

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120224\
 Data File : VX044062.D
 Acq On : 02 Dec 2024 13:44
 Operator : JC/MD
 Sample : P5021-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-13

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Title : SW846 8260

Signal : TIC: VX044062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	27	rBV	12524	13508	1.65%	0.211%
2	1.374	42	47	52	rVB	19385	21471	2.62%	0.336%
3	1.453	56	60	65	rVB	47842	54315	6.63%	0.850%
4	1.502	65	68	71	rBV2	5684	8981	1.10%	0.140%
5	1.581	71	81	82	rBV3	10680	22533	2.75%	0.352%
6	1.721	99	104	114	rVB	73270	107296	13.10%	1.678%
7	1.941	135	140	146	rVB	22654	33557	4.10%	0.525%
8	2.380	208	212	220	rVB	6539	11309	1.38%	0.177%
9	2.770	268	276	280	rBV5	7222	17245	2.11%	0.270%
10	2.819	280	284	288	rVV	13517	27210	3.32%	0.426%
11	2.855	288	290	299	rVB3	6452	10424	1.27%	0.163%
12	3.105	321	331	340	rBV4	18388	52674	6.43%	0.824%
13	3.434	378	385	394	rBV2	7477	16746	2.04%	0.262%
14	4.294	515	526	539	rVB3	16972	49611	6.06%	0.776%
15	5.379	692	704	714	rBV2	95179	284951	34.80%	4.457%
16	5.544	721	731	748	rVB	147768	424897	51.88%	6.646%
17	5.946	788	797	804	rBV	113601	303518	37.06%	4.748%
18	6.031	804	811	825	rVB	87955	241060	29.44%	3.771%
19	6.348	854	863	866	rBV9	2903	8389	1.02%	0.131%
20	6.757	921	930	941	rBV	243332	600787	73.36%	9.397%
21	7.373	1023	1031	1043	rVB4	10265	26527	3.24%	0.415%
22	8.647	1233	1240	1248	rBV	516258	818933	100.00%	12.810%
23	8.720	1249	1252	1256	rVB2	6519	9910	1.21%	0.155%
24	9.043	1298	1305	1310	rBV5	3761	8641	1.06%	0.135%
25	10.049	1465	1470	1486	rBV	500878	720740	88.01%	11.274%
26	10.189	1488	1493	1507	rVV	251754	359339	43.88%	5.621%
27	10.299	1507	1511	1521	rVB	44676	66801	8.16%	1.045%
28	10.640	1560	1567	1574	rBV	61485	83268	10.17%	1.302%
29	10.957	1614	1619	1626	rBV	19811	29406	3.59%	0.460%
30	11.079	1634	1639	1653	rBV	410996	535320	65.37%	8.373%
31	11.305	1671	1676	1683	rBV	28427	39353	4.81%	0.616%
32	11.378	1683	1688	1696	rBV	75891	132549	16.19%	2.073%
33	11.610	1721	1726	1736	rVB	119147	152548	18.63%	2.386%
34	11.750	1745	1749	1755	rVB	20277	25522	3.12%	0.399%
35	12.018	1788	1793	1800	rVV	509921	631878	77.16%	9.884%
36	12.085	1800	1804	1809	rVB	39704	51816	6.33%	0.811%

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ClientSampleId :
MW-13

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\82X112124W.M
Title : SW846 8260

37	12.244	1823	1830	1837	rBV2	112737	174997	21.37%	2.737%
38	12.317	1837	1842	1849	rVB2	25211	36051	4.40%	0.564%
39	12.408	1852	1857	1863	rBV4	6417	9468	1.16%	0.148%
40	12.609	1884	1890	1894	rBV	21582	28819	3.52%	0.451%
41	12.695	1900	1904	1911	rVB2	34557	48876	5.97%	0.765%
42	12.847	1925	1929	1934	rBV	10461	14307	1.75%	0.224%
43	12.920	1934	1941	1945	rVV3	9318	11935	1.46%	0.187%
44	13.170	1978	1982	1989	rVB	9910	12501	1.53%	0.196%
45	13.292	1992	2002	2008	rBV2	38790	53069	6.48%	0.830%

Sum of corrected areas: 6393056

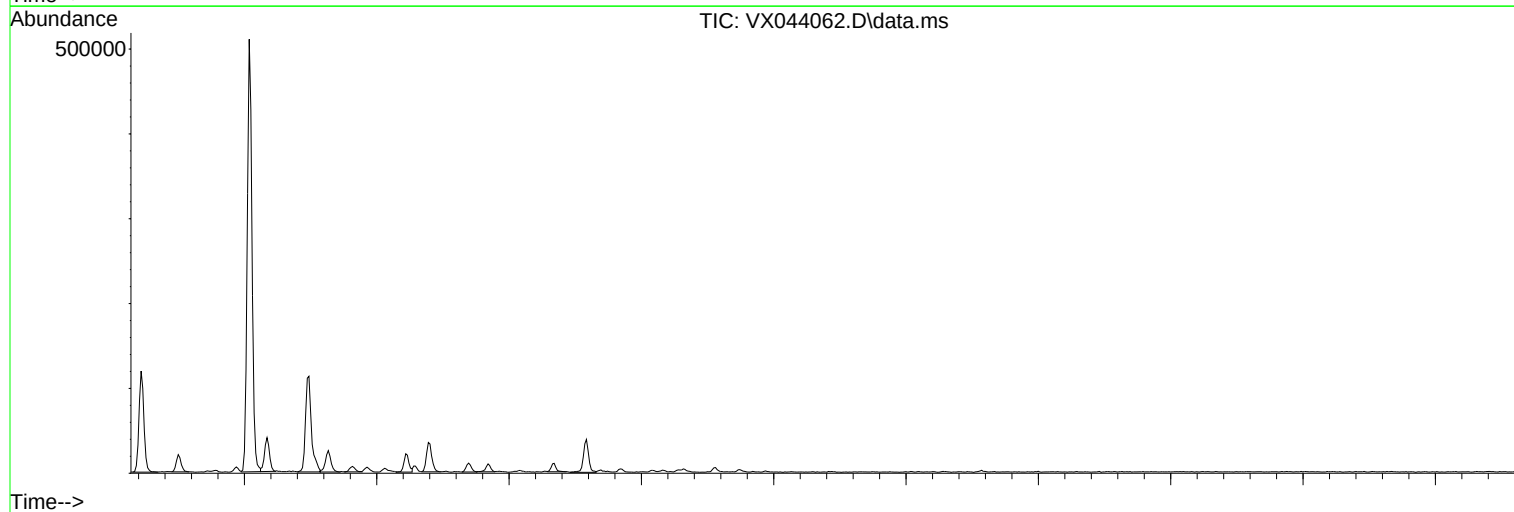
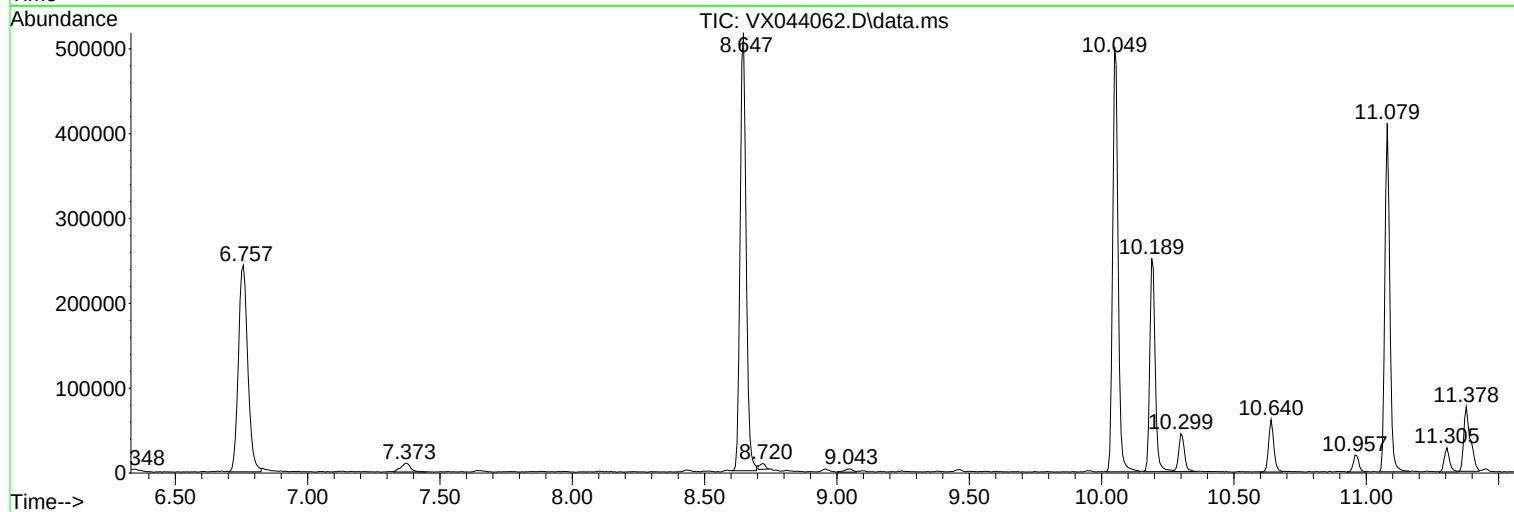
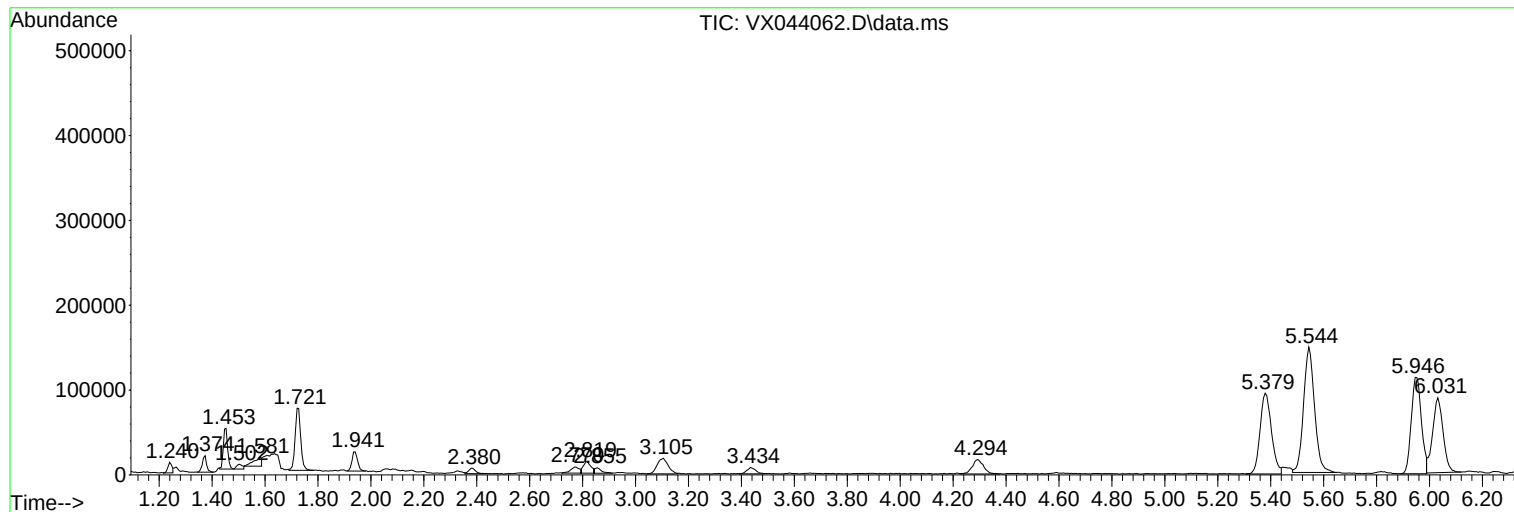
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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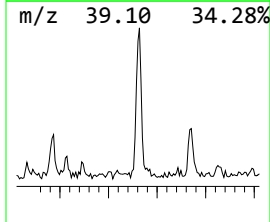
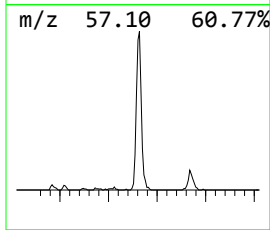
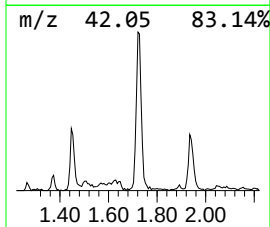
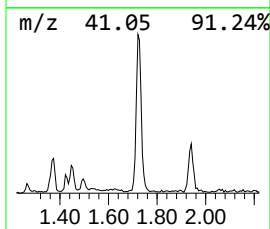
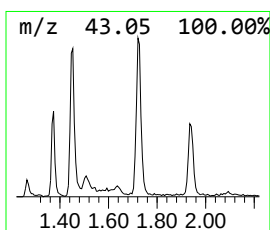
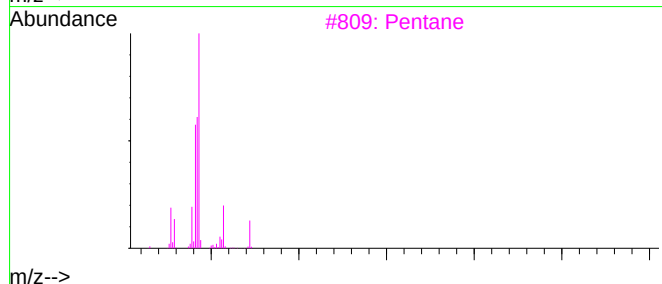
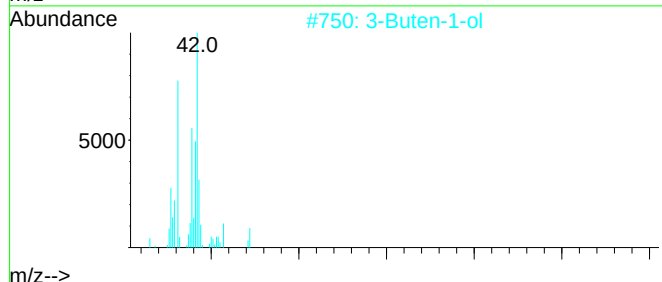
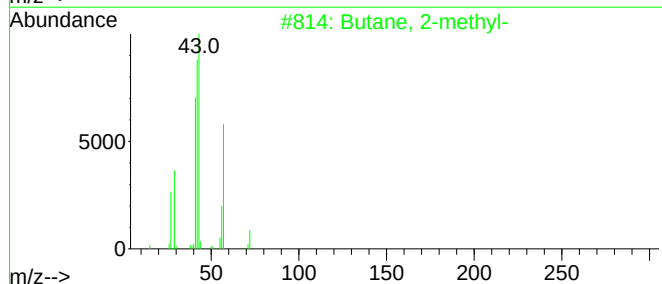
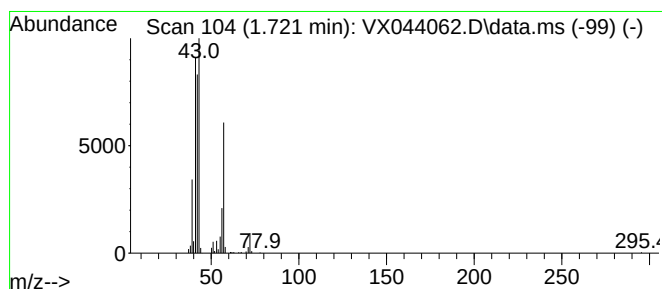
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.721	12.63 ug/l	107296	Pentafluorobenzene	5.544

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	38
3	Pentane	72	C5H12	000109-66-0	33
4	1-Butene	56	C4H8	000106-98-9	9
5	Azetidine	57	C3H7N	000503-29-7	9



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13

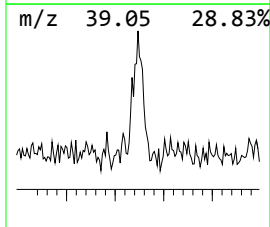
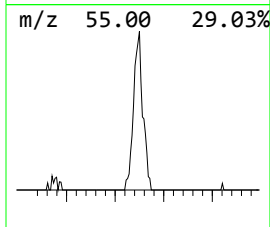
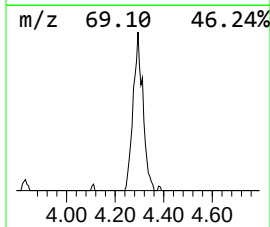
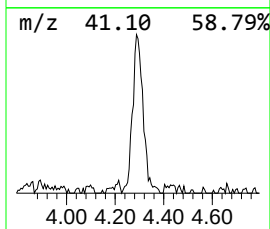
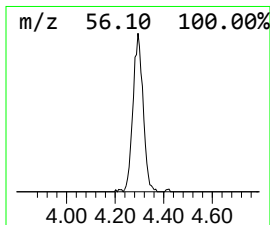
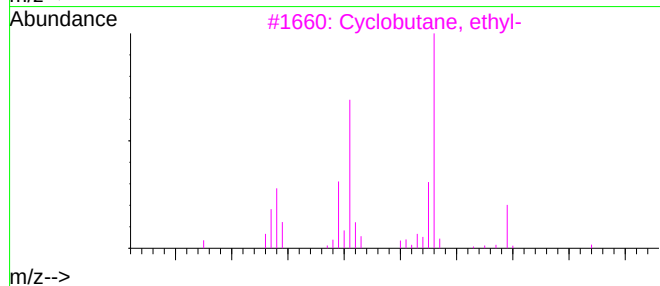
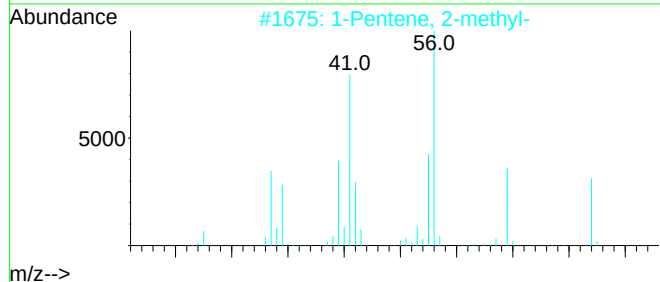
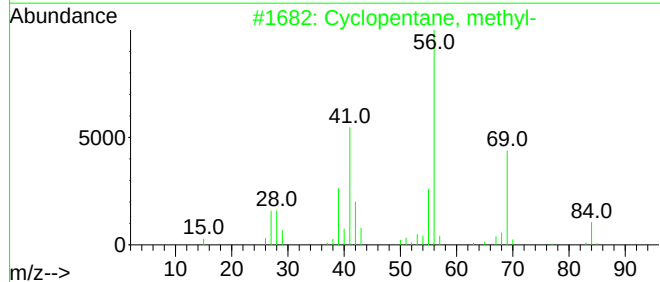
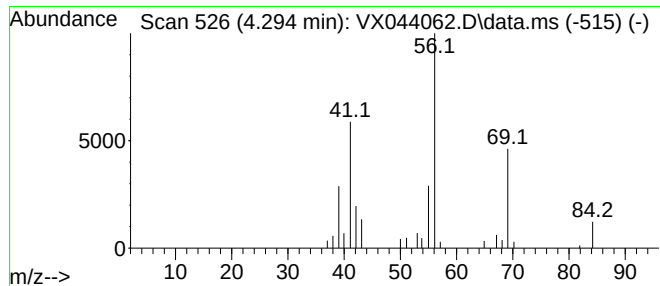
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	5.84 ug/l	49611	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclobutane	56	C4H8	000287-23-0	53
5	2-Butene	56	C4H8	000107-01-7	37



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

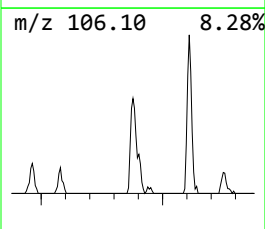
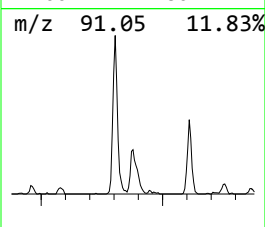
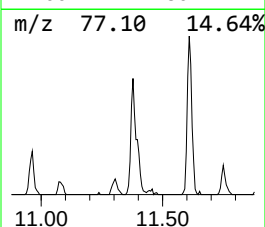
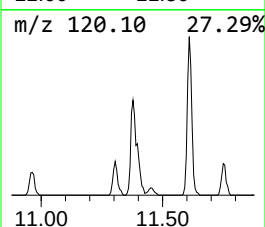
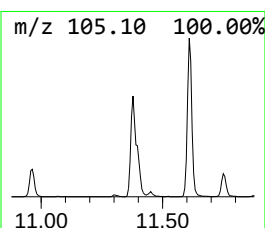
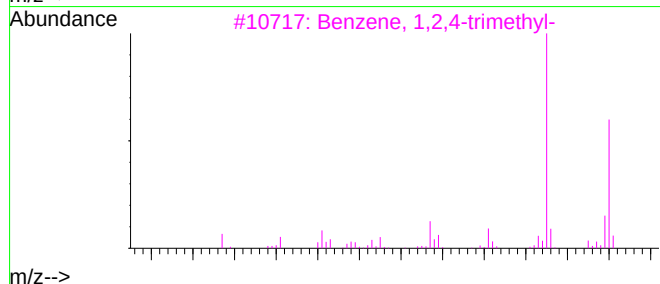
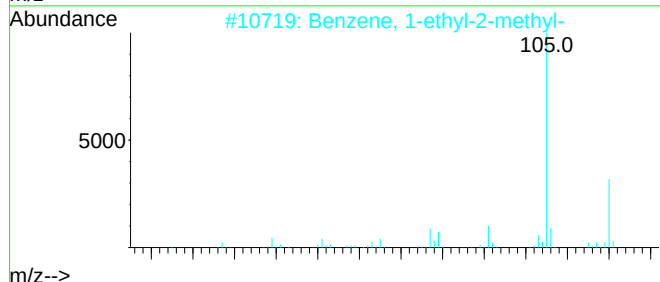
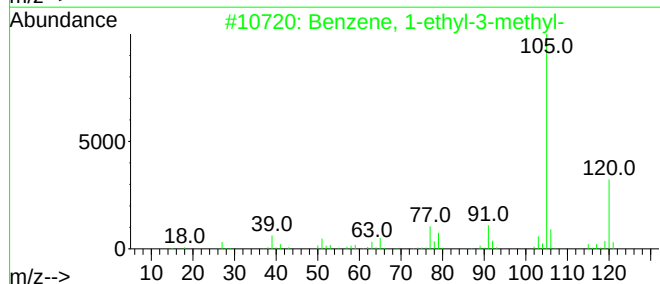
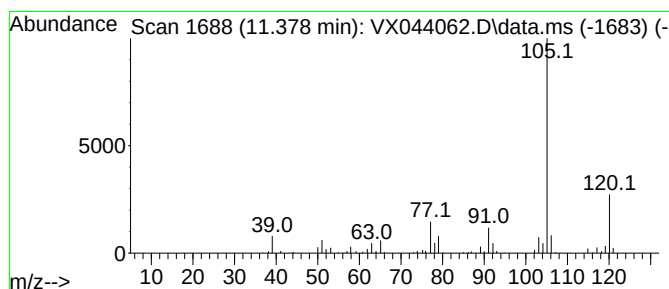
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	10.49 ug/l	132549	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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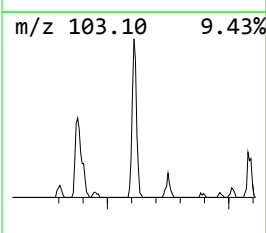
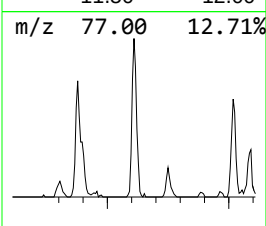
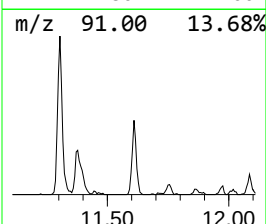
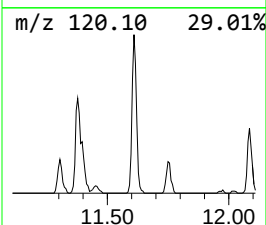
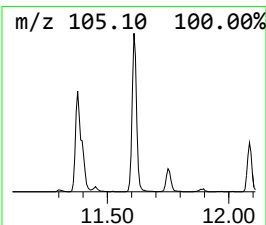
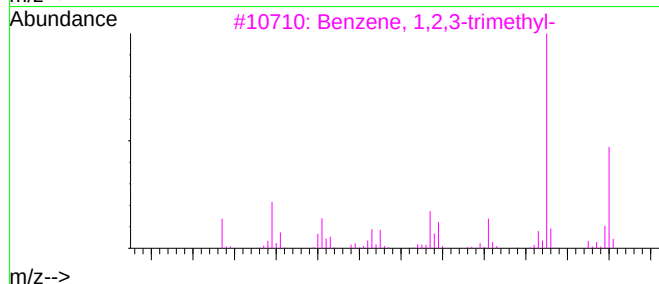
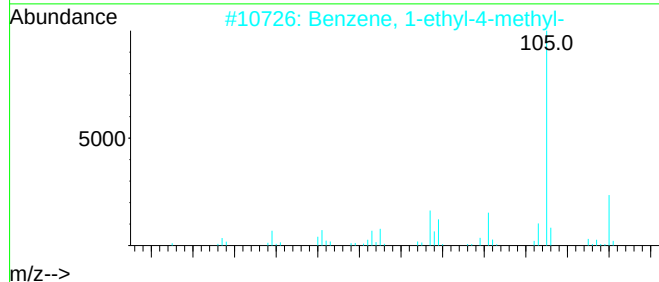
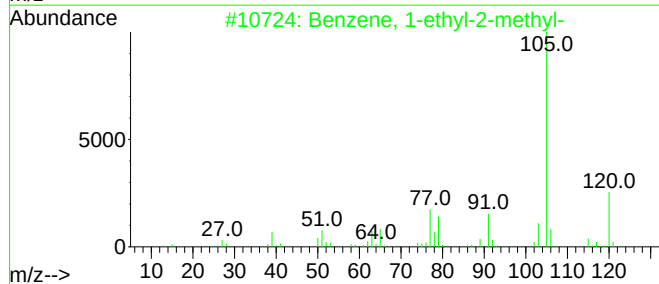
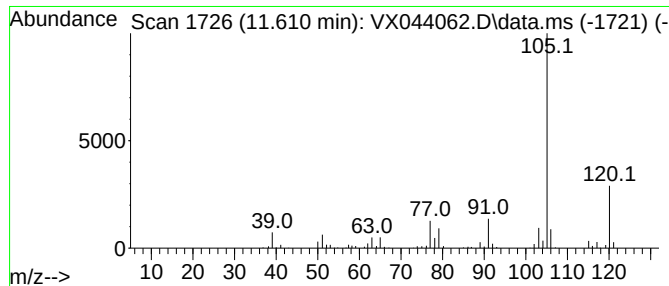
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	12.07 ug/l	152548	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

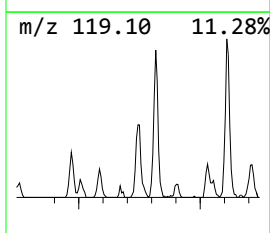
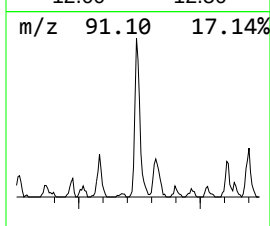
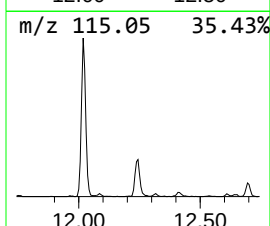
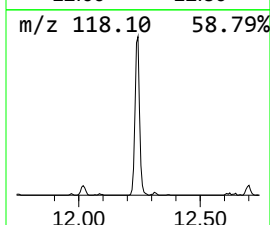
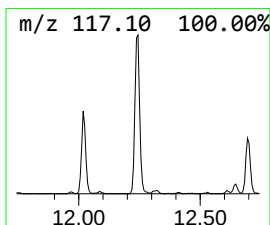
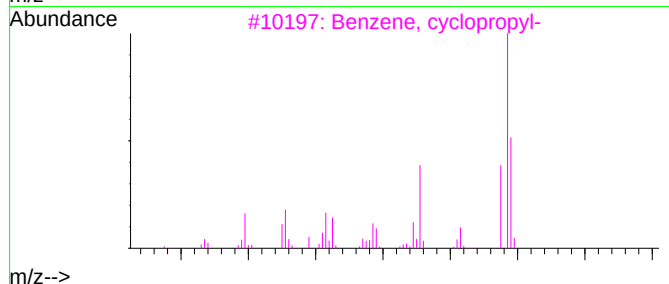
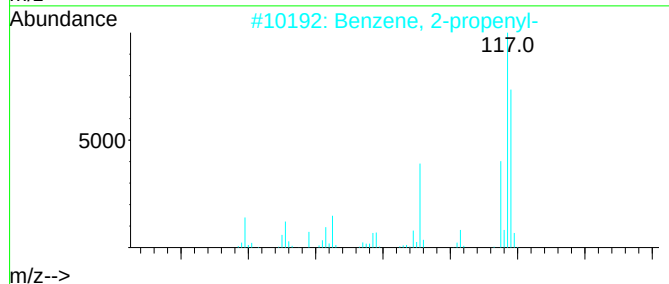
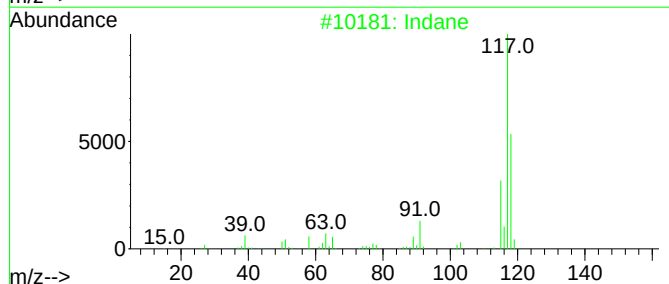
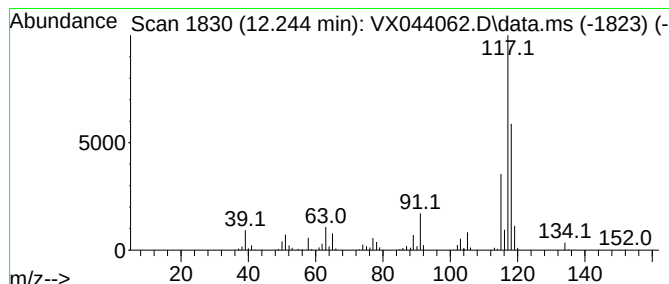
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	13.85 ug/l	174997	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120224\
Data File : VX044062.D
Acq On : 02 Dec 2024 13:44
Operator : JC/MD
Sample : P5021-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.721	12.6	ug/l	107296	1	5.544	424897	50.0
Cyclopentane, m...	4.294	5.8	ug/l	49611	1	5.544	424897	50.0
Benzene, 1-ethy...	11.378	10.5	ug/l	132549	4	12.018	631878	50.0
Benzene, 1-ethy...	11.610	12.1	ug/l	152548	4	12.018	631878	50.0
Indane	12.244	13.9	ug/l	174997	4	12.018	631878	50.0