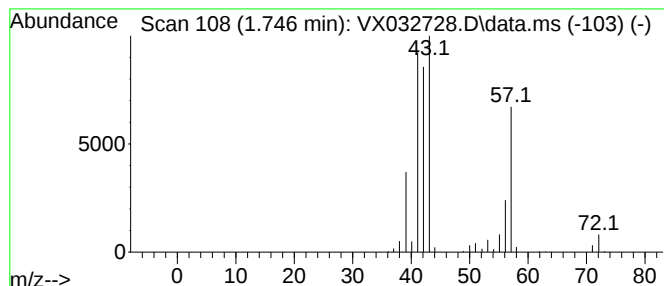
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	17.91 ug/l	120750	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	80
2	3-Buten-1-ol			72	C4H8O	000627-27-0	47
3	Pentane			72	C5H12	000109-66-0	36
4	2(3H)-Furanone, dihydro-4-methyl-			100	C5H8O2	001679-49-8	28
5	1-Butene			56	C4H8	000106-98-9	10



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ALS Vial : 12 Sample Multiplier: 1

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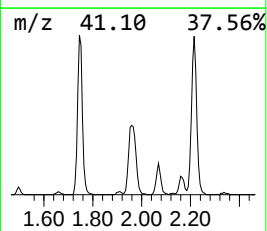
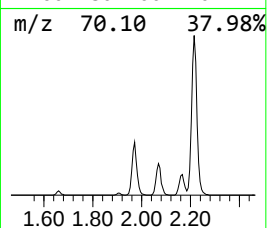
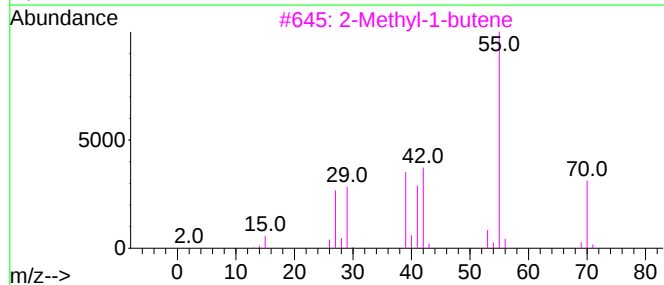
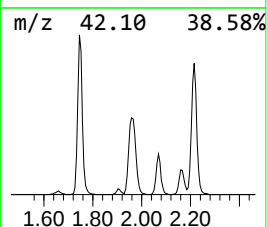
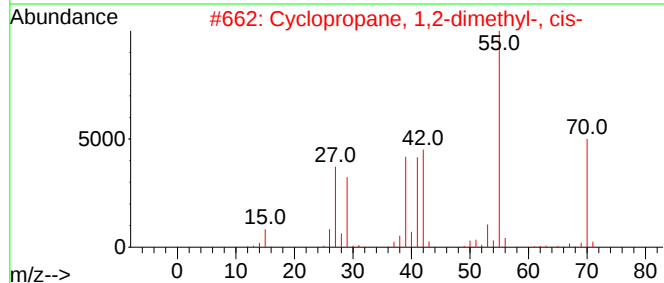
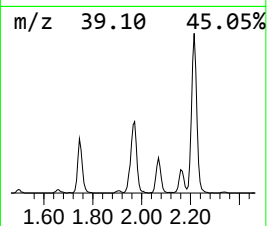
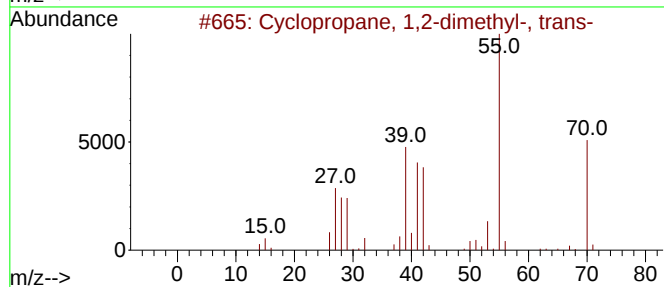
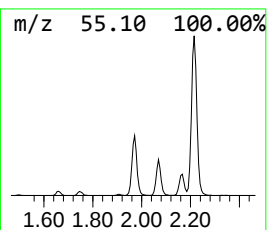
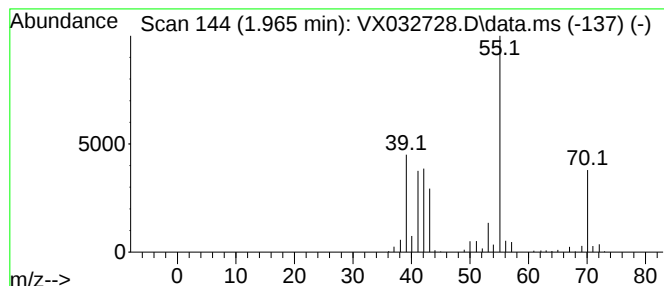
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	20.67 ug/l	139375	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
3			2-Methyl-1-butene	70	C5H10	000563-46-2	86
4			2-Pentene, (E)-	70	C5H10	000646-04-8	86
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	86



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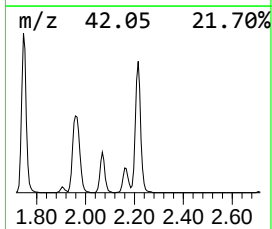
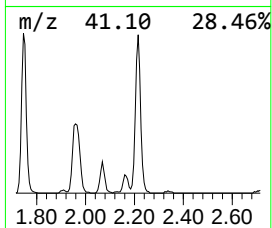
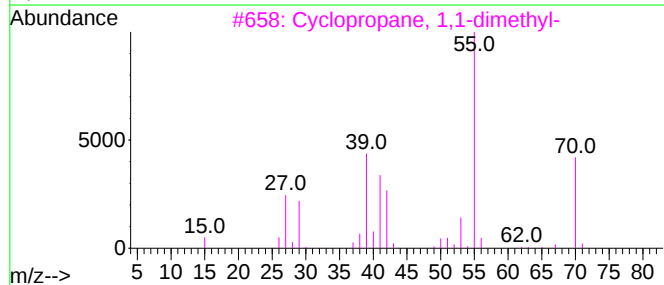
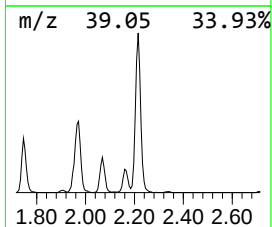
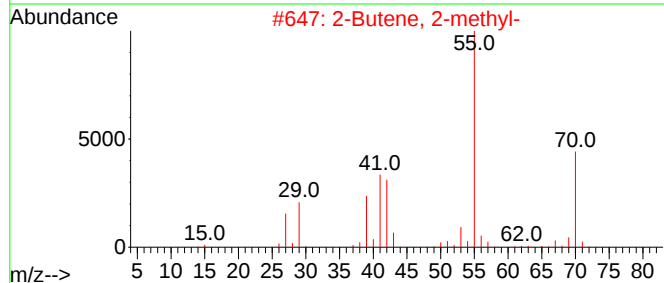
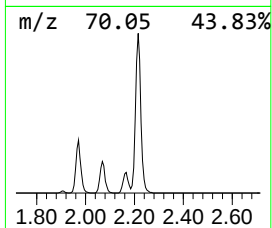
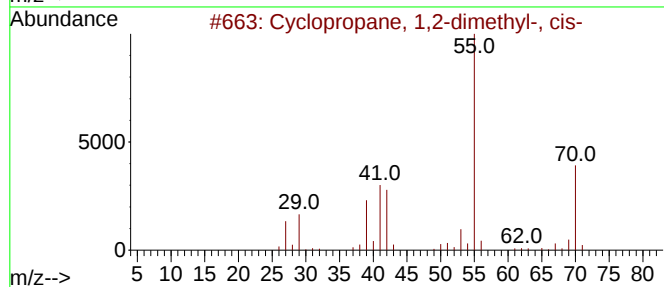
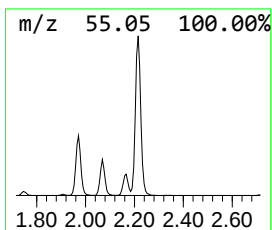
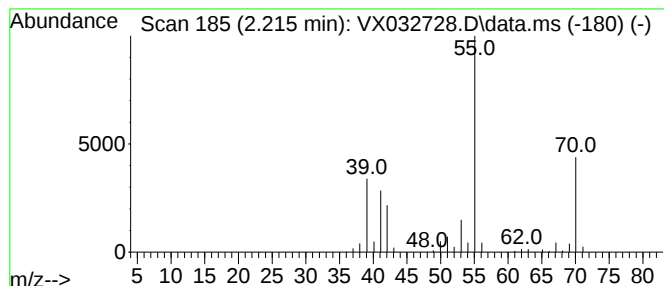
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	41.43 ug/l	279333	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			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

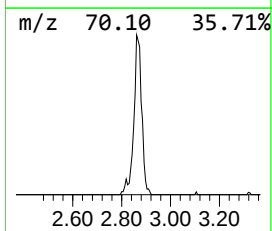
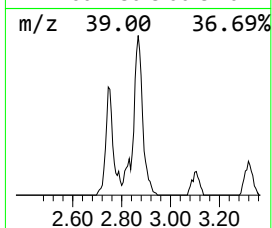
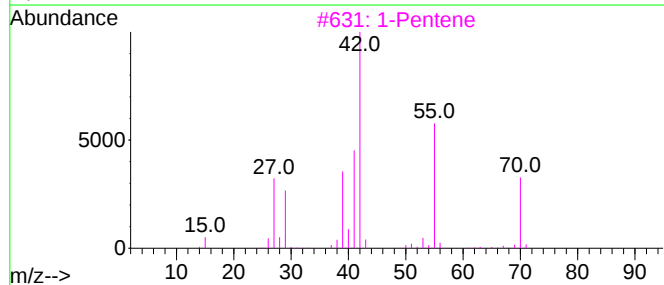
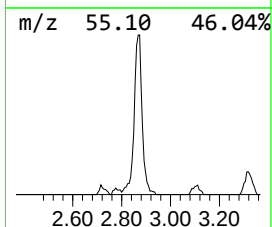
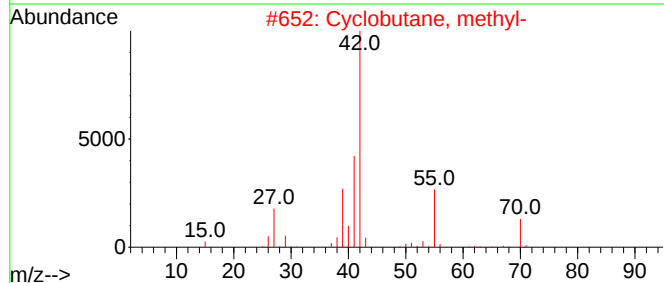
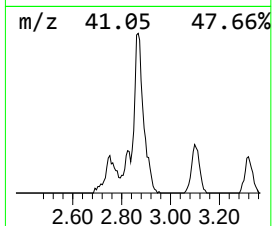
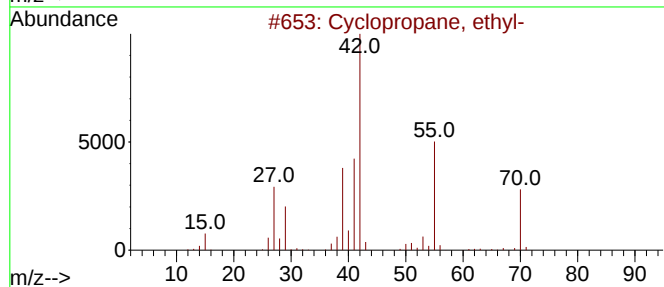
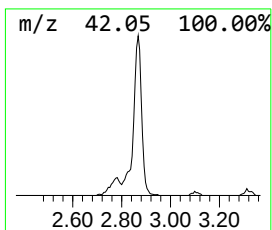
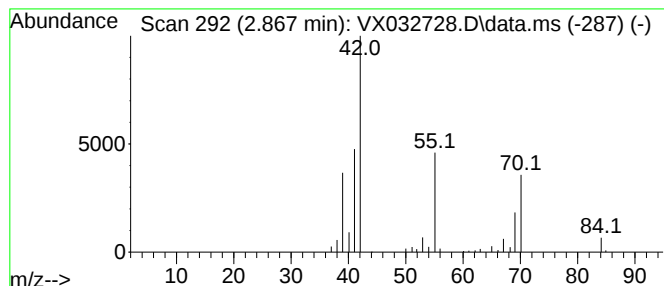
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	11.86 ug/l	79943	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	80
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3			1-Pentene	70	C5H10	000109-67-1	64
4			Cyclopentane	70	C5H10	000287-92-3	50
5			2-Butene-1,4-diol, (Z)-	88	C4H8O2	006117-80-2	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

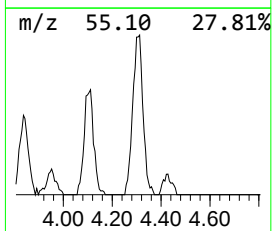
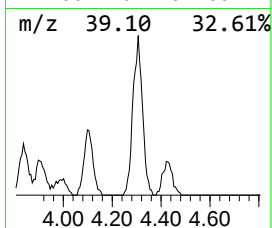
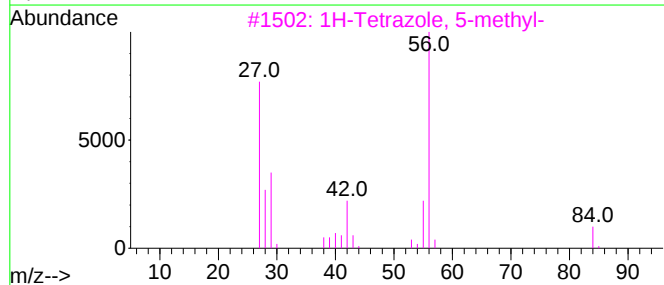
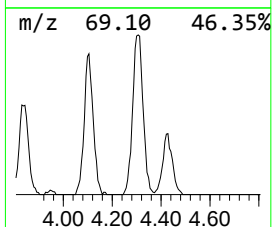
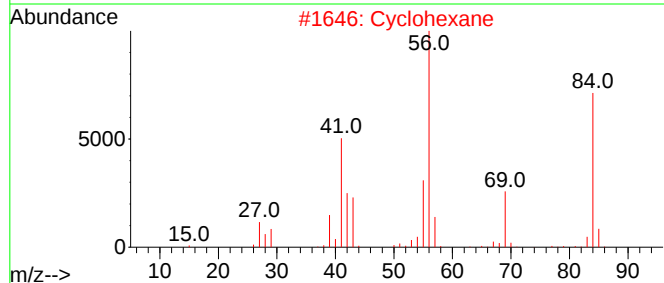
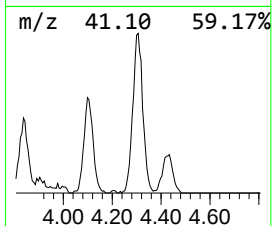
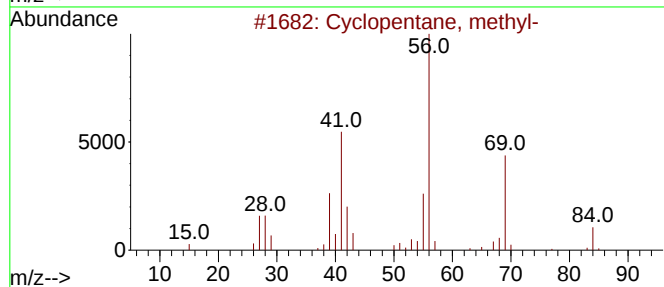
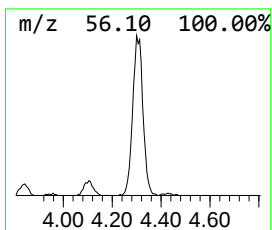
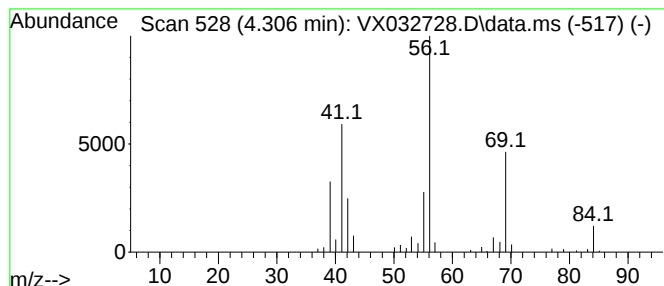
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	15.85 ug/l	106893	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			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

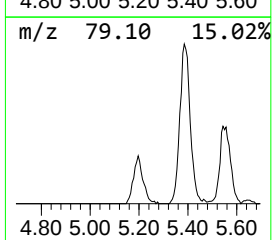
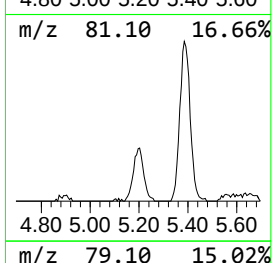
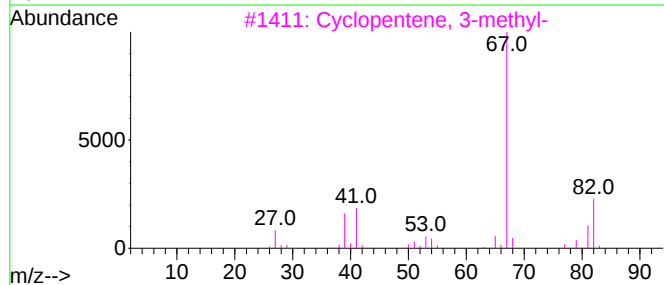
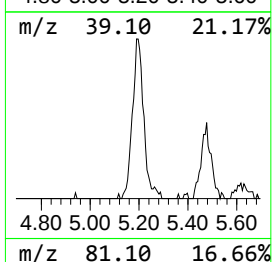
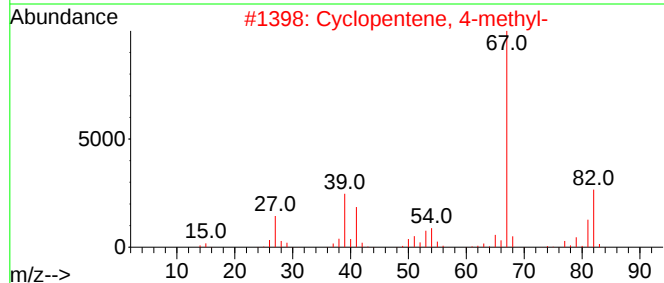
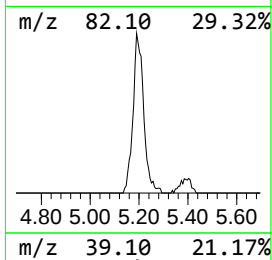
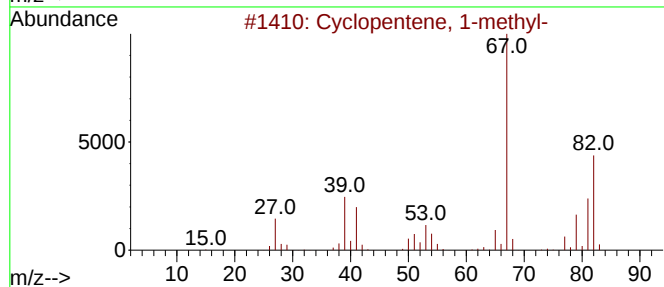
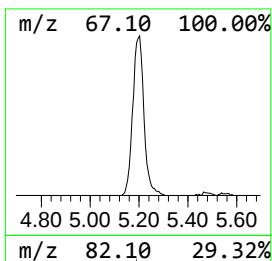
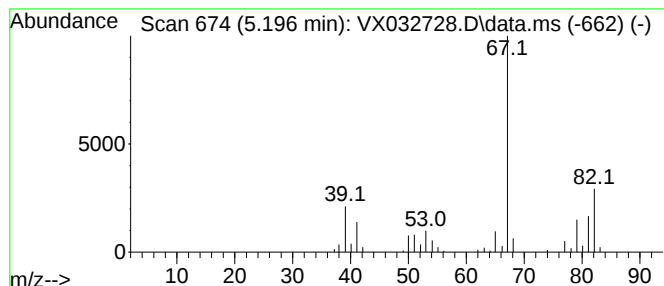
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.196	12.72 ug/l	85777	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	90
2			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	86
3			Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4			1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	86
5			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

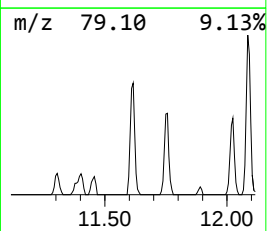
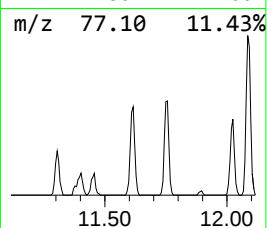
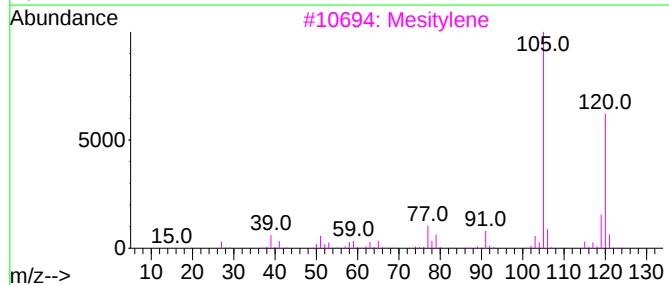
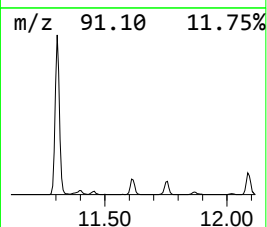
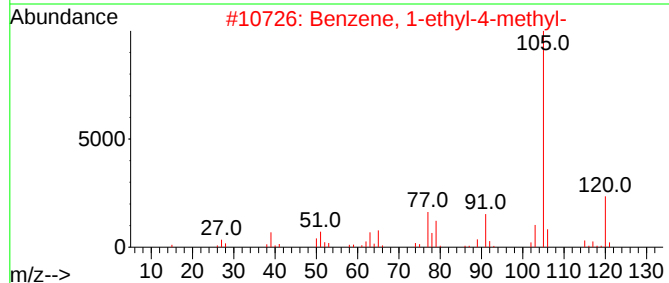
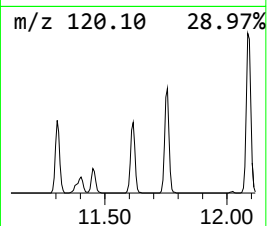
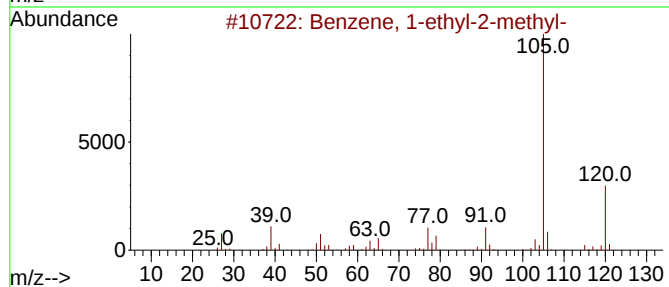
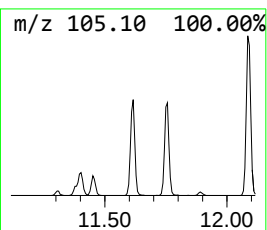
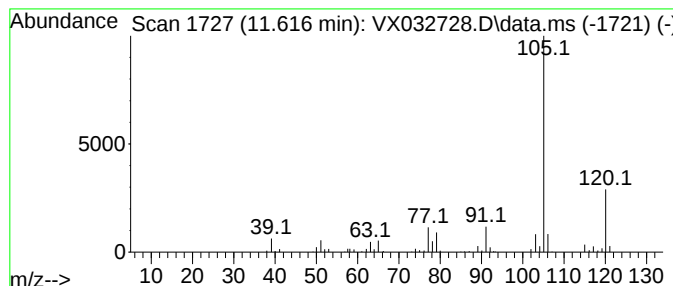
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	9.69 ug/l	94069	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	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

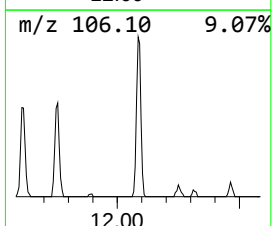
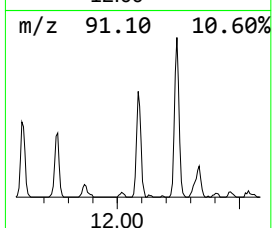
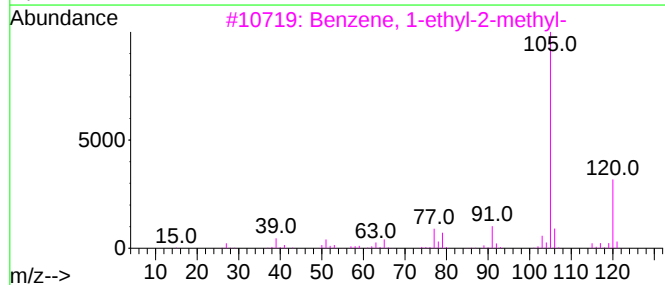
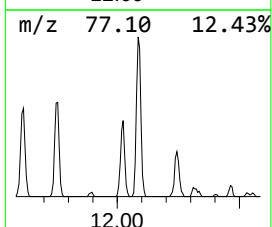
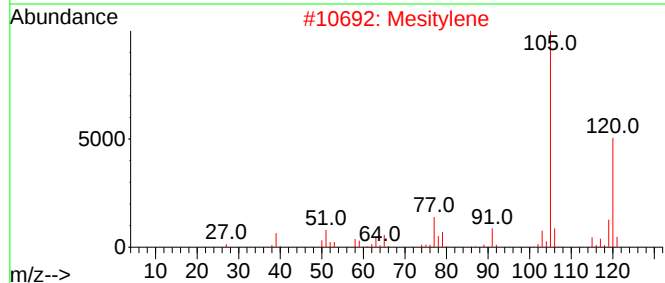
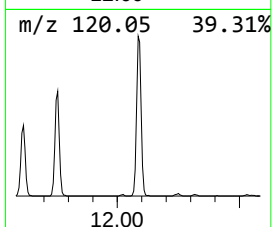
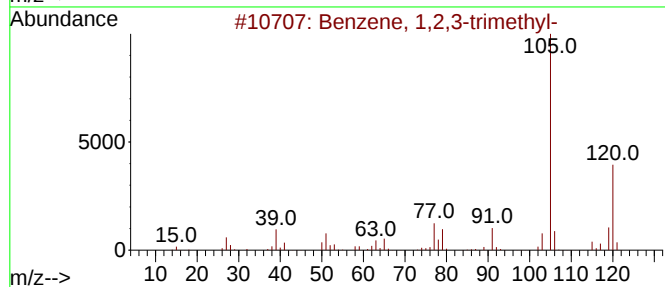
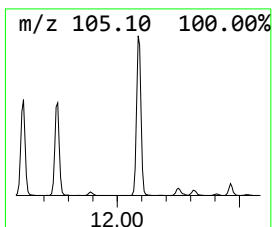
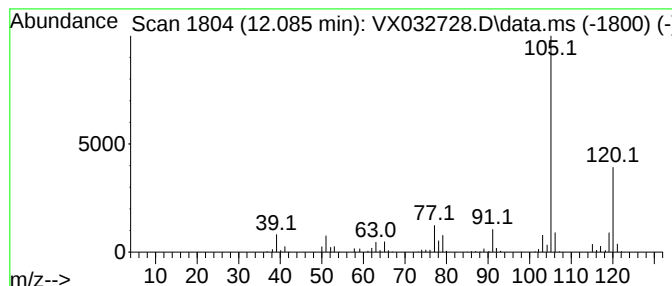
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	17.75 ug/l	172400	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	97
2			Mesitylene	120	C9H12	000108-67-8	95
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

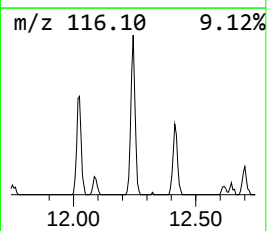
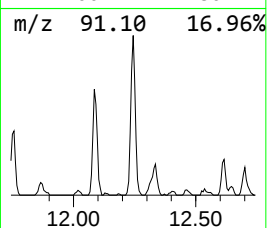
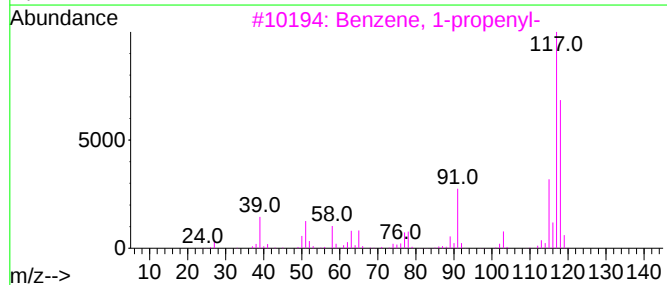
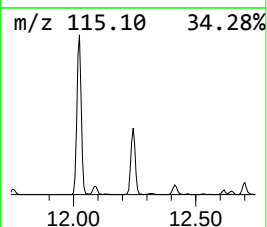
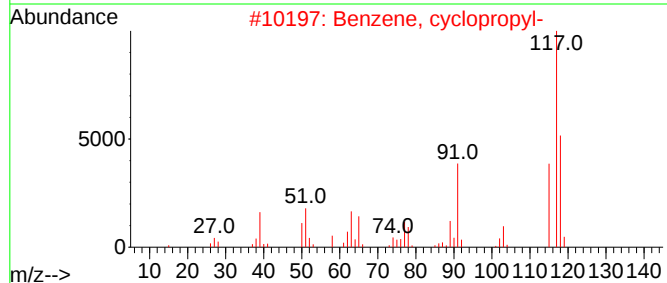
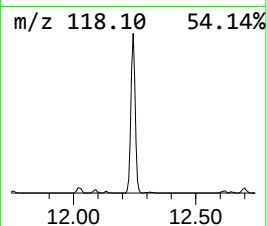
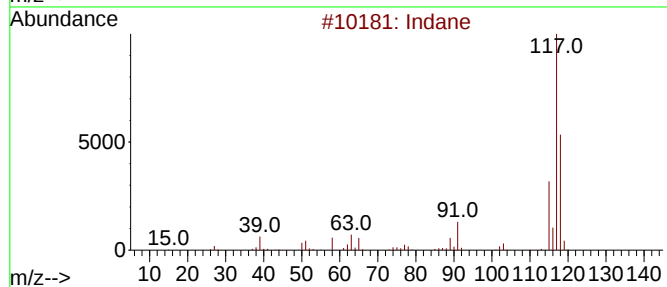
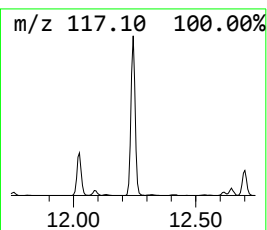
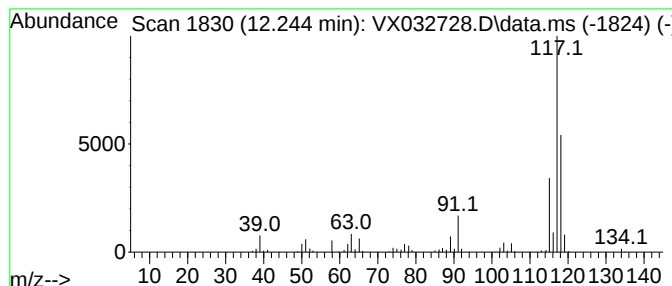
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	19.18 ug/l	186256	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111022\
Data File : VX032728.D
Acq On : 10 Nov 2022 15:10
Operator : JC/MD
Sample : N5551-15 40X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-21

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, 2-methyl-	1.746	17.9	ug/l	120750	1	5.556	337127	50.0
Cyclopropane, 1...	1.965	20.7	ug/l	139375	1	5.556	337127	50.0
Cyclopropane, 1...	2.215	41.4	ug/l	279333	1	5.556	337127	50.0
Cyclopropane, e...	2.867	11.9	ug/l	79943	1	5.556	337127	50.0
Cyclopentane, m...	4.306	15.9	ug/l	106893	1	5.556	337127	50.0
Cyclopentene, 1...	5.196	12.7	ug/l	85777	1	5.556	337127	50.0
Benzene, 1-ethy...	11.616	9.7	ug/l	94069	4	12.024	485639	50.0
Benzene, 1,2,3-...	12.085	17.8	ug/l	172400	4	12.024	485639	50.0
Indane	12.244	19.2	ug/l	186256	4	12.024	485639	50.0