

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
 Data File : VX044048.D
 Acq On : 27 Nov 2024 18:06
 Operator : JC/MD
 Sample : P5021-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 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

Signal : TIC: VX044048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	52	rBV	20638	26860	3.62%	0.434%
2	1.447	56	59	64	rVB	61986	67881	9.15%	1.096%
3	1.593	70	83	84	rBV4	15620	45184	6.09%	0.729%
4	1.721	98	104	112	rBV	81120	114891	15.48%	1.855%
5	1.941	135	140	146	rVB	26384	39085	5.27%	0.631%
6	2.203	179	183	190	rVB4	3935	8027	1.08%	0.130%
7	2.380	208	212	222	rVB	6594	12696	1.71%	0.205%
8	2.770	266	276	278	rBV5	8186	16625	2.24%	0.268%
9	2.813	280	283	288	rVB	11589	19969	2.69%	0.322%
10	3.093	319	329	341	rBV3	20122	59228	7.98%	0.956%
11	3.441	376	386	394	rBV4	5350	12988	1.75%	0.210%
12	4.288	517	525	537	rVB3	18627	53773	7.25%	0.868%
13	5.379	694	704	716	rBV	87018	261689	35.27%	4.225%
14	5.544	722	731	749	rVB2	130872	388567	52.37%	6.273%
15	5.952	788	798	805	rBV	103083	281416	37.93%	4.543%
16	6.032	805	811	825	rVB	87304	235151	31.69%	3.796%
17	6.336	854	861	873	rVB9	4006	13588	1.83%	0.219%
18	6.757	921	930	942	rBV	225278	544979	73.45%	8.798%
19	7.367	1020	1030	1039	rVB5	12233	33373	4.50%	0.539%
20	8.647	1233	1240	1248	rVV	456625	741976	100.00%	11.978%
21	8.714	1249	1251	1257	rVB2	6996	11614	1.57%	0.187%
22	10.049	1465	1470	1485	rBV	462156	653952	88.14%	10.557%
23	10.189	1488	1493	1504	rVV	262172	362567	48.87%	5.853%
24	10.299	1506	1511	1519	rVB	46792	72004	9.70%	1.162%
25	10.640	1562	1567	1575	rBV	61775	82388	11.10%	1.330%
26	10.964	1615	1620	1624	rBV	23615	31704	4.27%	0.512%
27	11.079	1634	1639	1652	rBV	363967	471055	63.49%	7.605%
28	11.305	1672	1676	1683	rBV	31380	40997	5.53%	0.662%
29	11.378	1683	1688	1697	rVV	90681	156979	21.16%	2.534%
30	11.610	1721	1726	1737	rBV	136804	169843	22.89%	2.742%
31	11.750	1745	1749	1756	rVB2	21395	29070	3.92%	0.469%
32	11.969	1779	1785	1788	rBV2	6645	8774	1.18%	0.142%
33	12.018	1788	1793	1800	rVV	442016	559735	75.44%	9.036%
34	12.085	1800	1804	1811	rVB	45642	59169	7.97%	0.955%
35	12.244	1823	1830	1838	rBV2	131980	190578	25.69%	3.077%
36	12.317	1838	1842	1849	rVB	30434	41838	5.64%	0.675%

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Integration Parameters: RTEINT.P

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37	12.415	1852	1858	1863	rBV3	8906	14300	1.93%	0.231%
38	12.463	1863	1866	1873	rVB	8447	10821	1.46%	0.175%
39	12.610	1885	1890	1894	rBV	27129	36084	4.86%	0.583%
40	12.646	1894	1896	1900	rVV	7370	7573	1.02%	0.122%
41	12.695	1900	1904	1912	rVB2	38456	56176	7.57%	0.907%
42	12.847	1922	1929	1934	rBV2	13176	18402	2.48%	0.297%
43	12.921	1936	1941	1945	rVV	13748	16350	2.20%	0.264%
44	13.170	1977	1982	1989	rVB	12667	17822	2.40%	0.288%
45	13.292	1997	2002	2007	rVB2	41019	54954	7.41%	0.887%
46	13.427	2019	2024	2031	rVB5	5007	7605	1.02%	0.123%
47	13.774	2075	2081	2088	rBV	21938	34087	4.59%	0.550%

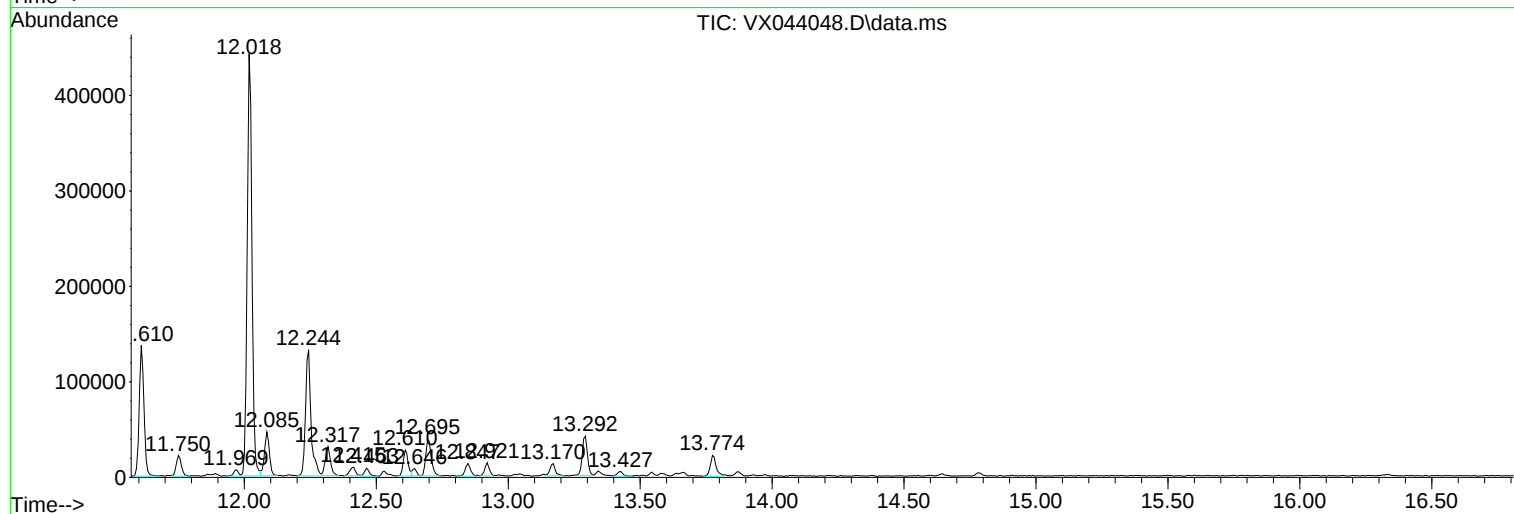
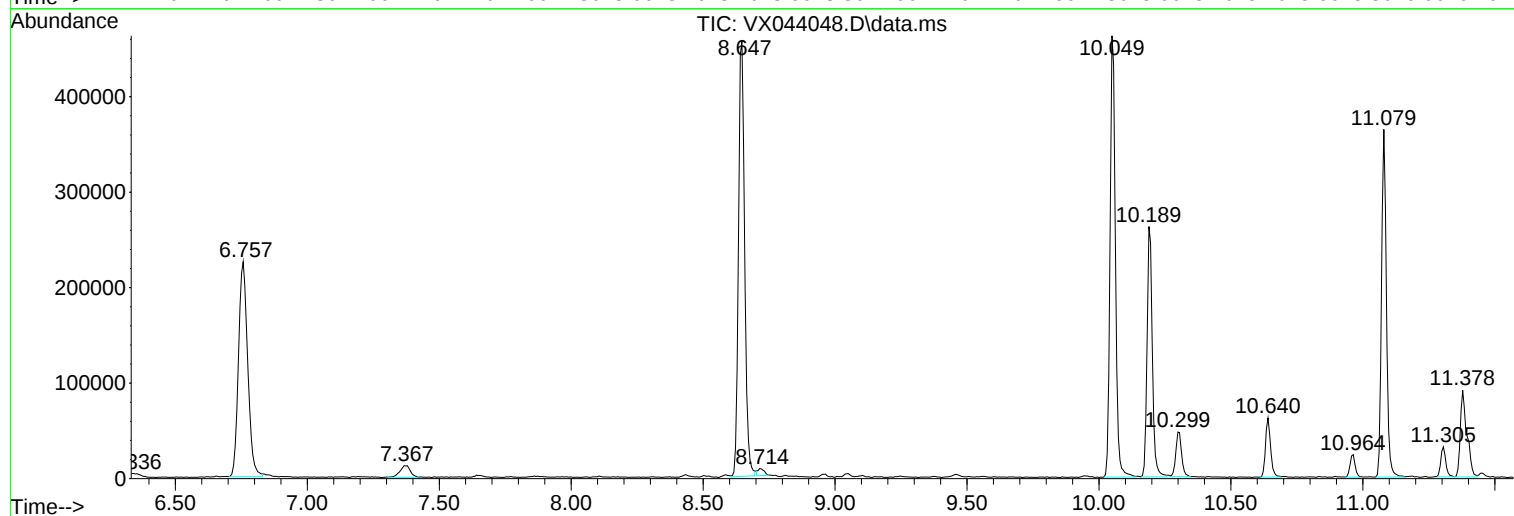
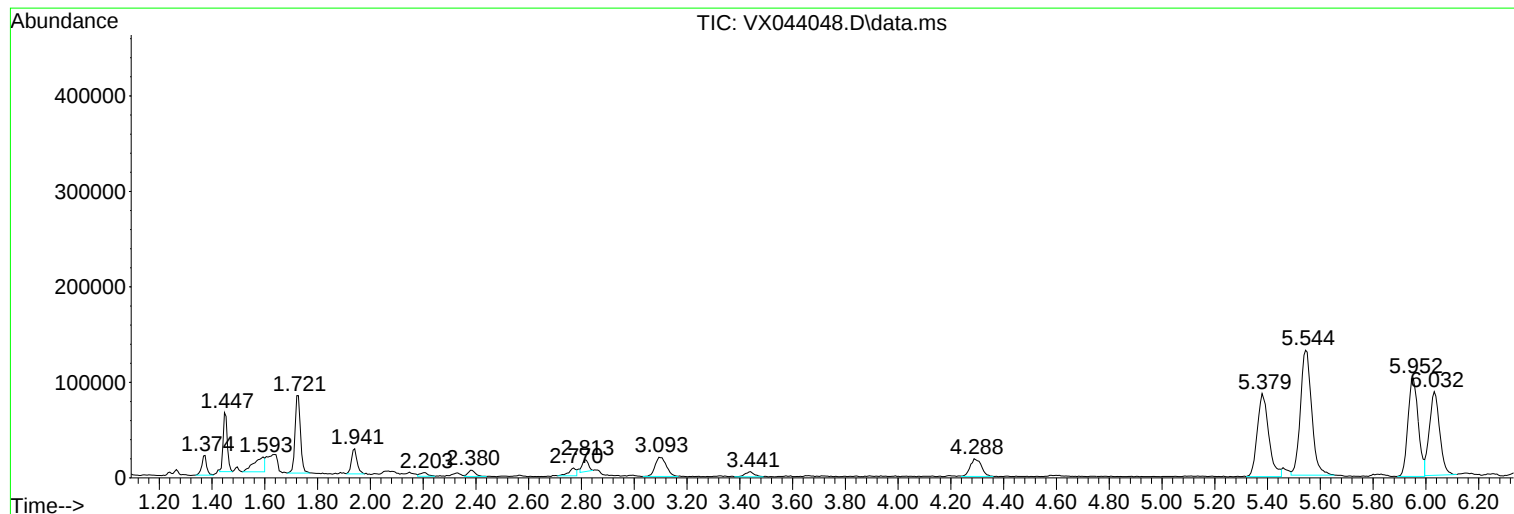
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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



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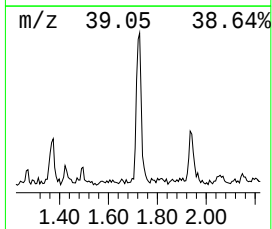
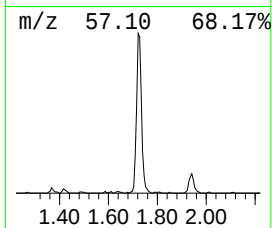
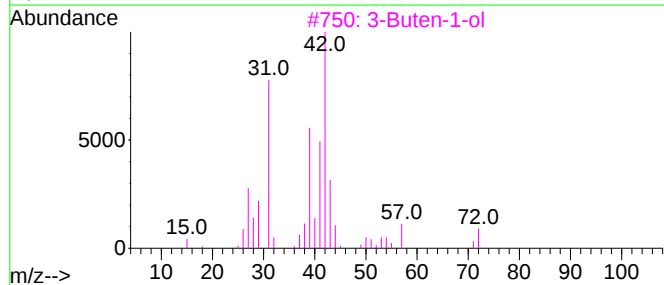
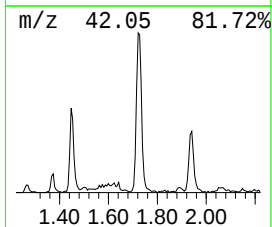
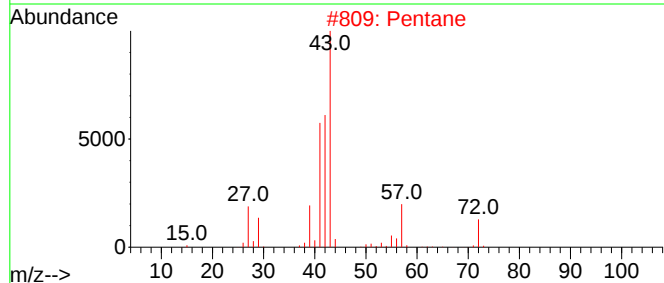
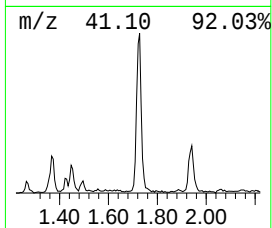
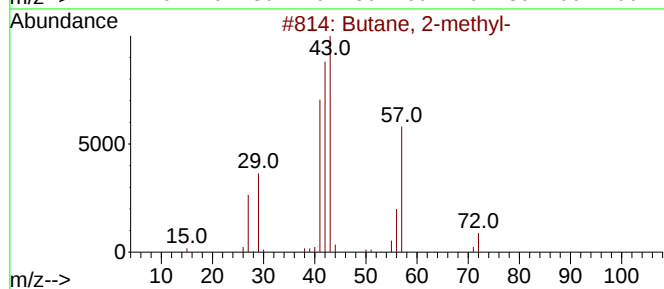
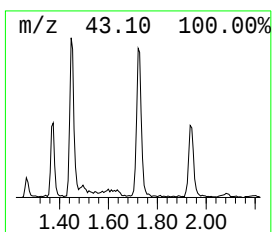
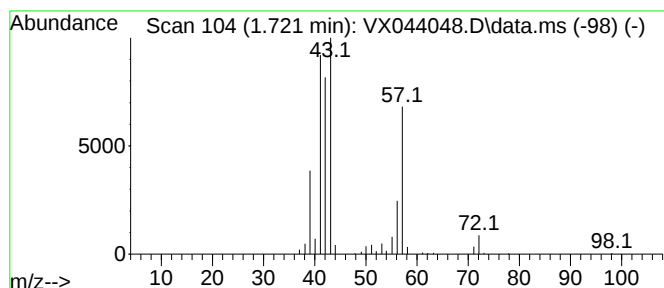
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.721	14.78 ug/l	114891	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	64
2		Pentane	72	C5H12	000109-66-0	36
3		3-Buten-1-ol	72	C4H8O	000627-27-0	33
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	30
5		1-Butene	56	C4H8	000106-98-9	30



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ALS Vial : 26 Sample Multiplier: 1

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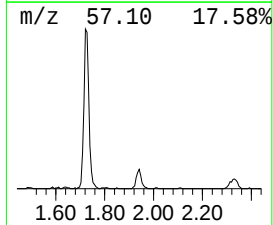
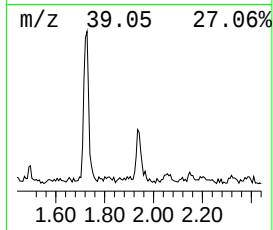
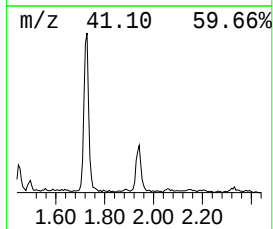
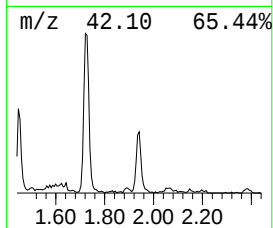
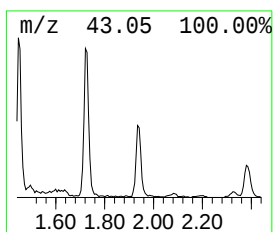
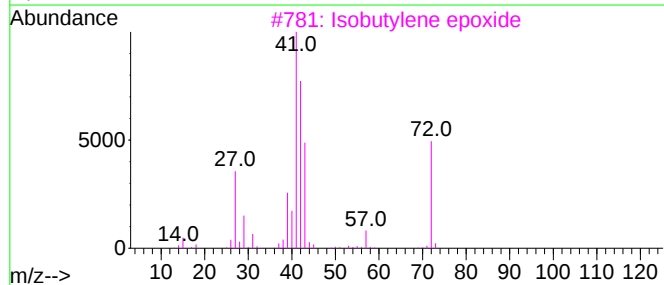
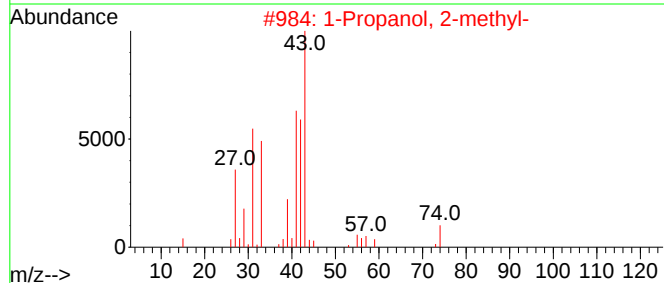
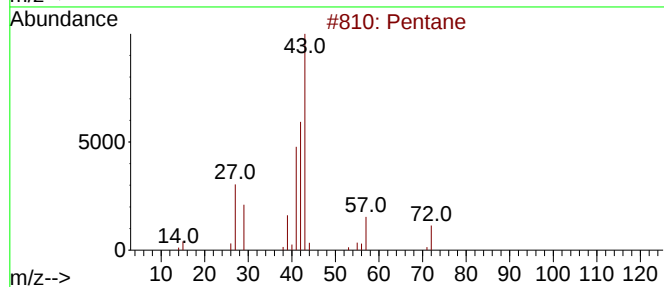
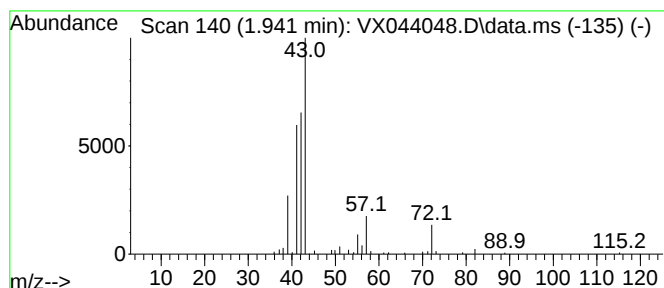
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.941	5.03 ug/l	39085	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	80
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	64
3			Isobutylene epoxide	72	C4H8O	000558-30-5	50
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	37



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

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ClientSampleId :
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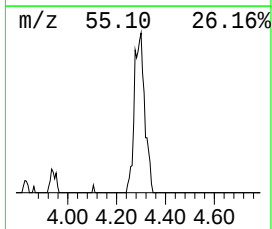
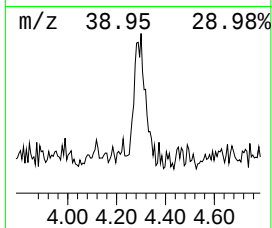
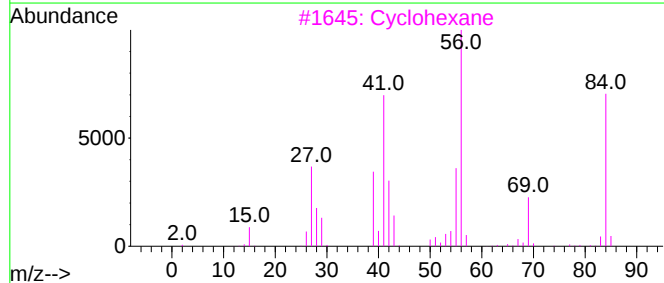
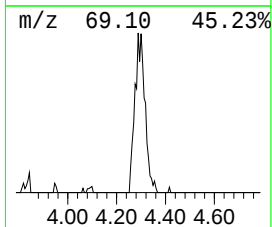
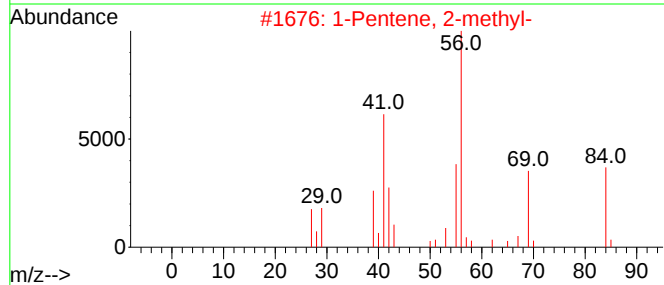
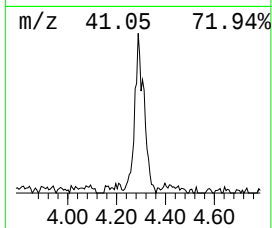
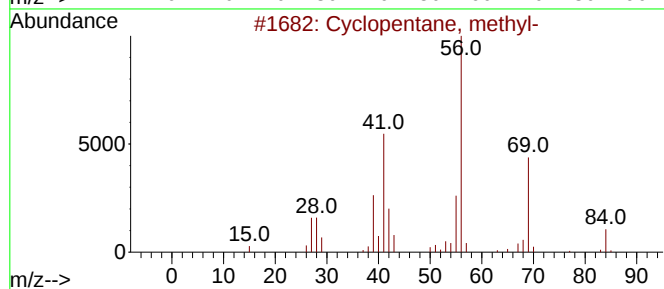
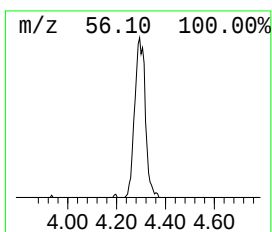
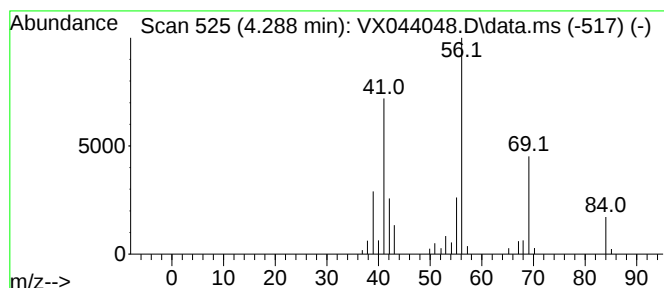
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.288	6.92 ug/l	53773	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	86
3			Cyclohexane	84	C6H12	000110-82-7	78
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	50
5			Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	30



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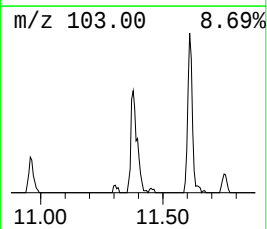
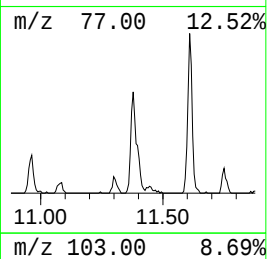
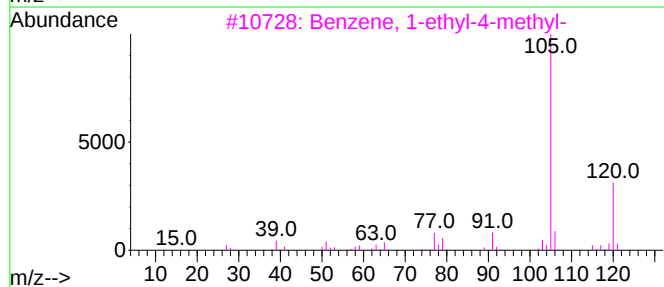
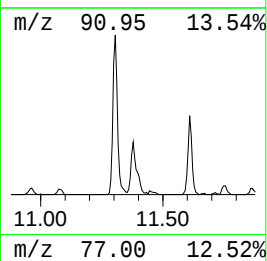
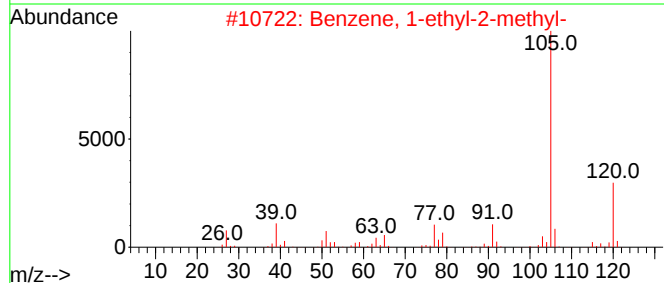
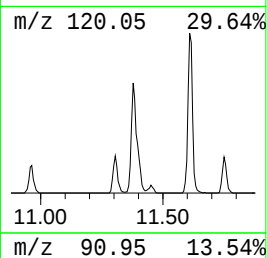
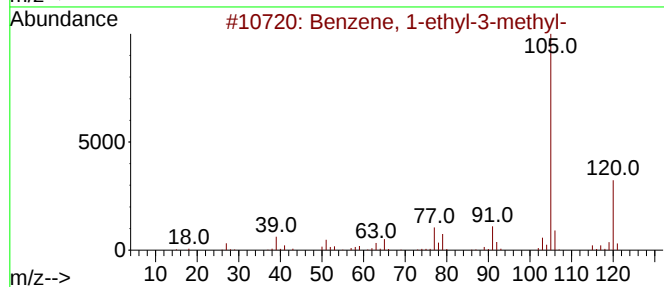
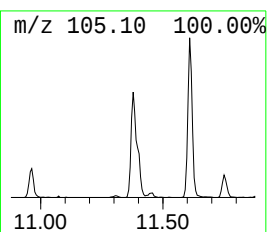
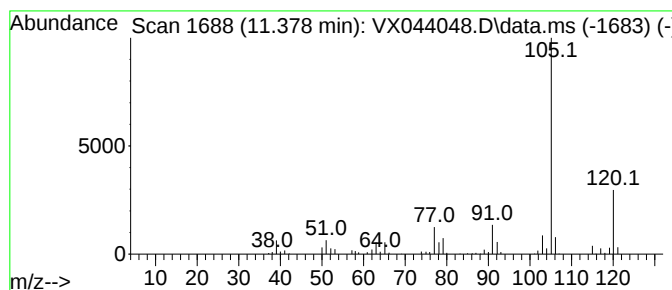
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	14.02 ug/l	156979	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	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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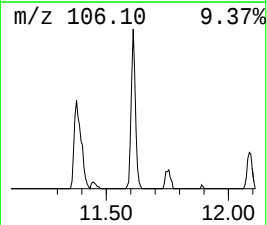
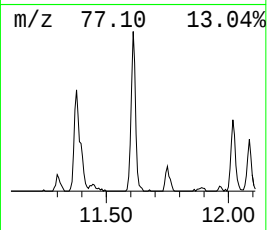
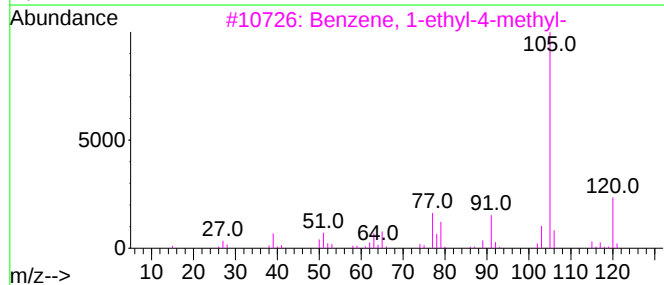
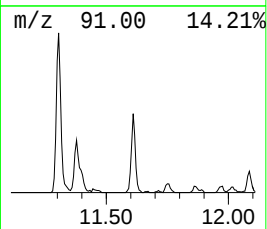
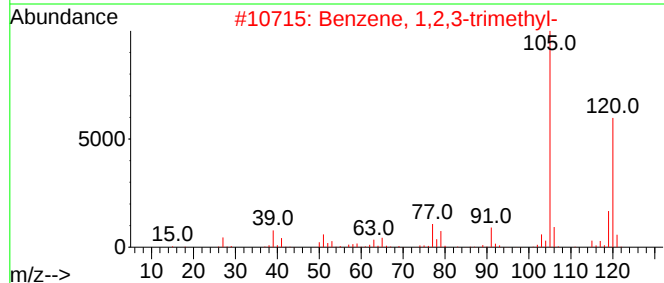
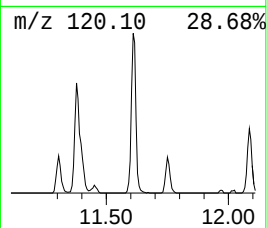
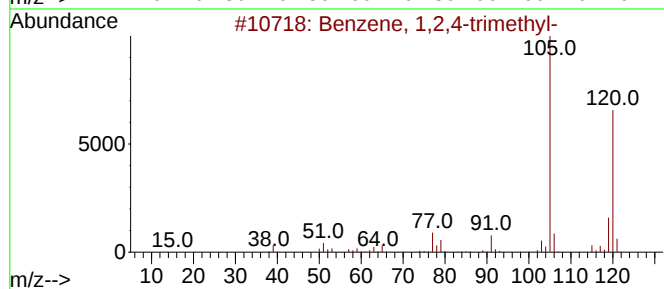
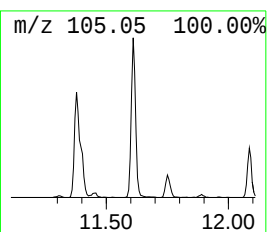
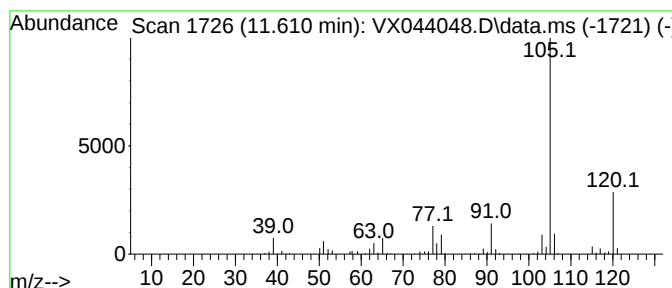
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	15.17 ug/l	169843	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044048.D
Acq On : 27 Nov 2024 18:06
Operator : JC/MD
Sample : P5021-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13

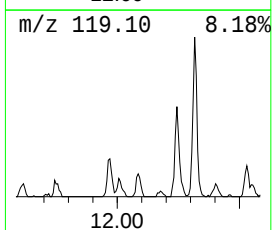
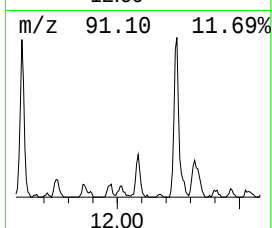
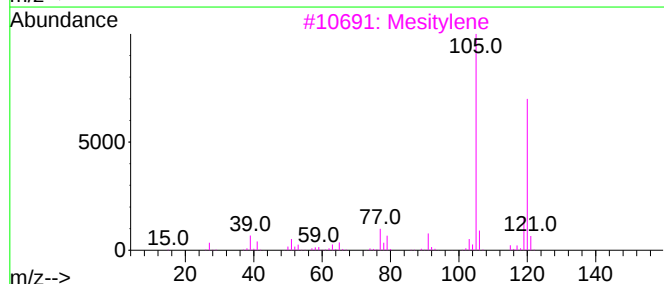
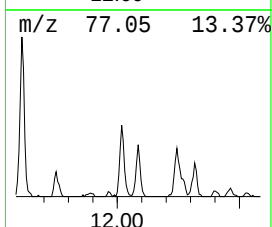
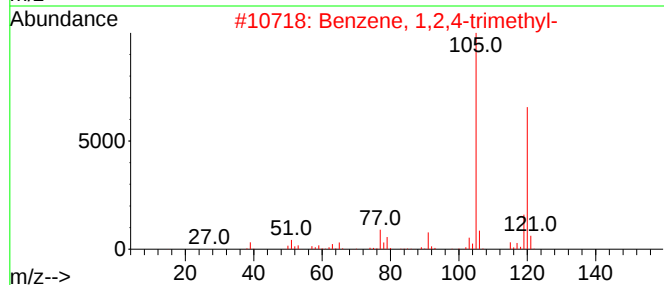
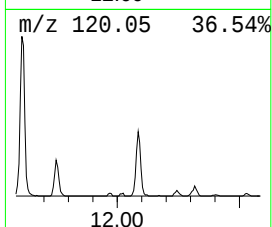
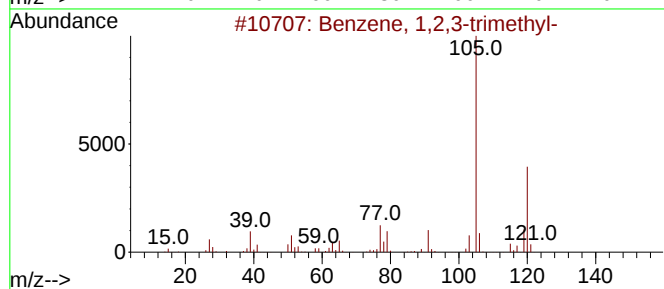
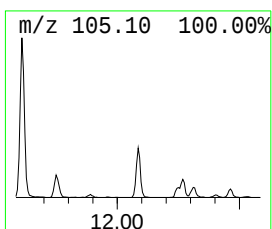
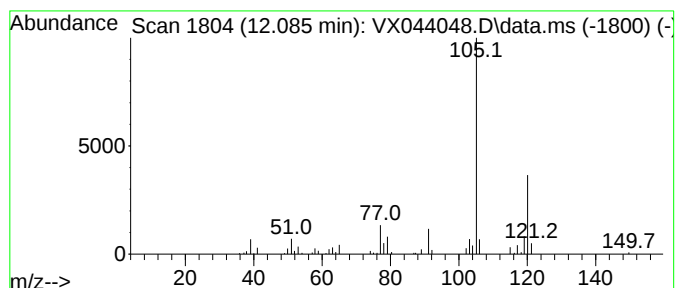
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	5.29 ug/l	59169	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044048.D
Acq On : 27 Nov 2024 18:06
Operator : JC/MD
Sample : P5021-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13

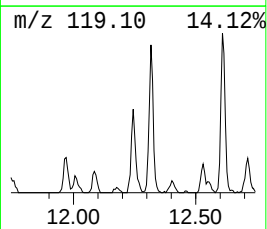
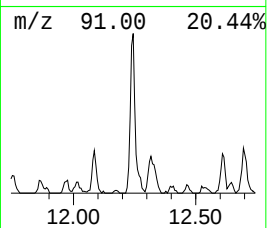
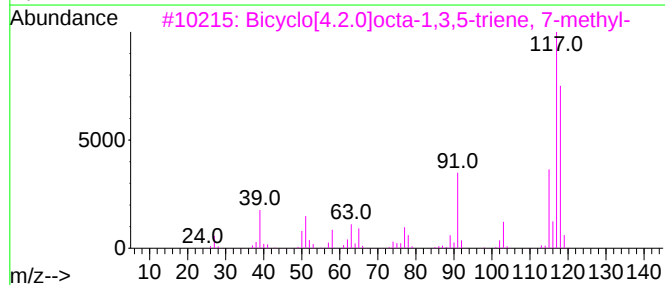
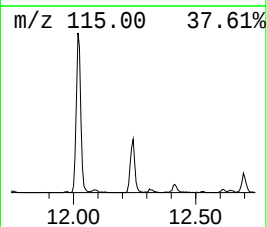
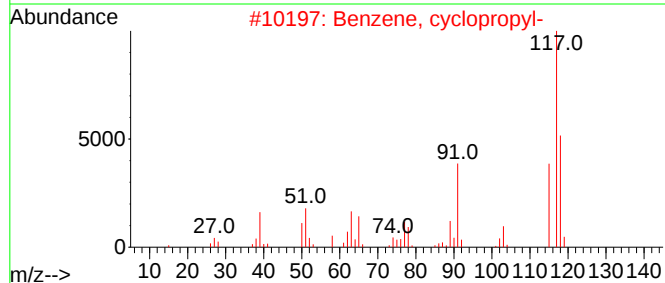
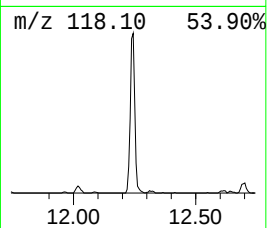
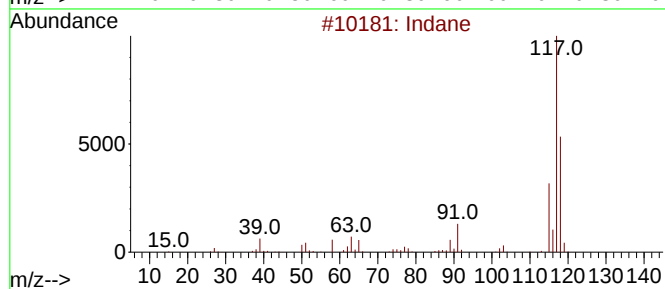
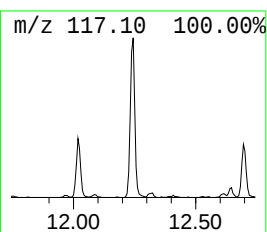
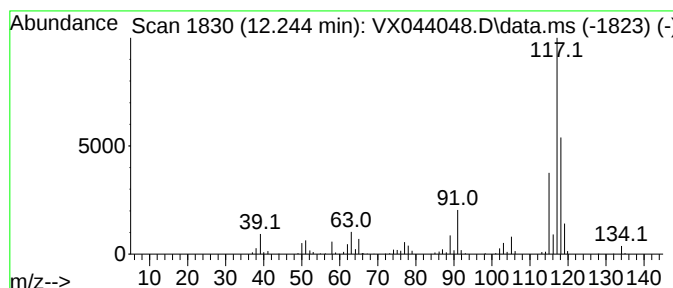
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	17.02 ug/l	190578	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, cyclopropyl-	118	C9H10	000873-49-4	76
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
4		Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
5		Deltacyclene	118	C9H10	007785-10-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044048.D
Acq On : 27 Nov 2024 18:06
Operator : JC/MD
Sample : P5021-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-13

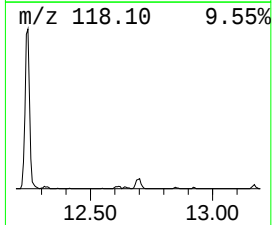
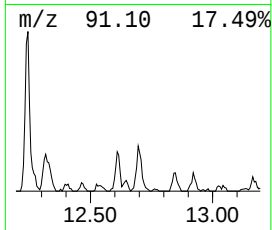
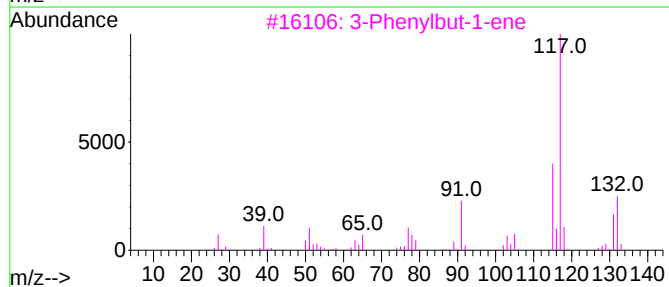
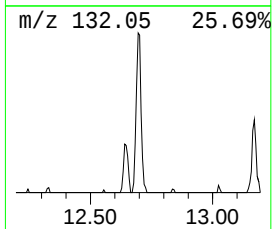
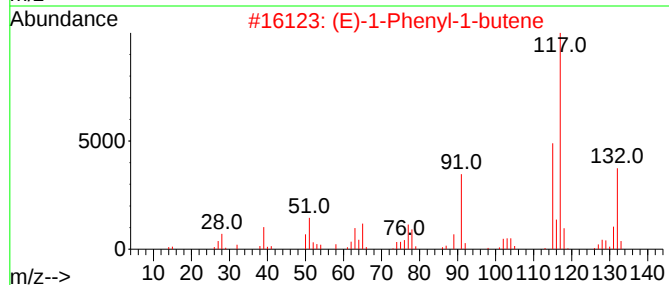
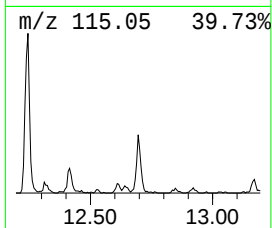
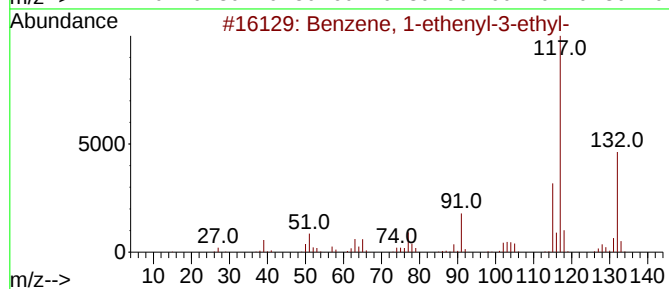
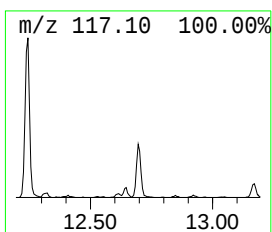
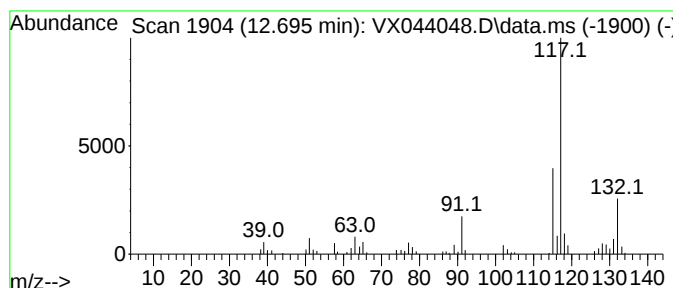
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	5.02 ug/l	56176	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2		(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	87
3		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5		Indan, 1-methyl-	132	C10H12	000767-58-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112724\
Data File : VX044048.D
Acq On : 27 Nov 2024 18:06
Operator : JC/MD
Sample : P5021-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.721	14.8	ug/l	114891	1	5.550	388567	50.0
Pentane	1.941	5.0	ug/l	39085	1	5.550	388567	50.0
Cyclopentane, m...	4.288	6.9	ug/l	53773	1	5.550	388567	50.0
Benzene, 1-ethy...	11.378	14.0	ug/l	156979	4	12.018	559735	50.0
Benzene, 1-ethy...	11.610	15.2	ug/l	169843	4	12.018	559735	50.0
Benzene, 1,2,3-...	12.085	5.3	ug/l	59169	4	12.018	559735	50.0
Indane	12.244	17.0	ug/l	190578	4	12.018	559735	50.0
Benzene, 1-ethe...	12.695	5.0	ug/l	56176	4	12.018	559735	50.0